

```

date Tue Mar 16 08:18:13 CET 2010
hostname despina
system Linux despina 2.6.30.10 #3 SMP PREEMPT Mon Dec 21 08:24:00 CET 2009 x86_64 Intel(R) Core(TM)2
Extreme CPU Q6850 @ 3.00GHz GenuineIntel GNU/Linux
user dtoebbens
executable in /home/dtoebbens/CRYSTAL/bin/Linux-ifort_mpich_1.2.7.fedora5_2.6/v1_0_2
temporary directory /home/dtoebbens/scr/tmp2639
output in /home/dtoebbens/CRYSTAL/test_cases/Cordierite-B3LYP-FREQ.out
input data /home/dtoebbens/CRYSTAL/test_cases/Cordierite-B3LYP-FREQ.d12
Cordierite, B3LYP optimized
Fractional coordinates for jmoledit
  -0.50<a<0.50
  -0.50<b<0.50
  -0.20<c<1.20
CRYSTAL
1 0 0
C c c m
  17.19628301   9.80014776   9.41154272
12
12  -1.628440693882E-01  5.000000000000E-01  2.500000000000E-01
13   2.500000000000E-01  2.500000000000E-01  2.502090230322E-01
13   5.061166050578E-02  3.086028727700E-01  0.000000000000E+00
14   0.000000000000E+00 -5.000000000000E-01  2.500000000000E-01
14   1.920774093107E-01  7.845658165449E-02  0.000000000000E+00
14   1.350164750857E-01 -2.372646960501E-01  0.000000000000E+00
 8   2.470393804899E-01 -1.033662256963E-01  3.584944396351E-01
 8   6.263705315058E-02 -4.170350836253E-01  3.492063126317E-01
 8  -1.734685455261E-01 -3.099688140280E-01  3.581599864041E-01
 8   4.312204313218E-02 -2.482616874061E-01  0.000000000000E+00
 8   1.218664333799E-01  1.850271811291E-01  0.000000000000E+00
 8   1.64447793599E-01 -7.929806548987E-02  0.000000000000E+00
FREQCALC
ANALYSIS
ENDFREQ
END
12 5      ! Mg(2+) (Valenzano) 85-11G(1), outer two sp and one d reoptimized in Mg-Cordierite LDA/VWN
0 0 8 2.0 1.0
68370.0    0.0002226
9661.0     0.001901
2041.0     0.011042
529.6      0.05005
159.17     0.1690
54.71      0.36695
21.236     0.4008
8.791      0.1487
0 1 5 8.0 1.0
143.7      -0.00671    0.00807
31.27      -0.07927    0.06401
9.661      -0.08088    0.2092
3.726      0.2947     0.3460
1.598      0.5714     0.3731
0 1 1 0.0 1.0
0.600      1.0000     1.0000

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0 1 1 0.0 1.0
    0.315    1.0000    1.0000
0 3 1 0.0 1.0
    0.426    1.0000
13 6      ! Al(1+) 88-311G(1) (N.M.Harrison 1993, 8-311G Al atom from scaled Si, outer two sp and one d
reoptimized in Mg-Cordierite LDA/VWN)
0 0 8 2.0 1.0
59852.6     0.0004
8507.9      0.0034
1902.55     0.0173
562.45      0.0617
202.931     0.168
77.6773     0.385
31.1496     0.5224
12.4308     0.2864
0 1 8 8.0 1.0
565.087     -0.0004    0.0011
144.448     -0.0059    0.0075
50.1458     -0.0385    0.0339
18.9981     -0.0964    0.116
8.036       0.0204    0.2451
3.5876      0.3772    0.3701
1.5884      0.5164    0.3554
0.7079      0.1783    0.1356
0 1 3 2.0 1.0
1.9603     -0.0607    0.0514
0.8551     -0.1183   -0.0938
0.2477      0.2007   -1.0297
0 1 1 0.0 1.0
    0.438    1.0000    1.0000
0 1 1 0.0 1.0
    0.212    1.0000    1.0000
0 3 1 0.0 1.0
    0.582    1.0000
14 6      ! Si(2+) (Pyrope) 86-311G(1) (Pyrope, outer two sp and one d reoptimized in Mg-Cordierite
LDA/VWN)
0 0 8 2.0 1.0
87645.8     0.000237
12851.8     0.00192
2786.28     0.0109
728.043     0.0496
219.516     0.1668
75.9006     0.363
29.4602     0.4051
11.9891     0.1504
0 1 6 8.0 1.0
165.958     -0.00884    0.00909
39.3727     -0.0859    0.0601
12.7112     -0.0712    0.1952
4.7177      0.4147    0.3384
1.8482      0.6168    0.3006
0.7365      0.1154    0.0648
0 1 3 2.0 1.0
4.1752     -0.0199   -0.0087

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1.4472 -0.1864 -0.00438
0.5023 0.0967 0.2207
0 1 1 0.0 1.0
0.344 1.0000 1.0000
0 1 1 0.0 1.0
0.13 1.0000 1.0000
0 3 1 0.0 1.0
0.677 1.0000
8 5 ! O(1-) (Andradite) 84-11G(1) (Andradite, outer two sp and one d reoptimized in Mg-Cordierite
LDA/VWN)
0 0 8 2.0 1.0
8020.0 0.00108
1338.0 0.00804
255.4 0.05324
69.22 0.1681
23.90 0.3581
9.264 0.3855
3.851 0.1468
1.212 0.0728
0 1 4 7.0 1.0
49.43 -0.00883 0.00958
10.47 -0.0915 0.0696
3.235 -0.0402 0.2065
1.217 0.379 0.347
0 1 1 0.0 1.0
0.466 1.0000 1.0000
0 1 1 0.0 1.0
0.195 1.0000 1.0000
0 3 1 0.0 1.0
0.538 1.0000
99 0
ENDBASIS
DFT
XLGRID
B3LYP
ENDDFT
MAXCYCLE
500
BIPOSIZE
7818200
EXCHSIZE
7876296
TOLINTEG
7 7 7 7 15
SCFDIR
SHRINK
4 4 4
FMIXING
80
BROYDEN
0.0001 50 2
ENDRUN
END

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*
*          *
*      CRYSTAL06          *
*      Release 1.0 - v1_0_2
*      Sequential executable          *
*
*          *
*      Compiled: 05 Apr 2007 10:31          *
*      Xmake: Linux-ifort_mpich_1.2.7.fedora5_2.6          *
*          *
*          *
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*      http://www.crystal.unito.it          *
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EEEEEEEEEE STARTING DATE 16 03 2010 TIME 08:18:13.9  
Cordierite, B3LYP optimized

CRYSTAL CALCULATION  
(INPUT ACCORDING TO THE INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY)  
CRYSTAL FAMILY : ORTHORHOMBIC  
CRYSTAL CLASS (GROTH - 1921) : ORTHORHOMBIC BIPYRAMIDAL

SPACE GROUP (CENTROSYMMETRIC) : C C C M

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - CONVENTIONAL CELL

A	B	C	ALPHA	BETA	GAMMA
17.19628	9.80015	9.41154	90.00000	90.00000	90.00000

NUMBER OF IRREDUCIBLE ATOMS IN THE CONVENTIONAL CELL: 12

INPUT COORDINATES

ATOM	AT. N.	COORDINATES
1	12	-1.628440693882E-01 5.000000000000E-01 2.500000000000E-01
2	13	2.500000000000E-01 2.500000000000E-01 2.502090230322E-01
3	13	5.061166050578E-02 3.086028727700E-01 0.000000000000E+00
4	14	0.000000000000E+00 -5.000000000000E-01 2.500000000000E-01

5 14 1.920774093107E-01 7.845658165449E-02 0.000000000000E+00  
6 14 1.350164750857E-01 -2.372646960501E-01 0.000000000000E+00  
7 8 2.470393804899E-01 -1.033662256963E-01 3.584944396351E-01  
8 8 6.263705315058E-02 -4.170350836253E-01 3.492063126317E-01  
9 8 -1.734685455261E-01 -3.099688140280E-01 3.581599864041E-01  
10 8 4.312204313218E-02 -2.482616874061E-01 0.000000000000E+00  
11 8 1.218664333799E-01 1.850271811291E-01 0.000000000000E+00  
12 8 1.644447793599E-01 -7.929806548987E-02 0.000000000000E+00

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<< INFORMATION >>: FROM NOW ON, ALL COORDINATES REFER TO THE PRIMITIVE CELL

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LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - PRIMITIVE CELL

A	B	C	ALPHA	BETA	GAMMA	VOLUME
9.89640	9.89640	9.41154	90.00000	90.00000	120.64244	793.045363

COORDINATES OF THE EQUIVALENT ATOMS (FRACTIONARY UNITS)

N. ATOM	EQUIV	AT. N.		X	Y	Z
1	1	1	12 MG	3.37155930612E-01	-3.37155930612E-01	2.50000000000E-01
2	1	2	12 MG	-3.37155930612E-01	3.37155930612E-01	2.50000000000E-01
3	1	3	12 MG	-3.37155930612E-01	3.37155930612E-01	-2.50000000000E-01
4	1	4	12 MG	3.37155930612E-01	-3.37155930612E-01	-2.50000000000E-01
5	2	1	13 AL	-5.00000000000E-01	0.00000000000E+00	2.50209023032E-01
6	2	2	13 AL	0.00000000000E+00	5.00000000000E-01	2.49790976968E-01
7	2	3	13 AL	5.00000000000E-01	0.00000000000E+00	-2.50209023032E-01
8	2	4	13 AL	0.00000000000E+00	-5.00000000000E-01	-2.49790976968E-01
9	3	1	13 AL	3.59214533276E-01	2.57991212264E-01	0.00000000000E+00
10	3	2	13 AL	-3.59214533276E-01	-2.57991212264E-01	0.00000000000E+00
11	3	3	13 AL	-2.57991212264E-01	-3.59214533276E-01	-5.00000000000E-01
12	3	4	13 AL	2.57991212264E-01	3.59214533276E-01	-5.00000000000E-01
13	4	1	14 SI	5.00000000000E-01	5.00000000000E-01	2.50000000000E-01
14	4	2	14 SI	-5.00000000000E-01	-5.00000000000E-01	-2.50000000000E-01
15	5	1	14 SI	2.70533990965E-01	-1.13620827656E-01	0.00000000000E+00
16	5	2	14 SI	-2.70533990965E-01	1.13620827656E-01	0.00000000000E+00
17	5	3	14 SI	1.13620827656E-01	-2.70533990965E-01	-5.00000000000E-01
18	5	4	14 SI	-1.13620827656E-01	2.70533990965E-01	-5.00000000000E-01
19	6	1	14 SI	-1.02248220964E-01	-3.72281171136E-01	0.00000000000E+00
20	6	2	14 SI	1.02248220964E-01	3.72281171136E-01	0.00000000000E+00
21	6	3	14 SI	3.72281171136E-01	1.02248220964E-01	-5.00000000000E-01
22	6	4	14 SI	-3.72281171136E-01	-1.02248220964E-01	-5.00000000000E-01
23	7	1	8 O	1.43673154794E-01	-3.50405606186E-01	3.58494439635E-01
24	7	2	8 O	-1.43673154794E-01	3.50405606186E-01	3.58494439635E-01
25	7	3	8 O	3.50405606186E-01	-1.43673154794E-01	1.41505560365E-01



NO.OF VECTORS CREATED 6999 STARS 1020 RMAX 207.45093 BOHR

GEOMETRY FOR WAVE FUNCTION - DIMENSIONALITY OF THE SYSTEM 3

(NON PERIODIC DIRECTION: LATTICE PARAMETER FORMALLY SET TO 500)

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LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM

PRIMITIVE CELL - CENTRING CODE 4/0 VOLUME= 793.045363 - DENSITY 2.444 g/cm<sup>3</sup>

A	B	C	ALPHA	BETA	GAMMA
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9.89640144	9.89640144	9.41154272	90.000000	90.000000	120.642439
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ATOMS IN THE ASYMMETRIC UNIT 12 - ATOMS IN THE UNIT CELL: 58

ATOM	X/A	Y/B	Z/C
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1 T	12 MG	3.371559306118E-01	-3.371559306118E-01	2.500000000000E-01
2 F	12 MG	-3.371559306118E-01	3.371559306118E-01	2.500000000000E-01
3 F	12 MG	-3.371559306118E-01	3.371559306118E-01	-2.500000000000E-01
4 F	12 MG	3.371559306118E-01	-3.371559306118E-01	-2.500000000000E-01
5 T	13 AL	-5.000000000000E-01	8.326672684689E-17	2.502090230322E-01
6 F	13 AL	0.000000000000E+00	-5.000000000000E-01	2.497909769678E-01
7 F	13 AL	-5.000000000000E-01	8.326672684689E-17	-2.502090230322E-01
8 F	13 AL	0.000000000000E+00	-5.000000000000E-01	-2.497909769678E-01
9 T	13 AL	3.592145332758E-01	2.579912122642E-01	0.000000000000E+00
10 F	13 AL	-3.592145332758E-01	-2.579912122642E-01	0.000000000000E+00
11 F	13 AL	-2.579912122642E-01	-3.592145332758E-01	-5.000000000000E-01
12 F	13 AL	2.579912122642E-01	3.592145332758E-01	-5.000000000000E-01
13 T	14 SI	-5.000000000000E-01	-5.000000000000E-01	2.500000000000E-01
14 F	14 SI	-5.000000000000E-01	-5.000000000000E-01	-2.500000000000E-01
15 T	14 SI	2.705339909652E-01	-1.136208276562E-01	0.000000000000E+00
16 F	14 SI	-2.705339909652E-01	1.136208276562E-01	0.000000000000E+00
17 F	14 SI	1.136208276562E-01	-2.705339909652E-01	-5.000000000000E-01
18 F	14 SI	-1.136208276562E-01	2.705339909652E-01	-5.000000000000E-01
19 T	14 SI	-1.022482209644E-01	-3.722811711358E-01	0.000000000000E+00
20 F	14 SI	1.022482209644E-01	3.722811711358E-01	0.000000000000E+00
21 F	14 SI	3.722811711358E-01	1.022482209644E-01	-5.000000000000E-01
22 F	14 SI	-3.722811711358E-01	-1.022482209644E-01	-5.000000000000E-01
23 T	8 O	1.436731547936E-01	-3.504056061862E-01	3.584944396351E-01
24 F	8 O	-1.436731547936E-01	3.504056061862E-01	3.584944396351E-01
25 F	8 O	3.504056061862E-01	-1.436731547936E-01	1.415055603649E-01
26 F	8 O	-3.504056061862E-01	1.436731547936E-01	1.415055603649E-01
27 F	8 O	-1.436731547936E-01	3.504056061862E-01	-3.584944396351E-01
28 F	8 O	1.436731547936E-01	-3.504056061862E-01	-3.584944396351E-01
29 F	8 O	-3.504056061862E-01	1.436731547936E-01	-1.415055603649E-01
30 F	8 O	3.504056061862E-01	-1.436731547936E-01	-1.415055603649E-01
31 T	8 O	-3.543980304747E-01	-4.796721367759E-01	3.492063126317E-01
32 F	8 O	3.543980304747E-01	4.796721367759E-01	3.492063126317E-01
33 F	8 O	4.796721367759E-01	3.543980304747E-01	1.507936873683E-01
34 F	8 O	-4.796721367759E-01	-3.543980304747E-01	1.507936873683E-01
35 F	8 O	3.543980304747E-01	4.796721367759E-01	-3.492063126317E-01
36 F	8 O	-3.543980304747E-01	-4.796721367759E-01	-3.492063126317E-01
37 F	8 O	-4.796721367759E-01	-3.543980304747E-01	-1.507936873683E-01
38 F	8 O	4.796721367759E-01	3.543980304747E-01	-1.507936873683E-01
39 T	8 O	-4.834373595541E-01	-1.365002685019E-01	3.581599864041E-01
40 F	8 O	4.834373595541E-01	1.365002685019E-01	3.581599864041E-01
41 F	8 O	1.365002685019E-01	4.834373595541E-01	1.418400135959E-01

42 F 8 O -1.365002685019E-01 -4.834373595541E-01 1.418400135959E-01  
43 F 8 O 4.834373595541E-01 1.365002685019E-01 -3.581599864041E-01  
44 F 8 O -4.834373595541E-01 -1.365002685019E-01 -3.581599864041E-01  
45 F 8 O -1.365002685019E-01 -4.834373595541E-01 -1.418400135959E-01  
46 F 8 O 1.365002685019E-01 4.834373595541E-01 -1.418400135959E-01  
47 T 8 O -2.051396442739E-01 -2.913837305383E-01 0.000000000000E+00  
48 F 8 O 2.051396442739E-01 2.913837305383E-01 0.000000000000E+00  
49 F 8 O 2.913837305383E-01 2.051396442739E-01 -5.000000000000E-01  
50 F 8 O -2.913837305383E-01 -2.051396442739E-01 -5.000000000000E-01  
51 T 8 O 3.068936145090E-01 6.316074774920E-02 0.000000000000E+00  
52 F 8 O -3.068936145090E-01 -6.316074774920E-02 0.000000000000E+00  
53 F 8 O -6.316074774920E-02 -3.068936145090E-01 -5.000000000000E-01  
54 F 8 O 6.316074774920E-02 3.068936145090E-01 -5.000000000000E-01  
55 T 8 O 8.514671387003E-02 -2.437428448498E-01 0.000000000000E+00  
56 F 8 O -8.514671387003E-02 2.437428448498E-01 0.000000000000E+00  
57 F 8 O 2.437428448498E-01 -8.514671387003E-02 -5.000000000000E-01  
58 F 8 O -2.437428448498E-01 8.514671387003E-02 -5.000000000000E-01

TRANSFORMATION MATRIX PRIMITIVE-CRYSTALLOGRAPHIC CELL  
1.0000 1.0000 0.0000 -1.0000 1.0000 0.0000 0.0000 0.0000 1.0000

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CRYSTALLOGRAPHIC CELL (VOLUME= 1586.09072531)  
A B C ALPHA BETA GAMMA  
17.19628301 9.80014776 9.41154272 90.000000 90.000000 90.000000

COORDINATES IN THE CRYSTALLOGRAPHIC CELL

ATOM	X/A	Y/B	Z/C
*****			
1 T 12 MG	-1.628440693882E-01	5.000000000000E-01	2.500000000000E-01
2 F 12 MG	1.628440693882E-01	5.000000000000E-01	2.500000000000E-01
3 F 12 MG	1.628440693882E-01	5.000000000000E-01	-2.500000000000E-01
4 F 12 MG	-1.628440693882E-01	5.000000000000E-01	-2.500000000000E-01
5 T 13 AL	2.500000000000E-01	2.500000000000E-01	2.502090230322E-01
6 F 13 AL	-2.500000000000E-01	2.500000000000E-01	2.497909769678E-01
7 F 13 AL	2.500000000000E-01	2.500000000000E-01	-2.502090230322E-01
8 F 13 AL	-2.500000000000E-01	2.500000000000E-01	-2.497909769678E-01
9 T 13 AL	5.061166050578E-02	3.086028727700E-01	0.000000000000E+00
10 F 13 AL	-5.061166050578E-02	-3.086028727700E-01	0.000000000000E+00
11 F 13 AL	5.061166050578E-02	-3.086028727700E-01	-5.000000000000E-01
12 F 13 AL	-5.061166050578E-02	3.086028727700E-01	-5.000000000000E-01
13 T 14 SI	0.000000000000E+00	-5.000000000000E-01	2.500000000000E-01
14 F 14 SI	0.000000000000E+00	-5.000000000000E-01	-2.500000000000E-01
15 T 14 SI	1.920774093107E-01	7.845658165449E-02	0.000000000000E+00
16 F 14 SI	-1.920774093107E-01	-7.845658165449E-02	0.000000000000E+00
17 F 14 SI	1.920774093107E-01	-7.845658165449E-02	-5.000000000000E-01
18 F 14 SI	-1.920774093107E-01	7.845658165449E-02	-5.000000000000E-01
19 T 14 SI	1.350164750857E-01	-2.372646960501E-01	0.000000000000E+00
20 F 14 SI	-1.350164750857E-01	2.372646960501E-01	0.000000000000E+00
21 F 14 SI	1.350164750857E-01	2.372646960501E-01	-5.000000000000E-01
22 F 14 SI	-1.350164750857E-01	-2.372646960501E-01	-5.000000000000E-01
23 T 8 O	2.470393804899E-01	-1.033662256963E-01	3.584944396351E-01
24 F 8 O	-2.470393804899E-01	1.033662256963E-01	3.584944396351E-01
25 F 8 O	2.470393804899E-01	1.033662256963E-01	1.415055603649E-01



26 F 8 O -2.470393804899E-01 -1.033662256963E-01 1.415055603649E-01  
27 F 8 O -2.470393804899E-01 1.033662256963E-01 -3.584944396351E-01  
28 F 8 O 2.470393804899E-01 -1.033662256963E-01 -3.584944396351E-01  
29 F 8 O -2.470393804899E-01 -1.033662256963E-01 -1.415055603649E-01  
30 F 8 O 2.470393804899E-01 1.033662256963E-01 -1.415055603649E-01  
31 T 8 O 6.263705315058E-02 -4.170350836253E-01 3.492063126317E-01  
32 F 8 O -6.263705315058E-02 4.170350836253E-01 3.492063126317E-01  
33 F 8 O 6.263705315058E-02 4.170350836253E-01 1.507936873683E-01  
34 F 8 O -6.263705315058E-02 -4.170350836253E-01 1.507936873683E-01  
35 F 8 O -6.263705315058E-02 4.170350836253E-01 -3.492063126317E-01  
36 F 8 O 6.263705315058E-02 -4.170350836253E-01 -3.492063126317E-01  
37 F 8 O -6.263705315058E-02 -4.170350836253E-01 -1.507936873683E-01  
38 F 8 O 6.263705315058E-02 4.170350836253E-01 -1.507936873683E-01  
39 T 8 O -1.734685455261E-01 -3.099688140280E-01 3.581599864041E-01  
40 F 8 O 1.734685455261E-01 3.099688140280E-01 3.581599864041E-01  
41 F 8 O -1.734685455261E-01 3.099688140280E-01 1.418400135959E-01  
42 F 8 O 1.734685455261E-01 -3.099688140280E-01 1.418400135959E-01  
43 F 8 O 1.734685455261E-01 3.099688140280E-01 -3.581599864041E-01  
44 F 8 O -1.734685455261E-01 -3.099688140280E-01 -3.581599864041E-01  
45 F 8 O 1.734685455261E-01 -3.099688140280E-01 -1.418400135959E-01  
46 F 8 O -1.734685455261E-01 3.099688140280E-01 -1.418400135959E-01  
47 T 8 O 4.312204313218E-02 -2.482616874061E-01 0.000000000000E+00  
48 F 8 O -4.312204313218E-02 2.482616874061E-01 0.000000000000E+00  
49 F 8 O 4.312204313218E-02 2.482616874061E-01 -5.000000000000E-01  
50 F 8 O -4.312204313218E-02 -2.482616874061E-01 -5.000000000000E-01  
51 T 8 O 1.218664333799E-01 1.850271811291E-01 0.000000000000E+00  
52 F 8 O -1.218664333799E-01 -1.850271811291E-01 0.000000000000E+00  
53 F 8 O 1.218664333799E-01 -1.850271811291E-01 -5.000000000000E-01  
54 F 8 O -1.218664333799E-01 1.850271811291E-01 -5.000000000000E-01  
55 T 8 O 1.644447793599E-01 -7.929806548987E-02 0.000000000000E+00  
56 F 8 O -1.644447793599E-01 7.929806548987E-02 0.000000000000E+00  
57 F 8 O 1.644447793599E-01 7.929806548987E-02 -5.000000000000E-01  
58 F 8 O -1.644447793599E-01 -7.929806548987E-02 -5.000000000000E-01

T = ATOM BELONGING TO THE ASYMMETRIC UNIT

\*\*\*\* 8 SYMMOPS - TRANSLATORS IN FRACTIONARY UNITS

V	INV	ROTATION MATRICES								TRANSLATOR			
1	1	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
2	2	-1.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
3	3	0.00	-1.00	0.00	-1.00	0.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.50
4	4	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.50
5	5	-1.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.00
6	6	1.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	-1.00	0.00	0.00	0.00
7	7	0.00	1.00	0.00	1.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.50
8	8	0.00	-1.00	0.00	-1.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.50

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

X	Y	Z
0.859814150500E+01	0.490007388000E+01	0.000000000000E+00
-0.859814150500E+01	0.490007388000E+01	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	0.941154272000E+01

# CARTESIAN COORDINATES - PRIMITIVE CELL

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* ATOM	X(ANGSTROM)	Y(ANGSTROM)	Z(ANGSTROM)
*****			
1	12 MG	-2.800312703700E+00	-4.900073880000E+00
2	12 MG	2.800312703700E+00	-4.900073880000E+00
3	12 MG	2.800312703700E+00	-4.900073880000E+00
4	12 MG	-2.800312703700E+00	-4.900073880000E+00
5	13 AL	4.299070752500E+00	2.450036940000E+00
6	13 AL	-4.299070752500E+00	2.450036940000E+00
7	13 AL	4.299070752500E+00	2.450036940000E+00
8	13 AL	-4.299070752500E+00	2.450036940000E+00
9	13 AL	8.703324376634E-01	3.024353752306E+00
10	13 AL	-8.703324376634E-01	3.024353752306E+00
11	13 AL	8.703324376634E-01	3.024353752306E+00
12	13 AL	-8.703324376634E-01	3.024353752306E+00
13	14 SI	0.000000000000E+00	4.900073880000E+00
14	14 SI	0.000000000000E+00	4.900073880000E+00
15	14 SI	3.303017490334E+00	7.688860929585E-01
16	14 SI	-3.303017490334E+00	7.688860929585E-01
17	14 SI	3.303017490334E+00	7.688860929585E-01
18	14 SI	-3.303017490334E+00	7.688860929585E-01
19	14 SI	2.321781516586E+00	-2.325229079522E+00
20	14 SI	-2.321781516586E+00	-2.325229079522E+00
21	14 SI	2.321781516586E+00	-2.325229079522E+00
22	14 SI	-2.321781516586E+00	-2.325229079522E+00
23	8 O	4.248159101519E+00	-1.013004285217E+00
24	8 O	-4.248159101519E+00	-1.013004285217E+00
25	8 O	4.248159101519E+00	-1.013004285217E+00
26	8 O	-4.248159101519E+00	-1.013004285217E+00
27	8 O	4.248159101519E+00	-1.013004285217E+00
28	8 O	-4.248159101519E+00	-1.013004285217E+00
29	8 O	4.248159101519E+00	-1.013004285217E+00
30	8 O	-4.248159101519E+00	-1.013004285217E+00
31	8 O	1.077124492890E+00	-4.087005440632E+00
32	8 O	-1.077124492890E+00	-4.087005440632E+00
33	8 O	1.077124492890E+00	-4.087005440632E+00
34	8 O	-1.077124492890E+00	-4.087005440632E+00
35	8 O	1.077124492890E+00	-4.087005440632E+00
36	8 O	-1.077124492890E+00	-4.087005440632E+00
37	8 O	1.077124492890E+00	-4.087005440632E+00
38	8 O	-1.077124492890E+00	-4.087005440632E+00
39	8 O	2.983014202200E+00	-3.037740178466E+00
40	8 O	-2.983014202200E+00	-3.037740178466E+00
41	8 O	2.983014202200E+00	-3.037740178466E+00
42	8 O	-2.983014202200E+00	-3.037740178466E+00
43	8 O	2.983014202200E+00	-3.037740178466E+00
44	8 O	-2.983014202200E+00	-3.037740178466E+00
45	8 O	2.983014202200E+00	-3.037740178466E+00
46	8 O	-2.983014202200E+00	-3.037740178466E+00
47	8 O	7.415388576704E-01	-2.433001219727E+00
48	8 O	-7.415388576704E-01	-2.433001219727E+00
49	8 O	7.415388576704E-01	-2.433001219727E+00
50	8 O	-7.415388576704E-01	-2.433001219727E+00

51	8 O	2.095649677820E+00	1.813293714681E+00	0.000000000000E+00
52	8 O	-2.095649677820E+00	-1.813293714681E+00	0.000000000000E+00
53	8 O	2.095649677820E+00	-1.813293714681E+00	4.705771360000E+00
54	8 O	-2.095649677820E+00	1.813293714681E+00	4.705771360000E+00
55	8 O	2.827838965390E+00	-7.771327588829E-01	0.000000000000E+00
56	8 O	-2.827838965390E+00	7.771327588829E-01	0.000000000000E+00
57	8 O	2.827838965390E+00	7.771327588829E-01	4.705771360000E+00
58	8 O	-2.827838965390E+00	-7.771327588829E-01	4.705771360000E+00

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# LOCAL ATOMIC FUNCTIONS BASIS SET

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ATOM	X(AU)	Y(AU)	Z(AU)	NO.	TYPE	EXPONENT	S COEF	P COEF	D/F/G COEF
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1 MG -5.292 -9.260 4.446

1 S

6.837E+04	2.226E-04	0.000E+00	0.000E+00
9.661E+03	1.901E-03	0.000E+00	0.000E+00
2.041E+03	1.104E-02	0.000E+00	0.000E+00
5.296E+02	5.005E-02	0.000E+00	0.000E+00
1.592E+02	1.690E-01	0.000E+00	0.000E+00
5.471E+01	3.669E-01	0.000E+00	0.000E+00
2.124E+01	4.008E-01	0.000E+00	0.000E+00
8.791E+00	1.487E-01	0.000E+00	0.000E+00

2- 5 SP

1.437E+02	-6.710E-03	8.070E-03	0.000E+00
3.127E+01	-7.927E-02	6.401E-02	0.000E+00
9.661E+00	-8.088E-02	2.092E-01	0.000E+00
3.726E+00	2.947E-01	3.460E-01	0.000E+00
1.598E+00	5.714E-01	3.731E-01	0.000E+00

6- 9 SP

6.000E-01	1.000E+00	1.000E+00	0.000E+00
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10- 13 SP

3.150E-01	1.000E+00	1.000E+00	0.000E+00
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14- 18 D

4.260E-01	0.000E+00	0.000E+00	1.000E+00
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2 MG 5.292 -9.260 4.446

3 MG 5.292 -9.260 -4.446

4 MG -5.292 -9.260 -4.446

5 AL 8.124 4.630 4.450

73 S

5.985E+04	4.000E-04	0.000E+00	0.000E+00
8.508E+03	3.400E-03	0.000E+00	0.000E+00
1.903E+03	1.730E-02	0.000E+00	0.000E+00
5.625E+02	6.170E-02	0.000E+00	0.000E+00
2.029E+02	1.680E-01	0.000E+00	0.000E+00
7.768E+01	3.850E-01	0.000E+00	0.000E+00
3.115E+01	5.224E-01	0.000E+00	0.000E+00
1.243E+01	2.864E-01	0.000E+00	0.000E+00

74- 77 SP

5.651E+02	-4.000E-04	1.100E-03	0.000E+00
1.444E+02	-5.900E-03	7.500E-03	0.000E+00
5.015E+01	-3.850E-02	3.390E-02	0.000E+00
1.900E+01	-9.640E-02	1.160E-01	0.000E+00

8.036E+00 2.040E-02 2.451E-01 0.000E+00  
 3.588E+00 3.772E-01 3.701E-01 0.000E+00  
 1.588E+00 5.164E-01 3.554E-01 0.000E+00  
 7.079E-01 1.783E-01 1.356E-01 0.000E+00  
 78- 81 SP  
 1.960E+00-6.070E-02 5.140E-02 0.000E+00  
 8.551E-01-1.183E-01-9.380E-02 0.000E+00  
 2.477E-01 2.007E-01-1.030E+00 0.000E+00  
 82- 85 SP  
 4.380E-01 1.000E+00 1.000E+00 0.000E+00  
 86- 89 SP  
 2.120E-01 1.000E+00 1.000E+00 0.000E+00  
 90- 94 D  
 5.820E-01 0.000E+00 0.000E+00 1.000E+00  
 6 AL -8.124 4.630 4.443  
 7 AL 8.124 4.630 -4.450  
 8 AL -8.124 4.630 -4.443  
 9 AL 1.645 5.715 0.000  
 10 AL -1.645 -5.715 0.000  
 11 AL 1.645 -5.715 8.893  
 12 AL -1.645 5.715 8.893  
 13 SI 0.000 9.260 4.446  
 249 S  
 8.765E+04 2.370E-04 0.000E+00 0.000E+00  
 1.285E+04 1.920E-03 0.000E+00 0.000E+00  
 2.786E+03 1.090E-02 0.000E+00 0.000E+00  
 7.280E+02 4.960E-02 0.000E+00 0.000E+00  
 2.195E+02 1.668E-01 0.000E+00 0.000E+00  
 7.590E+01 3.630E-01 0.000E+00 0.000E+00  
 2.946E+01 4.051E-01 0.000E+00 0.000E+00  
 1.199E+01 1.504E-01 0.000E+00 0.000E+00  
 250- 253 SP  
 1.660E+02-8.840E-03 9.090E-03 0.000E+00  
 3.937E+01-8.590E-02 6.010E-02 0.000E+00  
 1.271E+01-7.120E-02 1.952E-01 0.000E+00  
 4.718E+00 4.147E-01 3.384E-01 0.000E+00  
 1.848E+00 6.168E-01 3.006E-01 0.000E+00  
 7.365E-01 1.154E-01 6.480E-02 0.000E+00  
 254- 257 SP  
 4.175E+00-1.990E-02-8.700E-03 0.000E+00  
 1.447E+00-1.864E-01-4.380E-03 0.000E+00  
 5.023E-01 9.670E-02 2.207E-01 0.000E+00  
 258- 261 SP  
 3.440E-01 1.000E+00 1.000E+00 0.000E+00  
 262- 265 SP  
 1.300E-01 1.000E+00 1.000E+00 0.000E+00  
 266- 270 D  
 6.770E-01 0.000E+00 0.000E+00 1.000E+00  
 14 SI 0.000 9.260 -4.446  
 15 SI 6.242 1.453 0.000  
 16 SI -6.242 -1.453 0.000  
 17 SI 6.242 -1.453 8.893  
 18 SI -6.242 1.453 8.893  
 19 SI 4.388 -4.394 0.000

20 SI -4.388 4.394 0.000  
 21 SI 4.388 4.394 8.893  
 22 SI -4.388 -4.394 8.893  
 23 O 8.028 -1.914 6.376  
     469 S  
         8.020E+03 1.080E-03 0.000E+00 0.000E+00  
         1.338E+03 8.040E-03 0.000E+00 0.000E+00  
         2.554E+02 5.324E-02 0.000E+00 0.000E+00  
         6.922E+01 1.681E-01 0.000E+00 0.000E+00  
         2.390E+01 3.581E-01 0.000E+00 0.000E+00  
         9.264E+00 3.855E-01 0.000E+00 0.000E+00  
         3.851E+00 1.468E-01 0.000E+00 0.000E+00  
         1.212E+00 7.280E-02 0.000E+00 0.000E+00  
 470- 473 SP  
         4.943E+01-8.830E-03 9.580E-03 0.000E+00  
         1.047E+01-9.150E-02 6.960E-02 0.000E+00  
         3.235E+00-4.020E-02 2.065E-01 0.000E+00  
         1.217E+00 3.790E-01 3.470E-01 0.000E+00  
 474- 477 SP  
         4.660E-01 1.000E+00 1.000E+00 0.000E+00  
 478- 481 SP  
         1.950E-01 1.000E+00 1.000E+00 0.000E+00  
 482- 486 D  
         5.380E-01 0.000E+00 0.000E+00 1.000E+00  
 24 O -8.028 1.914 6.376  
 25 O 8.028 1.914 2.517  
 26 O -8.028 -1.914 2.517  
 27 O -8.028 1.914 -6.376  
 28 O 8.028 -1.914 -6.376  
 29 O -8.028 -1.914 -2.517  
 30 O 8.028 1.914 -2.517  
 31 O 2.035 -7.723 6.211  
 32 O -2.035 7.723 6.211  
 33 O 2.035 7.723 2.682  
 34 O -2.035 -7.723 2.682  
 35 O -2.035 7.723 -6.211  
 36 O 2.035 -7.723 -6.211  
 37 O -2.035 -7.723 -2.682  
 38 O 2.035 7.723 -2.682  
 39 O -5.637 -5.740 6.370  
 40 O 5.637 5.740 6.370  
 41 O -5.637 5.740 2.523  
 42 O 5.637 -5.740 2.523  
 43 O 5.637 5.740 -6.370  
 44 O -5.637 -5.740 -6.370  
 45 O 5.637 -5.740 -2.523  
 46 O -5.637 5.740 -2.523  
 47 O 1.401 -4.598 0.000  
 48 O -1.401 4.598 0.000  
 49 O 1.401 4.598 8.893  
 50 O -1.401 -4.598 8.893  
 51 O 3.960 3.427 0.000  
 52 O -3.960 -3.427 0.000  
 53 O 3.960 -3.427 8.893

54 O -3.960 3.427 8.893  
55 O 5.344 -1.469 0.000  
56 O -5.344 1.469 0.000  
57 O 5.344 1.469 8.893  
58 O -5.344 -1.469 8.893  
INFORMATION \*\*\*\* MAXCYCLE \*\*\*\* MAX NUMBER OF SCF CYCLES SET TO 500  
INFORMATION \*\*\*\* BIPOSIZE \*\*\*\* COULOMB BIPOLAR BUFFER SET TO 7818200  
INFORMATION \*\*\*\* EXCHSIZE \*\*\*\* EXCHANGE BIPOLAR BUFFER SIZE SET TO 7876296  
INFORMATION \*\*\*\* TOLINTEG \*\*\*\* COULOMB AND EXCHANGE SERIES TOLERANCES MODIFIED  
INFORMATION \*\*\*\* READM2 \*\*\*\* FULL DIRECT SCF (MONO AND BIEL INT) SELECTED

MODIFIED BROYDEN MIXING OF THE FOCK MATRIX

WO PARAMETER(D.D. Johnson, PRB38, 12807,(1988) 1.0000E-04  
% OF FOCK/KS MATRICES MIXING WHEN BROYDEN METHOD IS ON 50  
NUMBER OF SCF ITERATIONS AFTER WHICH BROYDEN METHOD IS ACTIVE 2  
\*\*\*\*\*  
N. OF ATOMS PER CELL 58 COULOMB OVERLAP TOL (T1) 10\*\* -7  
NUMBER OF SHELLS 308 COULOMB PENETRATION TOL (T2) 10\*\* -7  
NUMBER OF AO 1116 EXCHANGE OVERLAP TOL (T3) 10\*\* -7  
N. OF ELECTRONS PER CELL 580 EXCHANGE PSEUDO OVP (F(G)) (T4) 10\*\* -7  
CORE ELECTRONS PER CELL 292 EXCHANGE PSEUDO OVP (P(G)) (T5) 10\*\* -15  
N. OF SYMMETRY OPERATORS 8 POLE ORDER IN MONO ZONE 4  
\*\*\*\*\*

TYPE OF CALCULATION : RESTRICTED CLOSED SHELL  
KOHN-SHAM HAMILTONIAN

(EXCHANGE)[CORRELATION] FUNCTIONAL:(BECKE)[LEE-YANG-PARR]

NON-LOCAL WEIGHTING FACTOR (EXCHANGE) = 0.9000  
NON-LOCAL WEIGHTING FACTOR [CORRELATION] = 0.8100

HYBRID EXCHANGE - PERCENTAGE OF FOCK EXCHANGE 20.0000

CAPPA: IS1= 4 IS2= 4 IS3= 4K POINTS MONKHORST NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

CAPPA1: ISJ1= 4 ISJ2= 4 ISJ3= 4K POINTS GILAT NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

\*\*\*\*\*  
MAX NUMBER OF SCF CYCLES 500 CONVERGENCE ON DELTAP 10\*\* -16  
WEIGHT OF F(I) IN F(I+1) 80% CONVERGENCE ON ENERGY 10\*\* -6  
SHRINK. FACT.(MONKH.) 4 4 4 NUMBER OF K POINTS IN THE IBZ 21  
SHRINKING FACTOR(GILAT NET) 4 NUMBER OF K POINTS(GILAT NET) 21  
\*\*\*\*\*

\*\*\* K POINTS COORDINATES (OBLIQUE COORDINATES IN UNITS OF IS = 4)

1-R( 0 0 0) 2-C( 1 0 0) 3-R( 2 0 0) 4-C( 1 1 0)  
5-C( 2 1 0) 6-C( 3 1 0) 7-R( 2 2 0) 8-C( 0 0 1)  
9-C( 1 0 1) 10-C( 2 0 1) 11-C( 1 1 1) 12-C( 2 1 1)  
13-C( 3 1 1) 14-C( 2 2 1) 15-R( 0 0 2) 16-C( 1 0 2)  
17-R( 2 0 2) 18-C( 1 1 2) 19-C( 2 1 2) 20-C( 3 1 2)  
21-R( 2 2 2)

DIRECT LATTICE VECTORS COMPON. (A.U.) RECIP. LATTICE VECTORS COMPON. (A.U.)

X	Y	Z	X	Y	Z
16.2481327	9.2597977	0.0000000	0.1933510	0.3392723	0.0000000
-16.2481327	9.2597977	0.0000000	-0.1933510	0.3392723	0.0000000
0.0000000	0.0000000	17.7852382	0.0000000	0.0000000	0.3532809

DISK SPACE FOR EIGENVECTORS (FTN 10) 44836416 REALS

SYMMETRY ADAPTION OF THE BLOCH FUNCTIONS ENABLED

DIMENSIONS P(G)= 2353196 F(G)= 378354 P(G),F(G) (IRR) 165393  
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TT INPUT TELAPSE 0.06 TCPU 0.04

NEIGHBORS OF THE NON-EQUIVALENT ATOMS

N = NUMBER OF NEIGHBORS AT DISTANCE R

ATOM	N	R/ANG	R/AU	NEIGHBORS (ATOM LABELS AND CELL INDICES)
1 MG	2	2.1143	3.9955	23 O -1 0 0 25 O -1 0 0
1 MG	2	2.1218	4.0097	32 O -1-1 0 34 O 0 0 0
1 MG	2	2.1302	4.0256	39 O 0 0 0 41 O -1-1 0
1 MG	1	2.8003	5.2918	13 SI -1-1 0
1 MG	2	2.8721	5.4275	5 AL -1 0 0 6 AL -1-1 0
1 MG	2	3.5144	6.6413	15 SI -1 0 0 17 SI -1 0 0
5 AL	2	1.7634	3.3324	39 O 1 0 0 40 O 0 0 0
5 AL	2	1.7647	3.3349	25 O 0 0 0 26 O 1 0 0
5 AL	2	2.8721	5.4275	1 MG 1 0 0 2 MG 1 1 0
5 AL	2	3.0600	5.7826	15 SI 0 0 0 16 SI 1 0 0
5 AL	2	3.0744	5.8098	21 SI 0 0 0 22 SI 1 0 0
5 AL	2	3.2388	6.1205	57 O 0 0 0 58 O 1 0 0
9 AL	1	1.7169	3.2445	48 O 0 0 0
9 AL	1	1.7228	3.2556	51 O 0 0 0
9 AL	2	1.7850	3.3731	33 O 0 0 0 38 O 0 0 0
9 AL	2	3.1324	5.9194	13 SI 0 0 0 14 SI 0 0 0
9 AL	1	3.2678	6.1752	20 SI 0 0 0
9 AL	1	3.3174	6.2690	15 SI 0 0 0
13 SI	4	1.6410	3.1011	31 O 1 1 0 32 O 0 0 0 33 O 0 0 0
				34 O 1 1 0
13 SI	2	2.8003	5.2918	1 MG 1 1 0 2 MG 1 1 0
13 SI	4	3.1324	5.9194	9 AL 0 0 0 10 AL 1 1 0 11 AL 1 1 0
				12 AL 0 0 0
13 SI	4	3.4889	6.5931	47 O 1 1 0 48 O 0 0 0 49 O 0 0 0
				50 O 1 1 0
13 SI	4	3.6610	6.9183	39 O 1 1 0 40 O 0 0 0 41 O 0 0 0
				42 O 1 1 0
13 SI	4	4.0062	7.5707	35 O 0 0 1 36 O 1 1 1 37 O 1 1 0
				38 O 0 0 0
15 SI	1	1.5964	3.0168	51 O 0 0 0
15 SI	1	1.6174	3.0564	55 O 0 0 0
15 SI	2	1.6512	3.1204	25 O 0 0 0 30 O 0 0 0

15 SI	2	3.0600	5.7826	5 AL	0 0 0	7 AL	0 0 0
15 SI	1	3.2460	6.1340	19 SI	0 0 0		
15 SI	1	3.3174	6.2690	9 AL	0 0 0		
19 SI	1	1.5839	2.9932	47 O	0 0 0		
19 SI	1	1.6287	3.0778	55 O	0 0 0		
19 SI	2	1.6513	3.1206	42 O	0 0 0	45 O	0 0 0
19 SI	2	3.0744	5.8098	6 AL	0-1 0	8 AL	0-1 0
19 SI	1	3.2460	6.1340	15 SI	0 0 0		
19 SI	1	3.2678	6.1752	10 AL	0 0 0		
23 O	1	1.6512	3.1204	17 SI	0 0 0		
23 O	1	1.7647	3.3349	6 AL	0-1 0		
23 O	1	2.1143	3.9955	1 MG	1 0 0		
23 O	1	2.5976	4.9088	41 O	0-1 0		
23 O	1	2.6449	4.9982	57 O	0 0 0		
23 O	1	2.6547	5.0166	53 O	0 0 0		
31 O	1	1.6410	3.1011	13 SI	-1-1 0		
31 O	1	1.7850	3.3731	11 AL	0 0 0		
31 O	1	2.1218	4.0097	2 MG	0 0 0		
31 O	1	2.4762	4.6793	33 O	-1-1 0		
31 O	1	2.6991	5.1005	32 O	-1-1 0		
31 O	1	2.8384	5.3638	36 O	0 0 1		
39 O	1	1.6513	3.1206	22 SI	0 0 0		
39 O	1	1.7634	3.3324	5 AL	-1 0 0		
39 O	1	2.1302	4.0256	1 MG	0 0 0		
39 O	1	2.5976	4.9088	25 O	-1 0 0		
39 O	1	2.6299	4.9698	58 O	0 0 0		
39 O	1	2.6699	5.0453	44 O	0 0 1		
47 O	1	1.5839	2.9932	19 SI	0 0 0		
47 O	1	1.7169	3.2445	10 AL	0 0 0		
47 O	1	2.6636	5.0334	55 O	0 0 0		
47 O	2	2.6781	5.0608	42 O	0 0 0	45 O	0 0 0
47 O	2	2.8386	5.3641	34 O	0 0 0	37 O	0 0 0
47 O	1	2.9041	5.4879	52 O	0 0 0		
51 O	1	1.5964	3.0168	15 SI	0 0 0		
51 O	1	1.7228	3.2556	9 AL	0 0 0		
51 O	2	2.6547	5.0166	25 O	0 0 0	30 O	0 0 0
51 O	1	2.6919	5.0870	55 O	0 0 0		
51 O	2	2.8673	5.4184	33 O	0 0 0	38 O	0 0 0
51 O	1	2.9041	5.4879	48 O	0 0 0		
55 O	1	1.6174	3.0564	15 SI	0 0 0		
55 O	1	1.6287	3.0778	19 SI	0 0 0		
55 O	2	2.6299	4.9698	42 O	0 0 0	45 O	0 0 0
55 O	2	2.6449	4.9982	25 O	0 0 0	30 O	0 0 0
55 O	1	2.6636	5.0334	47 O	0 0 0		
55 O	1	2.6919	5.0870	51 O	0 0 0		



SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM TELAPSE 0.31 TCPU 0.27  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT\_SCREEN TELAPSE 0.35 TCPU 0.32

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*
*      FFFFF RRRR EEEE EEE U U EEEE N N CCC Y Y      *
*      F  R R E  E E U U E  NN N C  YY      *
*      FFF  RRRR EEEE E E U U EEEE N N N C  Y      *
*      F  R R E  E EE U U E  N NN C  Y      *
*      F  R R EEEE EE E UUU EEEE N N CCC  Y      *
*
*
*      *
*
* CALCULATION OF PHONON FREQUENCIES AT THE GAMMA POINT.      *
*
*
* SYMMETRY IS EXPLOITED TO BUILD THE TOTAL HESSIAN MATRIX.      *
* (F. PASCALE PHD THESIS TURIN-PARIS 2002)      *
*
*
*****
*
*
* REFERENCES TO BE QUOTED WHEN USING THIS MODULE:      *
*
*
* F. Pascale, C.M. Zicovich-Wilson, F. Lopez, B. Civalleri      *
* R. Orlando, R. Dovesi      *
* The calculation of the vibration frequencies of crystalline      *
* compounds and its implementation in the CRYSTAL code      *
* J. Comput. Chem. 25 (2004) 888-897      *
*
*
* C.M. Zicovich-Wilson, F. Pascale, C. Roetti, V.R. Saunders,      *
* R. Orlando, R. Dovesi      *
* The calculation of the vibration frequencies of alpha-quartz:      *
* the effect of hamiltonian and basis set      *
* J. Comput. Chem. 25 (2004) 1873-1881      *
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## ATOMS ISOTOPIC MASS (AMU) FOR FREQUENCY CALCULATION

1 MG	23.985040	2 MG	23.985040	3 MG	23.985040	4 MG	23.985040
5 AL	26.981530	6 AL	26.981530	7 AL	26.981530	8 AL	26.981530
9 AL	26.981530	10 AL	26.981530	11 AL	26.981530	12 AL	26.981530
13 SI	27.976930	14 SI	27.976930	15 SI	27.976930	16 SI	27.976930
17 SI	27.976930	18 SI	27.976930	19 SI	27.976930	20 SI	27.976930
21 SI	27.976930	22 SI	27.976930	23 O	15.994910	24 O	15.994910
25 O	15.994910	26 O	15.994910	27 O	15.994910	28 O	15.994910
29 O	15.994910	30 O	15.994910	31 O	15.994910	32 O	15.994910
33 O	15.994910	34 O	15.994910	35 O	15.994910	36 O	15.994910
37 O	15.994910	38 O	15.994910	39 O	15.994910	40 O	15.994910
41 O	15.994910	42 O	15.994910	43 O	15.994910	44 O	15.994910
45 O	15.994910	46 O	15.994910	47 O	15.994910	48 O	15.994910
49 O	15.994910	50 O	15.994910	51 O	15.994910	52 O	15.994910
53 O	15.994910	54 O	15.994910	55 O	15.994910	56 O	15.994910

57 O 15.994910 58 O 15.994910

STEP SIZE 0.0030  
USE OF RESIDUAL SYMMETRY AFTER DISPLACEMENT

NUMERICAL GRADIENT COMPUTED WITH DIFFERENT QUOTIENT FORMULA  
NUMBER OF IRREDUCIBLE ATOMS 12  
NUMBER OF SCF+GRADIENT CALCULATIONS 37

ATOM SYMOP ORDER

1	2	2
5	2	2
9	2	2
13	4	2
15	2	2
19	2	2
23	1	1
31	1	1
39	1	1
47	2	2
51	2	2
55	2	2

ATOM : IRREDUCIBLE ATOM  
SYMOP : NUMBER OF SYMMETRY OPERATORS THAT DOESN'T MOVE THE IRREDUCIBLE ATOM  
ORDER : MAXIMUM ORDER AMONG THE OPERATORS OF THE IRREDUCIBLE ATOM

\*\*\*\*\*

GCALCO - MAX INDICES DIRECT LATTICE VECTOR 15 15 14  
NO.OF VECTORS CREATED 6999 STARS 1020 RMAX 207.45093 BOHR

CAPPA: IS1= 4 IS2= 4 IS3= 4K POINTS MONKHORST NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

CAPPA1: ISJ1= 4 ISJ2= 4 ISJ3= 4K POINTS GILAT NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

DIMENSIONS P(G)= 2353196 F(G)= 378354 P(G),F(G) (IRR) 165393  
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TT INPUT TELAPSE 0.38 TCPU 0.35

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23

TT SYMM	TELAPSE	0.64	TCPU	0.60
TT INT_SCREEN	TELAPSE	0.69	TCPU	0.65

INFORMATION \*\*\*\* EXCBUF \*\*\*\* EXCH. BIPO BUFFER: WORDS USED = 6237756

DFT PARAMETERS

ATOM	ELECTRONS	NET CHARGE	R(ANGSTROM)
1 12 MG	10.0000	2.0000	0.72000000

5 13 AL 12.0000 1.0000 1.13333333  
13 14 SI 12.0000 2.0000 0.78500000  
23 8 O 9.0000 -1.0000 1.07000000

SIZE OF GRID= 195985

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MAKEGRID TELAPSE 34.31 TCPU 34.28

BECKE WEIGHT FUNCTION

RADSAFE = 2.00

TOLERANCES - DENSITY:10\*\*- 6; POTENTIAL:10\*\*- 9; GRID WGT:10\*\*-14

RADIAL INTEGRATION - INTERVALS (POINTS,UPPER LIMIT): 1( 75, 4.0\*R)

ANGULAR INTEGRATION - INTERVALS (ACCURACY LEVEL [N. POINTS] UPPER LIMIT):

1( 4[ 86] 0.2) 2( 8[ 194] 0.5) 3( 12[ 350] 0.9) 4( 16[ 974] 3.5)

5( 12[ 350]9999.0)

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT\_CALC TELAPSE 34.42 TCPU 34.39

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Cordierite, B3LYP optimized

CRYSTAL - SCF - TYPE OF CALCULATION : RESTRICTED CLOSED SHELL

\*\*\*\*\*

CAPPA: IS1= 4 IS2= 4 IS3= 4K POINTS MONKHORST NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

CAPPA1: ISJ1= 4 ISJ2= 4 ISJ3= 4K POINTS GILAT NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SDIK TELAPSE 48.52 TCPU 48.48

AA  
AAAAAAAAAAAAAAAAAA

ATOMIC WAVEFUNCTION(S)

NUCLEAR CHARGE 12.0 SYMMETRY SPECIES S P

N. ELECTRONS 10.0 NUMBER OF PRIMITIVE GTOS 15 7

NUMBER OF CONTRACTED GTOS 4 3

NUMBER OF CLOSED SHELLS 2 1

OPEN SHELL OCCUPATION 0 0

ZNUC SCFIT TOTAL HF ENERGY KINETIC ENERGY VIRIAL THEOREM ACCURACY

12.0 8 -1.988191155E+02 1.990028320E+02 -1.999076815E+00 2.5E-06

NUCLEAR CHARGE 13.0 SYMMETRY SPECIES S P

N. ELECTRONS 12.0 NUMBER OF PRIMITIVE GTOS 21 13

NUMBER OF CONTRACTED GTOS 5 4

NUMBER OF CLOSED SHELLS 3 1

OPEN SHELL OCCUPATION 0 0

ZNUC SCFIT TOTAL HF ENERGY KINETIC ENERGY VIRIAL THEOREM ACCURACY

13.0 10 -2.416210442E+02 2.418765826E+02 -1.998943518E+00 1.0E-06

NUCLEAR CHARGE 14.0 SYMMETRY SPECIES S P

N. ELECTRONS 12.0 NUMBER OF PRIMITIVE GTOS 19 11  
NUMBER OF CONTRACTED GTOS 5 4  
NUMBER OF CLOSED SHELLS 3 1  
OPEN SHELL OCCUPATION 0 0

ZNUC SCFIT TOTAL HF ENERGY KINETIC ENERGY VIRIAL THEOREM ACCURACY  
14.0 9 -2.879787081E+02 2.880726364E+02 -1.999673942E+00 2.8E-06

NUCLEAR CHARGE 8.0 SYMMETRY SPECIES S P  
N. ELECTRONS 9.0 NUMBER OF PRIMITIVE GTOS 14 6  
NUMBER OF CONTRACTED GTOS 4 3  
NUMBER OF CLOSED SHELLS 2 0  
OPEN SHELL OCCUPATION 0 5

ZNUC SCFIT TOTAL HF ENERGY KINETIC ENERGY VIRIAL THEOREM ACCURACY  
8.0 23 -7.475928154E+01 7.474563283E+01 -2.000182602E+00 4.3E-06

AA  
AAAAAAAAAAAAAAAA

CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 49.29 TCPU 49.25  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 415.88 TCPU 415.92  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 430.41 TCPU 430.45  
NUMERICALLY INTEGRATED DENSITY 579.9999998797  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 457.31 TCPU 457.36  
CYC 0 ETOT(AU) -8.361014906685E+03 DETOT -8.36E+03 tst 0.00E+00 PX 1.00E+00  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 735.45 TCPU 735.53  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.9860798E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 760.26 TCPU 760.34  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 761.03 TCPU 761.12  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 1162.22 TCPU 1162.41  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 1176.66 TCPU 1176.85  
NUMERICALLY INTEGRATED DENSITY 579.9999935333  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 1248.06 TCPU 1248.27  
CYC 1 ETOT(AU) -8.344918071947E+03 DETOT 1.61E+01 tst 0.00E+00 PX 1.00E+00  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 1341.91 TCPU 1342.14  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.7392147E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 1367.25 TCPU 1367.49  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 1368.04 TCPU 1368.28  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 1774.18 TCPU 1774.52  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 1788.62 TCPU 1788.96  
NUMERICALLY INTEGRATED DENSITY 579.9999930351  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 1859.96 TCPU 1860.32  
CYC 2 ETOT(AU) -8.346267795356E+03 DETOT -1.35E+00 tst 4.90E-04 PX 4.21E-02  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 4.483069704428E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 1962.25 TCPU 1962.62  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.1255020E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 1987.21 TCPU 1987.57  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 1987.98 TCPU 1988.35  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 2393.08 TCPU 2393.50

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TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3   TELAPSE   2407.51 TCPU   2407.94
NUMERICALLY INTEGRATED DENSITY   579.9999933048
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT   TELAPSE   2480.52 TCPU   2480.96
CYC  3 ETOT(AU) -8.346818671550E+03 DETOT -5.51E-01 tst 1.30E-03 PX 1.14E-01
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 1.425740354868E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK     TELAPSE   2562.05 TCPU   2562.47
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.9058641E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG     TELAPSE   2586.98 TCPU   2587.39
CHARGE NORMALIZATION FACTOR 1.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD   TELAPSE   2587.75 TCPU   2588.17
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX   TELAPSE   2991.69 TCPU   2992.20
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3   TELAPSE   3006.19 TCPU   3006.69
NUMERICALLY INTEGRATED DENSITY   579.9999931620
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT   TELAPSE   3079.76 TCPU   3080.28
CYC  4 ETOT(AU) -8.346606820589E+03 DETOT 2.12E-01 tst 1.16E-04 PX 6.57E-02
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 8.074133601912E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK     TELAPSE   3161.76 TCPU   3162.27
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.1244359E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG     TELAPSE   3186.94 TCPU   3187.46
CHARGE NORMALIZATION FACTOR 1.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD   TELAPSE   3187.72 TCPU   3188.24
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX   TELAPSE   3591.14 TCPU   3591.76
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3   TELAPSE   3605.61 TCPU   3606.23
NUMERICALLY INTEGRATED DENSITY   579.9999930854
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT   TELAPSE   3678.78 TCPU   3679.42
CYC  5 ETOT(AU) -8.346815778539E+03 DETOT -2.09E-01 tst 1.32E-04 PX 5.55E-02
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 1.513101977543E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK     TELAPSE   3763.28 TCPU   3763.92
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.2589710E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG     TELAPSE   3788.27 TCPU   3788.91
CHARGE NORMALIZATION FACTOR 1.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD   TELAPSE   3789.04 TCPU   3789.68
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX   TELAPSE   4194.13 TCPU   4194.85
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3   TELAPSE   4208.60 TCPU   4209.32
NUMERICALLY INTEGRATED DENSITY   579.9999931819
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT   TELAPSE   4281.88 TCPU   4282.62
CYC  6 ETOT(AU) -8.346888462452E+03 DETOT -7.27E-02 tst 3.79E-05 PX 3.07E-02
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 3.108989138593E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK     TELAPSE   4362.79 TCPU   4363.54
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.4224833E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG     TELAPSE   4387.95 TCPU   4388.70
CHARGE NORMALIZATION FACTOR 1.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD   TELAPSE   4388.73 TCPU   4389.48
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX   TELAPSE   4793.96 TCPU   4794.81
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3   TELAPSE   4808.43 TCPU   4809.28
NUMERICALLY INTEGRATED DENSITY   579.9999933124
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT   TELAPSE   4881.61 TCPU   4882.49
CYC  7 ETOT(AU) -8.346907388205E+03 DETOT -1.89E-02 tst 6.05E-05 PX 3.20E-02
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 9.824654259656E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK     TELAPSE   4959.50 TCPU   4960.39
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3379928E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG     TELAPSE   4984.66 TCPU   4985.55
CHARGE NORMALIZATION FACTOR 1.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD   TELAPSE   4985.43 TCPU   4986.32

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TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 5389.63 TCPU 5390.62  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 5404.07 TCPU 5405.07  
NUMERICALLY INTEGRATED DENSITY 579.9999932347  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 5475.68 TCPU 5476.70  
CYC 8 ETOT(AU) -8.346906656196E+03 DETOT 7.32E-04 tst 1.78E-05 PX 1.32E-02  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 8.330529229055E+00  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 5555.80 TCPU 5556.83  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3855356E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 5580.63 TCPU 5581.67  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 5581.40 TCPU 5582.44  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 5986.68 TCPU 5987.82  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 6001.17 TCPU 6002.32  
NUMERICALLY INTEGRATED DENSITY 579.9999932847  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 6074.90 TCPU 6076.06  
CYC 9 ETOT(AU) -8.346909726400E+03 DETOT -3.07E-03 tst 5.36E-06 PX 8.77E-03  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 2.309145216689E+02  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 6153.27 TCPU 6154.44  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3841800E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 6178.15 TCPU 6179.32  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 6178.92 TCPU 6180.10  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 6585.00 TCPU 6584.16  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 6599.41 TCPU 6598.57  
NUMERICALLY INTEGRATED DENSITY 579.9999932748  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 6673.82 TCPU 6670.72  
CYC 10 ETOT(AU) -8.346909745663E+03 DETOT -1.93E-05 tst 1.47E-08 PX 1.69E-03  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 2.286197345519E+02  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 6757.18 TCPU 6753.03  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3841788E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 6782.28 TCPU 6778.14  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 6783.06 TCPU 6778.91  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 7190.28 TCPU 7183.44  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 7205.05 TCPU 7197.92  
NUMERICALLY INTEGRATED DENSITY 579.9999932833  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 7279.55 TCPU 7270.91  
CYC 11 ETOT(AU) -8.346909749597E+03 DETOT -3.93E-06 tst 6.41E-09 PX 4.23E-04  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 7.032368388975E+02  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 7355.53 TCPU 7344.87  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3840405E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 7381.71 TCPU 7370.16  
CHARGE NORMALIZATION FACTOR 1.00000000  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 7382.49 TCPU 7370.94  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 7786.20 TCPU 7773.91  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 7800.68 TCPU 7788.40  
NUMERICALLY INTEGRATED DENSITY 579.9999932811  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 7874.40 TCPU 7862.13  
CYC 12 ETOT(AU) -8.346909749564E+03 DETOT 3.31E-08 tst 4.39E-10 PX 1.82E-04  
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 4.270050418356E+03  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 7945.08 TCPU 7932.82  
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -2.3839992E-01  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 7970.47 TCPU 7958.21  
CHARGE NORMALIZATION FACTOR 1.00000000

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 7971.25 TCPU 7958.99  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 8377.90 TCPU 8365.74  
::: PSEUDO TOTAL ENERGY -7.7520404196521E+03  
::: VIRIAL COEFFICIENT 1.0350842894022E+00  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 8392.41 TCPU 8380.25  
NUMERICALLY INTEGRATED DENSITY 579.9999932811  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 8466.04 TCPU 8453.91  
CYC 13 ETOT(AU) -8.346909749472E+03 DETOT 9.18E-08 tst 9.68E-12 PX 1.82E-04

== SCF ENDED - CONVERGENCE ON ENERGY E(AU) -8.3469097494718E+03 CYCLES 13

ENERGY EXPRESSION=HARTREE+FOCK EXCH\*0.20000+(BECKE EXCH)\*0.80000+LYP CORR

TOTAL ENERGY(DFT)(AU)( 13) -8.3469097494718E+03 DE 9.2E-08 tester 9.7E-12

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EDFT TELAPSE 8466.05 TCPU 8453.91

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\* FORCE CALCULATION \*  
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TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFG TELAPSE 8784.33 TCPU 8772.26  
INFORMATION \*\*\*\* EXCPOG \*\*\*\* EXCH. BIPO BUFFER LENGTH (WORDS) = 24951024  
INFORMATION \*\*\*\* GENPOG \*\*\*\* BIPO BUFFER LENGTH (WORDS) = 2528200  
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELXG TELAPSE 11772.34 TCPU 11749.35

#### CARTESIAN FORCES (ANALYTICAL)

ATOM	X	Y	Z
1 12	-4.431858298892E-05	9.381384558083E-15	-6.106226635438E-16
2 12	4.431858299492E-05	-5.551115123126E-17	-2.109423746788E-15
3 12	4.431858298493E-05	1.887379141863E-15	4.107825191113E-15
4 12	-4.431858298359E-05	8.215650382226E-15	2.359223927328E-15
5 13	5.329070518201E-15	-1.265654248073E-14	-9.639434747855E-05
6 13	-2.220446049250E-16	4.440892098501E-16	9.639434748165E-05
7 13	4.884981308351E-15	-1.532107773983E-14	9.639434748143E-05
8 13	-1.554312234475E-15	1.110223024625E-15	-9.639434748521E-05
9 13	7.544665995241E-05	-2.659833439722E-05	1.096554675099E-15
10 13	-7.544665995729E-05	2.659833439544E-05	3.285752841907E-15
11 13	7.544665995196E-05	2.659833439012E-05	-1.895162146223E-15
12 13	-7.544665995107E-05	-2.659833439367E-05	-4.532683969567E-16
13 14	-1.235123114895E-14	-1.332267629550E-14	1.576516694968E-14
14 14	-1.204591981718E-14	-9.992007221626E-16	-1.421085471520E-14
15 14	-2.552527285182E-05	-7.015940931865E-05	-1.404294554939E-15
16 14	2.552527285005E-05	7.015940931776E-05	1.759371381434E-15
17 14	-2.552527284116E-05	7.015940931998E-05	-1.072294531279E-14
18 14	2.552527285360E-05	-7.015940932487E-05	3.674939307271E-15
19 14	3.201947748188E-05	2.418682964311E-05	2.440901979397E-15
20 14	-3.201947747833E-05	-2.418682963690E-05	2.124863406612E-15
21 14	3.201947749787E-05	-2.418682964134E-05	3.015876756424E-15
22 14	-3.201947749787E-05	2.418682964134E-05	4.832364954769E-15
23 8	-1.127077690632E-05	-8.446008348262E-06	-4.998773037546E-05
24 8	1.127077689422E-05	8.446008345597E-06	-4.998773038434E-05
25 8	-1.127077689578E-05	8.446008351370E-06	4.998773038034E-05





ATOM	STEP	ENERGY (AU)	N.CYC	DE	SYM	
CENTRAL POINT		-8.346909749472E+03	13	0.0000E+00	8	
1 MG DX	1 *	5.6692E-03	-8.346909748038E+03	3	1.4342E-06	2
1 MG DY	1 *	5.6692E-03	-8.346909747440E+03	3	2.0317E-06	1
1 MG DZ	1 *	5.6692E-03	-8.346909748048E+03	3	1.4236E-06	1
5 AL DX	1 *	5.6692E-03	-8.346909744952E+03	3	4.5199E-06	1
5 AL DY	1 *	5.6692E-03	-8.346909743726E+03	3	5.7463E-06	1
5 AL DZ	1 *	5.6692E-03	-8.346909743776E+03	3	5.6958E-06	2
9 AL DX	1 *	5.6692E-03	-8.346909743558E+03	3	5.9137E-06	2
9 AL DY	1 *	5.6692E-03	-8.346909744183E+03	3	5.2886E-06	2
9 AL DZ	1 *	5.6692E-03	-8.346909745083E+03	3	4.3887E-06	1
13 SI DX	1 *	5.6692E-03	-8.346909739835E+03	3	9.6373E-06	2
13 SI DY	1 *	5.6692E-03	-8.346909743005E+03	3	6.4669E-06	2
13 SI DZ	1 *	5.6692E-03	-8.346909741530E+03	3	7.9417E-06	2
15 SI DX	1 *	5.6692E-03	-8.346909740776E+03	3	8.6960E-06	2
15 SI DY	1 *	5.6692E-03	-8.346909739714E+03	3	9.7580E-06	2
15 SI DZ	1 *	5.6692E-03	-8.346909742003E+03	3	7.4690E-06	1
19 SI DX	1 *	5.6692E-03	-8.346909738234E+03	3	1.1238E-05	2
19 SI DY	1 *	5.6692E-03	-8.346909741896E+03	3	7.5758E-06	2
19 SI DZ	1 *	5.6692E-03	-8.346909742028E+03	3	7.4434E-06	1
23 O DX	1 *	5.6692E-03	-8.346909746426E+03	3	3.0459E-06	1
23 O DY	1 *	5.6692E-03	-8.346909745897E+03	3	3.5745E-06	1
23 O DZ	1 *	5.6692E-03	-8.346909744707E+03	3	4.7646E-06	1
31 O DX	1 *	5.6692E-03	-8.346909746340E+03	3	3.1322E-06	1
31 O DY	1 *	5.6692E-03	-8.346909745918E+03	3	3.5535E-06	1
31 O DZ	1 *	5.6692E-03	-8.346909744572E+03	3	4.8999E-06	1
39 O DX	1 *	5.6692E-03	-8.346909745915E+03	3	3.5569E-06	1
39 O DY	1 *	5.6692E-03	-8.346909746841E+03	3	2.6311E-06	1
39 O DZ	1 *	5.6692E-03	-8.346909744719E+03	3	4.7527E-06	1
47 O DX	1 *	5.6692E-03	-8.346909739590E+03	3	9.8821E-06	2
47 O DY	1 *	5.6692E-03	-8.346909748431E+03	3	1.0412E-06	2
47 O DZ	1 *	5.6692E-03	-8.346909748381E+03	3	1.0913E-06	1
51 O DX	1 *	5.6692E-03	-8.346909744093E+03	3	5.3783E-06	2
51 O DY	1 *	5.6692E-03	-8.346909744231E+03	3	5.2412E-06	2
51 O DZ	1 *	5.6692E-03	-8.346909748381E+03	3	1.0909E-06	1
55 O DX	1 *	5.6692E-03	-8.346909748058E+03	3	1.4133E-06	2
55 O DY	1 *	5.6692E-03	-8.346909739115E+03	3	1.0357E-05	2
55 O DZ	1 *	5.6692E-03	-8.346909748318E+03	3	1.1539E-06	1

GCALCO - MAX INDICES DIRECT LATTICE VECTOR 15 15 14  
NO.OF VECTORS CREATED 6999 STARS 1020 RMAX 207.45093 BOHR

CAPPA: IS1= 4 IS2= 4 IS3= 4K POINTS MONKHORST NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

CAPPA1: ISJ1= 4 ISJ2= 4 ISJ3= 4K POINTS GILAT NET 21 SYMMOPS K SPACE 8 SYMMOPS G SPACE 8

DIMENSIONS P(G)= 2353196 F(G)= 378354 P(G),F(G) (IRR) 165393  
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TT INPUT TELAPSE 1163368.46 TCPU 1154880.93

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23

[illegible][illegible]

### +++ SYMMETRY ADAPTION OF VIBRATIONAL MODES +++

SYMMETRY INFORMATION:

K-LITTLE GROUP: CLASS TABLE, CHARACTER TABLE.

IRREP-(DIMENSION, NO. IRREDUCIBLE SETS)

[WARNINGS: (1) ONLY ACTIVE IRREPS ARE GENERATED AND LISTED.

(2) ONLY RELEVANT CLASSES ARE CONSIDERED IN THE CHARACTER TABLE

(3) SYMBOLS MAY NOT FULLY COINCIDE WITH THOSE FROM TEXT BOOKS]

(P, D, RP, RD, STAND FOR PAIRING, DOUBLING, REAL PAIRING AND REAL DOUBLING OF THE IRREPS (SEE MANUAL))

CLASS | GROUP OPERATORS (SEE SYMMOPS KEYWORD)

C2	2;
C2'	3;
C2''	4;
I	5;
SGH	6;
SGV	7;
SGV'	8;

IRREP/CLA E C2 C2' C2'' I SGH SGV SGV'

AG		1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
B1G		1.00	1.00	-1.00	-1.00	1.00	1.00	-1.00	-1.00
B2G		1.00	-1.00	1.00	-1.00	1.00	-1.00	1.00	-1.00
B3G		1.00	-1.00	-1.00	1.00	1.00	-1.00	-1.00	1.00
AU		1.00	1.00	1.00	1.00	-1.00	-1.00	-1.00	-1.00
B1U		1.00	1.00	-1.00	-1.00	-1.00	-1.00	1.00	1.00
B2U		1.00	-1.00	1.00	-1.00	-1.00	1.00	-1.00	1.00
B3U		1.00	-1.00	-1.00	1.00	-1.00	1.00	1.00	-1.00

AG -(1, 23); B1G-(1, 25); B2G-(1, 19); B3G-(1, 20);  
AU -(1, 17); B1U-(1, 19); B2U-(1, 25); B3U-(1, 26);

[illegible]

EIGENVALUES (EIGV) OF THE MASS WEIGHTED HESSIAN MATRIX AND HARMONIC FREQUENCIES. IRREP LABELS REFER TO SYMMETRY REPRESENTATION ANALYSIS; A AND I INDICATE WHETHER THE MODE IS ACTIVE OR INACTIVE, RESPECTIVELY, FOR IR AND RAMAN; IR INTENSITIES IN BRACKETS.

### CONVERSION FACTORS FOR FREOUENCIES:

1 CM\*\*(-1) = 0.2194746E+06 HARTREE

$$1 \text{ THZ} = 0.2997925\text{E-01 CM}^{**}(-1)$$
[illegible]

MODES		EIGV	FREQUENCIES		IRREP	IR	INTENS	RAMAN
		(HARTREE**2)	(CM**-1)	(THZ)		(KM/MOL)		
1-	1	-0.1474E-09	-2.6647	-0.0799	(B3U)	A (	0.00)	I
2-	2	-0.1164E-09	-2.3679	-0.0710	(B2U)	A (	0.00)	I
3-	3	-0.5300E-10	-1.5978	-0.0479	(B1U)	A (	0.00)	I
4-	4	0.1850E-06	94.4058	2.8302	(B2G)	I (	0.00)	A
5-	5	0.2042E-06	99.1761	2.9732	(B3G)	I (	0.00)	A
6-	6	0.2688E-06	113.7806	3.4111	(B1U)	A (	0.00)	I
7-	7	0.2853E-06	117.2195	3.5142	(AU )	I (	0.00)	I
8-	8	0.2928E-06	118.7551	3.5602	(B3G)	I (	0.00)	A
9-	9	0.3399E-06	127.9532	3.8359	(B1G)	I (	0.00)	A
10-	10	0.3550E-06	130.7718	3.9204	(B3U)	A (	0.00)	I
11-	11	0.3666E-06	132.8795	3.9836	(B2G)	I (	0.00)	A
12-	12	0.3681E-06	133.1652	3.9922	(AG )	I (	0.00)	A
13-	13	0.3751E-06	134.4129	4.0296	(B3G)	I (	0.00)	A
14-	14	0.5143E-06	157.3905	4.7184	(B2U)	A (	0.00)	I
15-	15	0.5416E-06	161.5240	4.8424	(B2G)	I (	0.00)	A
16-	16	0.5462E-06	162.1986	4.8626	(AG )	I (	0.00)	A
17-	17	0.5846E-06	167.8058	5.0307	(B3U)	A (	0.00)	I
18-	18	0.5968E-06	169.5537	5.0831	(B1G)	I (	0.00)	A
19-	19	0.6231E-06	173.2418	5.1937	(B2U)	A (	0.00)	I
20-	20	0.6316E-06	174.4224	5.2291	(B3U)	A (	0.00)	I
21-	21	0.6390E-06	175.4357	5.2594	(B1U)	A (	0.00)	I
22-	22	0.6507E-06	177.0357	5.3074	(B3G)	I (	0.00)	A
23-	23	0.7059E-06	184.3933	5.5280	(B3G)	I (	0.00)	A
24-	24	0.7146E-06	185.5350	5.5622	(AU )	I (	0.00)	I
25-	25	0.7377E-06	188.5069	5.6513	(B1G)	I (	0.00)	A
26-	26	0.7456E-06	189.5125	5.6814	(B2G)	I (	0.00)	A
27-	27	0.7628E-06	191.6874	5.7466	(B3U)	A (	0.00)	I
28-	28	0.7733E-06	193.0028	5.7861	(B1U)	A (	0.00)	I
29-	29	0.7774E-06	193.5166	5.8015	(B2U)	A (	0.00)	I
30-	30	0.7942E-06	195.5946	5.8638	(AU )	I (	0.00)	I
31-	31	0.8328E-06	200.2927	6.0046	(B1U)	A (	0.00)	I
32-	32	0.8539E-06	202.8034	6.0799	(B2G)	I (	0.00)	A
33-	33	0.9424E-06	213.0640	6.3875	(B3G)	I (	0.00)	A
34-	34	0.9688E-06	216.0196	6.4761	(AU )	I (	0.00)	I
35-	35	0.1014E-05	221.0290	6.6263	(B2G)	I (	0.00)	A
36-	36	0.1236E-05	243.9804	7.3143	(B3G)	I (	0.00)	A
37-	37	0.1242E-05	244.6423	7.3342	(AG )	I (	0.00)	A
38-	38	0.1246E-05	244.9633	7.3438	(B3U)	A (	0.00)	I
39-	39	0.1253E-05	245.6747	7.3651	(B1G)	I (	0.00)	A
40-	40	0.1272E-05	247.5349	7.4209	(B1U)	A (	0.00)	I
41-	41	0.1295E-05	249.7646	7.4878	(B1G)	I (	0.00)	A
42-	42	0.1325E-05	252.6410	7.5740	(B1U)	A (	0.00)	I
43-	43	0.1351E-05	255.0728	7.6469	(B2U)	A (	0.00)	I
44-	44	0.1404E-05	260.0582	7.7963	(B2G)	I (	0.00)	A
45-	45	0.1465E-05	265.6859	7.9651	(B3G)	I (	0.00)	A
46-	46	0.1470E-05	266.1101	7.9778	(AG )	I (	0.00)	A
47-	47	0.1481E-05	267.1075	8.0077	(AU )	I (	0.00)	I
48-	48	0.1486E-05	267.5339	8.0205	(B2U)	A (	0.00)	I
49-	49	0.1531E-05	271.5718	8.1415	(B1G)	I (	0.00)	A
50-	50	0.1531E-05	271.5913	8.1421	(B3U)	A (	0.00)	I
51-	51	0.1724E-05	288.1528	8.6386	(B2G)	I (	0.00)	A
52-	52	0.1777E-05	292.5584	8.7707	(B1U)	A (	0.00)	I

53-	53	0.1835E-05	297.2705	8.9119	(B1G)	I (	0.00)	A
54-	54	0.1840E-05	297.7295	8.9257	(AG )	I (	0.00)	A
55-	55	0.1843E-05	297.9305	8.9317	(B3G)	I (	0.00)	A
56-	56	0.1845E-05	298.1540	8.9384	(B2U)	A (	0.00)	I
57-	57	0.1848E-05	298.3238	8.9435	(AU )	I (	0.00)	I
58-	58	0.1902E-05	302.6463	9.0731	(B1G)	I (	0.00)	A
59-	59	0.1947E-05	306.2413	9.1809	(B3G)	I (	0.00)	A
60-	60	0.2054E-05	314.5589	9.4302	(AG )	I (	0.00)	A
61-	61	0.2154E-05	322.1347	9.6574	(AU )	I (	0.00)	I
62-	62	0.2220E-05	326.9807	9.8026	(B2U)	A (	0.00)	I
63-	63	0.2261E-05	330.0326	9.8941	(AG )	I (	0.00)	A
64-	64	0.2262E-05	330.1225	9.8968	(B2G)	I (	0.00)	A
65-	65	0.2282E-05	331.5545	9.9398	(B3U)	A (	0.00)	I
66-	66	0.2407E-05	340.4812	10.2074	(B3U)	A (	0.00)	I
67-	67	0.2431E-05	342.1781	10.2582	(B1U)	A (	0.00)	I
68-	68	0.2434E-05	342.3809	10.2643	(B1G)	I (	0.00)	A
69-	69	0.2670E-05	358.6119	10.7509	(B3U)	A (	0.00)	I
70-	70	0.2673E-05	358.8567	10.7583	(B1G)	I (	0.00)	A
71-	71	0.2686E-05	359.6766	10.7828	(B2U)	A (	0.00)	I
72-	72	0.2736E-05	363.0313	10.8834	(AG )	I (	0.00)	A
73-	73	0.2747E-05	363.7686	10.9055	(B2U)	A (	0.00)	I
74-	74	0.2847E-05	370.3269	11.1021	(B1U)	A (	0.00)	I
75-	75	0.2849E-05	370.4221	11.1050	(AG )	I (	0.00)	A
76-	76	0.2866E-05	371.5579	11.1390	(AU )	I (	0.00)	I
77-	77	0.2971E-05	378.3199	11.3417	(B3G)	I (	0.00)	A
78-	78	0.2994E-05	379.7765	11.3854	(B3U)	A (	0.00)	I
79-	79	0.3089E-05	385.7357	11.5641	(B2G)	I (	0.00)	A
80-	80	0.3284E-05	397.7195	11.9233	(B2G)	I (	0.00)	A
81-	81	0.3407E-05	405.1104	12.1449	(B2U)	A (	0.00)	I
82-	82	0.3488E-05	409.8758	12.2878	(B3U)	A (	0.00)	I
83-	83	0.3613E-05	417.1618	12.5062	(B2U)	A (	0.00)	I
84-	84	0.3738E-05	424.3305	12.7211	(B1G)	I (	0.00)	A
85-	85	0.3865E-05	431.4552	12.9347	(B3U)	A (	0.00)	I
86-	86	0.3935E-05	435.3946	13.0528	(AG )	I (	0.00)	A
87-	87	0.4194E-05	449.4940	13.4755	(B2U)	A (	0.00)	I
88-	88	0.4408E-05	460.7723	13.8136	(B2G)	I (	0.00)	A
89-	89	0.4432E-05	462.0409	13.8516	(B1G)	I (	0.00)	A
90-	90	0.4502E-05	465.6648	13.9603	(B3G)	I (	0.00)	A
91-	91	0.4539E-05	467.5831	14.0178	(AU )	I (	0.00)	I
92-	92	0.4699E-05	475.7624	14.2630	(AU )	I (	0.00)	I
93-	93	0.4753E-05	478.4843	14.3446	(B3G)	I (	0.00)	A
94-	94	0.4923E-05	486.9799	14.5993	(B1U)	A (	0.00)	I
95-	95	0.4981E-05	489.8360	14.6849	(AG )	I (	0.00)	A
96-	96	0.5085E-05	494.9119	14.8371	(B3G)	I (	0.00)	A
97-	97	0.5135E-05	497.3200	14.9093	(B1G)	I (	0.00)	A
98-	98	0.5151E-05	498.1088	14.9329	(B1U)	A (	0.00)	I
99-	99	0.5155E-05	498.3209	14.9393	(B3U)	A (	0.00)	I
100-	100	0.5194E-05	500.1748	14.9949	(B2G)	I (	0.00)	A
101-	101	0.5219E-05	501.3866	15.0312	(B3U)	A (	0.00)	I
102-	102	0.5384E-05	509.2356	15.2665	(B1U)	A (	0.00)	I
103-	103	0.5893E-05	532.7653	15.9719	(B2U)	A (	0.00)	I
104-	104	0.6081E-05	541.2014	16.2248	(AU )	I (	0.00)	I
105-	105	0.6421E-05	556.1276	16.6723	(B1G)	I (	0.00)	A
106-	106	0.6562E-05	562.2235	16.8550	(AG )	I (	0.00)	A

107- 107	0.6773E-05	571.1942	17.1240	(B2U)	A (	0.00)	I
108- 108	0.6786E-05	571.7168	17.1396	(B1U)	A (	0.00)	I
109- 109	0.6831E-05	573.6112	17.1964	(B1G)	I (	0.00)	A
110- 110	0.6897E-05	576.3712	17.2792	(AU )	I (	0.00)	I
111- 111	0.7008E-05	581.0193	17.4185	(B3U)	A (	0.00)	I
112- 112	0.7127E-05	585.9221	17.5655	(AG )	I (	0.00)	A
113- 113	0.7502E-05	601.1202	18.0211	(B3U)	A (	0.00)	I
114- 114	0.7540E-05	602.6717	18.0676	(B1G)	I (	0.00)	A
115- 115	0.8031E-05	621.9862	18.6467	(AU )	I (	0.00)	I
116- 116	0.8132E-05	625.8584	18.7628	(B1U)	A (	0.00)	I
117- 117	0.8266E-05	630.9981	18.9168	(B3G)	I (	0.00)	A
118- 118	0.8404E-05	636.2483	19.0742	(AG )	I (	0.00)	A
119- 119	0.9151E-05	663.9417	19.9045	(B3G)	I (	0.00)	A
120- 120	0.9372E-05	671.8840	20.1426	(B2G)	I (	0.00)	A
121- 121	0.9397E-05	672.8022	20.1701	(B3U)	A (	0.00)	I
122- 122	0.9838E-05	688.4036	20.6378	(AG )	I (	0.00)	A
123- 123	0.9895E-05	690.3724	20.6968	(B2U)	A (	0.00)	I
124- 124	0.1033E-04	705.3465	21.1458	(B1G)	I (	0.00)	A
125- 125	0.1037E-04	706.7811	21.1888	(AU )	I (	0.00)	I
126- 126	0.1052E-04	711.8569	21.3409	(B2U)	A (	0.00)	I
127- 127	0.1067E-04	716.9671	21.4941	(B1U)	A (	0.00)	I
128- 128	0.1101E-04	728.3854	21.8364	(AG )	I (	0.00)	A
129- 129	0.1128E-04	737.0089	22.0950	(B1G)	I (	0.00)	A
130- 130	0.1143E-04	741.9026	22.2417	(AG )	I (	0.00)	A
131- 131	0.1186E-04	755.6839	22.6548	(B3G)	I (	0.00)	A
132- 132	0.1198E-04	759.7064	22.7754	(B1G)	I (	0.00)	A
133- 133	0.1205E-04	761.9336	22.8422	(B3U)	A (	0.00)	I
134- 134	0.1232E-04	770.2159	23.0905	(B2G)	I (	0.00)	A
135- 135	0.1258E-04	778.4303	23.3368	(B2U)	A (	0.00)	I
136- 136	0.1275E-04	783.8259	23.4985	(B3U)	A (	0.00)	I
137- 137	0.1385E-04	816.8635	24.4890	(B2G)	I (	0.00)	A
138- 138	0.1487E-04	846.2795	25.3708	(B2U)	A (	0.00)	I
139- 139	0.1690E-04	902.1617	27.0461	(B3G)	I (	0.00)	A
140- 140	0.1705E-04	906.2879	27.1698	(B2G)	I (	0.00)	A
141- 141	0.1715E-04	908.8577	27.2469	(B1U)	A (	0.00)	I
142- 142	0.1717E-04	909.3702	27.2622	(B3G)	I (	0.00)	A
143- 143	0.1720E-04	910.1619	27.2860	(AU )	I (	0.00)	I
144- 144	0.1738E-04	915.1047	27.4341	(B3U)	A (	0.00)	I
145- 145	0.1800E-04	931.1252	27.9144	(AG )	I (	0.00)	A
146- 146	0.1854E-04	945.1382	28.3345	(B1U)	A (	0.00)	I
147- 147	0.1927E-04	963.5452	28.8864	(B1G)	I (	0.00)	A
148- 148	0.1932E-04	964.7716	28.9231	(B3U)	A (	0.00)	I
149- 149	0.1955E-04	970.3805	29.0913	(B2U)	A (	0.00)	I
150- 150	0.1984E-04	977.5961	29.3076	(B3G)	I (	0.00)	A
151- 151	0.1990E-04	979.1124	29.3531	(B2U)	A (	0.00)	I
152- 152	0.2012E-04	984.4347	29.5126	(AU )	I (	0.00)	I
153- 153	0.2026E-04	987.8548	29.6151	(AG )	I (	0.00)	A
154- 154	0.2026E-04	987.8705	29.6156	(B2G)	I (	0.00)	A
155- 155	0.2029E-04	988.6330	29.6385	(B1G)	I (	0.00)	A
156- 156	0.2138E-04	1014.8141	30.4234	(AG )	I (	0.00)	A
157- 157	0.2140E-04	1015.1952	30.4348	(B2G)	I (	0.00)	A
158- 158	0.2140E-04	1015.2143	30.4354	(B3U)	A (	0.00)	I
159- 159	0.2181E-04	1025.0226	30.7294	(B1U)	A (	0.00)	I
160- 160	0.2228E-04	1035.9359	31.0566	(B1G)	I (	0.00)	A

[illegible]

1) EACH PAIR OF BONDED ATOMS (I.E. WITHIN THEIR VAN DER WAALS DISTANCE) A AND B IS EXAMINED TO SEE IF THERE IS A LARGE RELATIVE MOTION BETWEEN THEM.  
2) IF SO, THE AB MOTION IS DECOMPOSED IN THREE COMPONENTS: ALONG A-B(LONG), ON THE PLANE CONTAINING A THIRD ATOM C (ANG) AND OUT OF THE PLANE (OUT).  
LONG+ANG+OUT=1.

[illegible]

file:///Volumes/...nsfers-TM/Data%20Backups/Roebling/05-12-2023/minsocam/MSA/AmMin/TOC/2011/Oct11\_Data/Kaindl\_p1568\_11\_1.txt[5/17/23, 10:16:25 PM]

(?) 58 O 22 SI(0.0) 39 O (0.7) 0.0

6 113.7806 (B1U)

(O) 32 O 1 MG(0.0) 39 O (0.5) 0.0

(O) 34 O 1 MG(0.0) 41 O (0.5) 0.0

(O) 31 O 2 MG(0.0) 40 O (0.5) 0.0

(O) 33 O 2 MG(0.0) 42 O (0.5) 0.0

(O) 36 O 3 MG(0.0) 43 O (0.5) 0.0

(O) 38 O 3 MG(0.0) 45 O (0.5) 0.0

(O) 35 O 4 MG(0.0) 44 O (0.5) 0.0

(O) 37 O 4 MG(0.0) 46 O (0.5) 0.0

(O) 48 O 9 AL(0.0) 33 O (0.7) 0.0

(O) 47 O 10 AL(0.0) 34 O (0.7) 0.0

(O) 50 O 11 AL(0.0) 31 O (0.7) 0.0

(O) 49 O 12 AL(0.0) 32 O (0.7) 0.0

7 117.2195 (AU )

(O) 55 O 19 SI(0.0) 42 O (0.7) 0.0

(O) 56 O 20 SI(0.0) 41 O (0.7) 0.0

(O) 57 O 21 SI(0.0) 40 O (0.7) 0.0

(O) 58 O 22 SI(0.0) 39 O (0.7) 0.0

8 118.7551 (B3G)

(O) 55 O 15 SI(0.0) 25 O (0.7) 0.0

(O) 56 O 16 SI(0.0) 26 O (0.7) 0.0

(O) 57 O 17 SI(0.0) 28 O (0.7) 0.0

(O) 58 O 18 SI(0.0) 24 O (0.7) 0.0

9 127.9532 (B1G)

(B) 15 SI 55 O (0.0) 19 SI(1.0) 0.0

(B) 16 SI 56 O (0.0) 20 SI(1.0) 0.0

(B) 17 SI 57 O (0.0) 21 SI(1.0) 0.0

(B) 18 SI 58 O (0.0) 22 SI(1.0) 0.0

(B) 19 SI 55 O (0.0) 15 SI(1.0) 0.0

(B) 20 SI 56 O (0.0) 16 SI(1.0) 0.0

(B) 21 SI 57 O (0.0) 17 SI(1.0) 0.0

(B) 22 SI 58 O (0.0) 18 SI(1.0) 0.0

10 130.7718 (B3U)

(B) 48 O 9 AL(0.0) 51 O (1.0) 0.0

(B) 47 O 10 AL(0.0) 52 O (1.0) 0.0

(B) 11 AL 50 O (0.0) 22 SI(1.0) 0.0

(B) 12 AL 49 O (0.0) 21 SI(1.0) 0.0

11 132.8795 (B2G)

(B) 32 O 1 MG(0.0) 39 O (1.0) 0.0

(B) 34 O 1 MG(0.0) 41 O (1.0) 0.0

(B) 31 O 2 MG(0.0) 40 O (1.0) 0.0

(B) 33 O 2 MG(0.0) 42 O (1.0) 0.0

(B) 36 O 3 MG(0.0) 43 O (1.0) 0.0

(B) 38 O 3 MG(0.0) 45 O (1.0) 0.0

(B) 35 O 4 MG(0.0) 44 O (1.0) 0.0

(B) 37 O 4 MG(0.0) 46 O (1.0) 0.0

(B) 33 O 9 AL(0.0) 38 O (1.0) 0.0

(B) 38 O 9 AL(0.0) 33 O (1.0) 0.0

(B) 34 O 10 AL(0.0) 37 O (1.0) 0.0

(B) 37 O 10 AL(0.0) 34 O (1.0) 0.0

(B) 31 O 11 AL(0.0) 36 O (1.0) 0.0

(B) 36 O 11 AL(0.0) 31 O (1.0) 0.0

(B) 32 O 12 AL(0.0) 35 O (1.0) 0.0

	(B)	35 O	12 AL(0.0)	32 O (1.0)	0.0
	(O)	31 O	13 SI(0.0)	34 O (0.7)	0.0
	(O)	32 O	13 SI(0.0)	33 O (0.7)	0.0
	(O)	33 O	13 SI(0.0)	32 O (0.7)	0.0
	(O)	34 O	13 SI(0.0)	31 O (0.7)	0.0
	(O)	35 O	14 SI(0.0)	38 O (0.7)	0.0
	(O)	36 O	14 SI(0.0)	37 O (0.7)	0.0
	(O)	37 O	14 SI(0.0)	36 O (0.7)	0.0
	(O)	38 O	14 SI(0.0)	35 O (0.7)	0.0
12	133.1652	(AG )			
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
13	134.4129	(B3G)			
	(B)	23 O	1 MG(0.0)	32 O (0.9)	0.0
	(B)	25 O	1 MG(0.0)	34 O (0.9)	0.0
	(B)	24 O	2 MG(0.0)	31 O (0.9)	0.0
	(B)	26 O	2 MG(0.0)	33 O (0.9)	0.0
	(B)	27 O	3 MG(0.0)	36 O (0.9)	0.0
	(B)	29 O	3 MG(0.0)	38 O (0.9)	0.0
	(B)	28 O	4 MG(0.0)	35 O (0.9)	0.0
	(B)	30 O	4 MG(0.0)	37 O (0.9)	0.0
	(O)	25 O	5 AL(0.0)	40 O (0.8)	0.0
	(O)	26 O	5 AL(0.0)	39 O (0.8)	0.0
	(O)	23 O	6 AL(0.0)	42 O (0.8)	0.0
	(O)	24 O	6 AL(0.0)	41 O (0.8)	0.0
	(O)	29 O	7 AL(0.0)	44 O (0.8)	0.0
	(O)	30 O	7 AL(0.0)	43 O (0.8)	0.0
	(O)	27 O	8 AL(0.0)	46 O (0.8)	0.0
	(O)	28 O	8 AL(0.0)	45 O (0.8)	0.0
	(B)	42 O	19 SI(0.0)	45 O (1.0)	0.0
	(B)	45 O	19 SI(0.0)	42 O (1.0)	0.0
	(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
	(B)	41 O	20 SI(0.0)	46 O (1.0)	0.0
	(B)	46 O	20 SI(0.0)	41 O (1.0)	0.0
	(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
	(B)	40 O	21 SI(0.0)	43 O (1.0)	-0.1
	(B)	43 O	21 SI(0.0)	40 O (1.0)	0.0
	(O)	49 O	21 SI(0.0)	40 O (0.8)	0.0
	(B)	39 O	22 SI(0.0)	44 O (1.0)	0.0
	(B)	44 O	22 SI(0.0)	39 O (1.0)	0.0
	(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0
14	157.3905	(B2U)			
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
15	161.5240	(B2G)			
	(O)	48 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	50 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
	(B)	42 O	19 SI(0.0)	47 O (1.0)	0.0



	(B)	45 O	19 SI(0.0)	47 O (1.0)	0.0
	(B)	41 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	46 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	40 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	43 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	39 O	22 SI(0.0)	50 O (1.0)	0.0
	(B)	44 O	22 SI(0.0)	50 O (1.0)	0.0
16	162.1986 (AG)				
	(B)	15 SI	55 O (0.0)	19 SI(1.0)	0.0
	(B)	16 SI	56 O (0.0)	20 SI(1.0)	0.0
	(B)	17 SI	57 O (0.0)	21 SI(1.0)	0.0
	(B)	18 SI	58 O (0.0)	22 SI(1.0)	0.0
	(B)	19 SI	55 O (0.0)	15 SI(1.0)	0.0
	(B)	20 SI	56 O (0.0)	16 SI(1.0)	0.0
	(B)	21 SI	57 O (0.0)	17 SI(1.0)	0.0
	(B)	22 SI	58 O (0.0)	18 SI(1.0)	0.0
17	167.8058 (B3U)				
	(B)	39 O	1 MG(0.1)	23 O (0.9)	0.0
	(B)	41 O	1 MG(0.1)	25 O (0.9)	0.0
	(B)	40 O	2 MG(0.1)	24 O (0.9)	0.0
	(B)	42 O	2 MG(0.1)	26 O (0.9)	0.0
	(B)	43 O	3 MG(0.1)	27 O (0.9)	0.0
	(B)	45 O	3 MG(0.1)	29 O (0.9)	0.0
	(B)	44 O	4 MG(0.1)	28 O (0.9)	0.0
	(B)	46 O	4 MG(0.1)	30 O (0.9)	0.0
	(B)	15 SI	55 O (0.0)	19 SI(1.0)	0.0
	(B)	16 SI	56 O (0.0)	20 SI(1.0)	0.0
	(B)	17 SI	57 O (0.0)	21 SI(1.0)	0.0
	(B)	18 SI	58 O (0.0)	22 SI(1.0)	0.0
18	169.5537 (B1G)				
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
19	173.2418 (B2U)				
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
20	174.4224 (B3U)				
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
21	175.4357 (B1U)				
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
22	177.0357 (B3G)				

	(B)	1 MG	5 AL(0.0)	40 O (1.0)	0.0
	(B)	1 MG	6 AL(0.0)	42 O (1.0)	0.0
	(B)	2 MG	5 AL(0.0)	39 O (1.0)	0.0
	(B)	2 MG	6 AL(0.0)	41 O (1.0)	0.0
	(B)	3 MG	7 AL(0.0)	44 O (1.0)	0.0
	(B)	3 MG	8 AL(0.0)	46 O (1.0)	0.0
	(B)	4 MG	7 AL(0.0)	43 O (1.0)	0.0
	(B)	4 MG	8 AL(0.0)	45 O (1.0)	0.0
23	184.3933	(B3G)			
	(O)	1 MG	5 AL(0.0)	26 O (0.8)	0.0
	(O)	1 MG	6 AL(0.0)	24 O (0.8)	0.0
	(O)	2 MG	5 AL(0.0)	25 O (0.8)	0.0
	(O)	2 MG	6 AL(0.0)	23 O (0.8)	0.0
	(O)	3 MG	7 AL(0.0)	30 O (0.8)	0.0
	(O)	3 MG	8 AL(0.0)	28 O (0.8)	0.0
	(O)	4 MG	7 AL(0.0)	29 O (0.8)	0.0
	(O)	4 MG	8 AL(0.0)	27 O (0.8)	0.0
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
24	185.5350	(AU)			
	(O)	51 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
25	188.5069	(B1G)			
	(O)	1 MG	5 AL(0.0)	26 O (0.6)	0.0
	(O)	1 MG	6 AL(0.0)	24 O (0.6)	0.0
	(O)	2 MG	5 AL(0.0)	25 O (0.6)	0.0
	(O)	2 MG	6 AL(0.0)	23 O (0.6)	0.0
	(O)	3 MG	7 AL(0.0)	30 O (0.6)	0.0
	(O)	3 MG	8 AL(0.0)	28 O (0.6)	0.0
	(O)	4 MG	7 AL(0.0)	29 O (0.6)	0.0
	(O)	4 MG	8 AL(0.0)	27 O (0.6)	0.0
26	189.5125	(B2G)			
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
27	191.6874	(B3U)			
	(B)	32 O	1 MG(0.1)	6 AL(0.8)	0.0
	(B)	34 O	1 MG(0.1)	5 AL(0.8)	0.0
	(B)	31 O	2 MG(0.1)	6 AL(0.8)	0.0
	(B)	33 O	2 MG(0.1)	5 AL(0.8)	0.0
	(B)	36 O	3 MG(0.1)	8 AL(0.8)	0.0

	(B)	38 O	3 MG(0.1)	7 AL(0.8)	0.0
	(B)	35 O	4 MG(0.1)	8 AL(0.8)	0.0
	(B)	37 O	4 MG(0.1)	7 AL(0.8)	0.0
28	193.0028	(B1U)			
	(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
	(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
	(O)	49 O	21 SI(0.0)	40 O (0.8)	-0.1
	(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0
29	193.5166	(B2U)			
	(B)	5 AL	1 MG(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	1 MG(0.0)	5 AL(1.0)	0.0
	(B)	5 AL	2 MG(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	2 MG(0.0)	5 AL(1.0)	0.0
	(B)	7 AL	3 MG(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	3 MG(0.0)	7 AL(1.0)	0.0
	(B)	7 AL	4 MG(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	4 MG(0.0)	7 AL(1.0)	0.0
30	195.5946	(AU)			
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
31	200.2927	(B1U)			
	(O)	51 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
32	202.8034	(B2G)			
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
33	213.0640	(B3G)			
	(O)	48 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	51 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	50 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
34	216.0196	(AU)			
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
	(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
	(O)	49 O	21 SI(0.0)	40 O (0.8)	-0.1
	(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0
35	221.0290	(B2G)			
	(B)	39 O	1 MG(0.0)	23 O (0.9)	0.0
	(B)	41 O	1 MG(0.0)	25 O (0.9)	0.0
	(B)	40 O	2 MG(0.0)	24 O (0.9)	-0.1

	(B)	42 O	2 MG(0.0)	26 O (0.9)	0.0
	(B)	43 O	3 MG(0.0)	27 O (0.9)	0.0
	(B)	45 O	3 MG(0.0)	29 O (0.9)	0.0
	(B)	44 O	4 MG(0.0)	28 O (0.9)	0.0
	(B)	46 O	4 MG(0.0)	30 O (0.9)	0.0
	(O)	39 O	5 AL(0.0)	40 O (0.7)	0.0
	(O)	40 O	5 AL(0.0)	39 O (0.7)	0.0
	(O)	41 O	6 AL(0.0)	42 O (0.7)	0.0
	(O)	42 O	6 AL(0.0)	41 O (0.7)	0.0
	(O)	43 O	7 AL(0.0)	44 O (0.7)	0.1
	(O)	44 O	7 AL(0.0)	43 O (0.7)	-0.1
	(O)	45 O	8 AL(0.0)	46 O (0.7)	0.0
	(O)	46 O	8 AL(0.0)	45 O (0.7)	0.0
36		243.9804	(B3G)		
	(B)	32 O	1 MG(0.0)	41 O (1.0)	0.0
	(B)	34 O	1 MG(0.0)	39 O (1.0)	0.0
	(B)	31 O	2 MG(0.0)	42 O (1.0)	0.0
	(B)	33 O	2 MG(0.0)	40 O (1.0)	0.0
	(B)	36 O	3 MG(0.0)	45 O (1.0)	0.0
	(B)	38 O	3 MG(0.0)	43 O (1.0)	0.0
	(B)	35 O	4 MG(0.0)	46 O (1.0)	0.0
	(B)	37 O	4 MG(0.0)	44 O (1.0)	0.0
	(O)	51 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
37		244.6423	(AG)		
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
38		244.9633	(B3U)		
	(O)	1 MG	5 AL(0.0)	26 O (0.6)	0.0
	(O)	1 MG	6 AL(0.0)	24 O (0.6)	0.0
	(O)	1 MG	23 O (0.2)	17 SI(0.5)	0.0
	(O)	1 MG	25 O (0.2)	15 SI(0.5)	0.0
	(O)	2 MG	5 AL(0.0)	25 O (0.6)	0.0
	(O)	2 MG	6 AL(0.0)	23 O (0.6)	0.0
	(O)	2 MG	24 O (0.2)	18 SI(0.5)	0.0
	(O)	2 MG	26 O (0.2)	16 SI(0.5)	0.0
	(O)	3 MG	7 AL(0.0)	30 O (0.6)	0.0
	(O)	3 MG	8 AL(0.0)	28 O (0.6)	0.0
	(O)	3 MG	27 O (0.2)	18 SI(0.5)	0.0
	(O)	3 MG	29 O (0.2)	16 SI(0.5)	0.0
	(O)	4 MG	7 AL(0.0)	29 O (0.6)	0.0
	(O)	4 MG	8 AL(0.0)	27 O (0.6)	0.0
	(O)	4 MG	28 O (0.2)	17 SI(0.5)	0.0
	(O)	4 MG	30 O (0.2)	15 SI(0.5)	0.0
39		245.6747	(B1G)		
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
40		247.5349	(B1U)		

	(O)	1 MG	5 AL(0.0)	25 O (0.6)	-0.1
	(O)	6 AL	1 MG(0.0)	23 O (0.6)	0.0
	(O)	1 MG	39 O (0.1)	22 SI(0.4)	-0.1
	(O)	1 MG	41 O (0.1)	20 SI(0.4)	0.0
	(O)	2 MG	5 AL(0.0)	26 O (0.6)	0.0
	(O)	6 AL	2 MG(0.0)	24 O (0.6)	0.0
	(O)	2 MG	40 O (0.1)	21 SI(0.4)	-0.2
	(O)	2 MG	42 O (0.1)	19 SI(0.4)	-0.1
	(O)	7 AL	3 MG(0.0)	29 O (0.6)	0.0
	(O)	8 AL	3 MG(0.0)	27 O (0.6)	0.0
	(O)	3 MG	43 O (0.1)	21 SI(0.4)	-0.1
	(O)	3 MG	45 O (0.1)	19 SI(0.4)	0.0
	(O)	7 AL	4 MG(0.0)	30 O (0.6)	0.0
	(O)	8 AL	4 MG(0.0)	28 O (0.6)	0.0
	(O)	4 MG	44 O (0.1)	22 SI(0.4)	0.0
	(O)	4 MG	46 O (0.1)	20 SI(0.4)	0.0
41	249.7646 (B1G)				
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
42	252.6410 (B1U)				
	(B)	23 O	1 MG(0.1)	32 O (0.8)	0.0
	(B)	25 O	1 MG(0.1)	34 O (0.8)	0.0
	(B)	24 O	2 MG(0.1)	31 O (0.8)	0.0
	(B)	26 O	2 MG(0.1)	33 O (0.8)	0.0
	(B)	27 O	3 MG(0.1)	36 O (0.8)	0.0
	(B)	29 O	3 MG(0.1)	38 O (0.8)	0.0
	(B)	28 O	4 MG(0.1)	35 O (0.8)	0.0
	(B)	30 O	4 MG(0.1)	37 O (0.8)	0.0
43	255.0728 (B2U)				
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
44	260.0582 (B2G)				
	(B)	23 O	1 MG(0.0)	32 O (0.9)	0.0
	(B)	25 O	1 MG(0.0)	34 O (0.9)	0.0
	(B)	24 O	2 MG(0.0)	31 O (0.9)	0.0
	(B)	26 O	2 MG(0.0)	33 O (0.9)	0.0
	(B)	27 O	3 MG(0.0)	36 O (0.9)	0.0
	(B)	29 O	3 MG(0.0)	38 O (0.9)	0.0
	(B)	28 O	4 MG(0.0)	35 O (0.9)	0.0
	(B)	30 O	4 MG(0.0)	37 O (0.9)	0.0
	(O)	25 O	5 AL(0.0)	40 O (0.7)	0.0
	(O)	26 O	5 AL(0.0)	39 O (0.7)	0.0
	(O)	23 O	6 AL(0.0)	42 O (0.7)	0.0
	(O)	24 O	6 AL(0.0)	41 O (0.7)	0.0
	(O)	29 O	7 AL(0.0)	44 O (0.7)	0.0
	(O)	30 O	7 AL(0.0)	43 O (0.7)	0.0
	(O)	27 O	8 AL(0.0)	46 O (0.7)	0.0
	(O)	28 O	8 AL(0.0)	45 O (0.7)	0.0
45	265.6859 (B3G)				
	(B)	39 O	1 MG(0.0)	23 O (0.9)	0.0

	(B)	41 O	1 MG(0.0)	25 O (0.9)	0.0
	(B)	40 O	2 MG(0.0)	24 O (0.9)	-0.1
	(B)	42 O	2 MG(0.0)	26 O (0.9)	0.0
	(B)	43 O	3 MG(0.0)	27 O (0.9)	0.0
	(B)	45 O	3 MG(0.0)	29 O (0.9)	0.0
	(B)	44 O	4 MG(0.0)	28 O (0.9)	0.0
	(B)	46 O	4 MG(0.0)	30 O (0.9)	0.0
46	266.1101 (AG)				
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
47	267.1075 (AU)				
	(B)	23 O	1 MG(0.0)	32 O (0.9)	0.0
	(B)	25 O	1 MG(0.0)	34 O (0.9)	0.0
	(B)	24 O	2 MG(0.0)	31 O (0.9)	0.0
	(B)	26 O	2 MG(0.0)	33 O (0.9)	0.0
	(B)	27 O	3 MG(0.0)	36 O (0.9)	0.0
	(B)	29 O	3 MG(0.0)	38 O (0.9)	0.0
	(B)	28 O	4 MG(0.0)	35 O (0.9)	0.0
	(B)	30 O	4 MG(0.0)	37 O (0.9)	0.0
	(O)	39 O	5 AL(0.0)	40 O (0.8)	0.0
	(O)	40 O	5 AL(0.0)	39 O (0.8)	0.0
	(O)	41 O	6 AL(0.0)	42 O (0.8)	0.0
	(O)	42 O	6 AL(0.0)	41 O (0.8)	0.0
	(O)	43 O	7 AL(0.0)	44 O (0.8)	0.0
	(O)	44 O	7 AL(0.0)	43 O (0.8)	0.0
	(O)	45 O	8 AL(0.0)	46 O (0.8)	0.0
	(O)	46 O	8 AL(0.0)	45 O (0.8)	0.0
48	267.5339 (B2U)				
	(B)	32 O	1 MG(0.0)	39 O (1.0)	0.0
	(B)	34 O	1 MG(0.0)	41 O (1.0)	0.0
	(B)	31 O	2 MG(0.0)	40 O (1.0)	0.0
	(B)	33 O	2 MG(0.0)	42 O (1.0)	0.0
	(B)	36 O	3 MG(0.0)	43 O (1.0)	0.0
	(B)	38 O	3 MG(0.0)	45 O (1.0)	0.0
	(B)	35 O	4 MG(0.0)	44 O (1.0)	0.0
	(B)	37 O	4 MG(0.0)	46 O (1.0)	0.0
	(B)	31 O	13 SI(0.0)	34 O (0.9)	0.0
	(B)	32 O	13 SI(0.0)	33 O (0.9)	0.0
	(B)	33 O	13 SI(0.0)	32 O (0.9)	0.0
	(B)	34 O	13 SI(0.0)	31 O (0.9)	0.0
	(B)	35 O	14 SI(0.0)	38 O (0.9)	0.0
	(B)	36 O	14 SI(0.0)	37 O (0.9)	0.0
	(B)	37 O	14 SI(0.0)	36 O (0.9)	0.0
	(B)	38 O	14 SI(0.0)	35 O (0.9)	0.0
49	271.5718 (B1G)				
	(B)	23 O	1 MG(0.4)	32 O (0.6)	0.0
	(B)	25 O	1 MG(0.4)	34 O (0.6)	0.0
	(B)	24 O	2 MG(0.4)	31 O (0.6)	0.0
	(B)	26 O	2 MG(0.4)	33 O (0.6)	0.0
	(B)	27 O	3 MG(0.4)	36 O (0.6)	0.0
	(B)	29 O	3 MG(0.4)	38 O (0.6)	0.0
	(B)	28 O	4 MG(0.4)	35 O (0.6)	0.0

	(B)	30 O	4 MG(0.4)	37 O (0.6)	0.0
50	271.5913	(B3U)			
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
51	288.1528	(B2G)			
	(B)	5 AL	1 MG(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	1 MG(0.0)	5 AL(1.0)	0.0
	(B)	5 AL	2 MG(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	2 MG(0.0)	5 AL(1.0)	0.0
	(B)	7 AL	3 MG(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	3 MG(0.0)	7 AL(1.0)	0.0
	(B)	7 AL	4 MG(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	4 MG(0.0)	7 AL(1.0)	0.0
52	292.5584	(B1U)			
	(S)	5 AL	1 MG(0.7)	6 AL(0.3)	0.0
	(S)	6 AL	1 MG(0.7)	5 AL(0.3)	0.0
	(B)	23 O	1 MG(0.2)	39 O (0.7)	0.0
	(B)	25 O	1 MG(0.2)	41 O (0.7)	0.0
	(S)	5 AL	2 MG(0.7)	6 AL(0.3)	0.0
	(S)	6 AL	2 MG(0.7)	5 AL(0.3)	0.0
	(B)	24 O	2 MG(0.2)	40 O (0.7)	0.0
	(B)	26 O	2 MG(0.2)	42 O (0.7)	0.0
	(S)	7 AL	3 MG(0.7)	8 AL(0.3)	0.0
	(S)	8 AL	3 MG(0.7)	7 AL(0.3)	0.0
	(B)	27 O	3 MG(0.2)	43 O (0.7)	0.0
	(B)	29 O	3 MG(0.2)	45 O (0.7)	0.0
	(S)	7 AL	4 MG(0.7)	8 AL(0.3)	0.0
	(S)	8 AL	4 MG(0.7)	7 AL(0.3)	0.0
	(B)	28 O	4 MG(0.2)	44 O (0.7)	0.0
	(B)	30 O	4 MG(0.2)	46 O (0.7)	0.0
53	297.2705	(B1G)			
	(B)	15 SI	55 O (0.0)	19 SI(1.0)	0.0
	(B)	16 SI	56 O (0.0)	20 SI(1.0)	0.0
	(B)	17 SI	57 O (0.0)	21 SI(1.0)	0.0
	(B)	18 SI	58 O (0.0)	22 SI(1.0)	0.0
	(B)	19 SI	55 O (0.0)	15 SI(1.0)	0.0
	(B)	20 SI	56 O (0.0)	16 SI(1.0)	0.0
	(B)	21 SI	57 O (0.0)	17 SI(1.0)	0.0
	(B)	22 SI	58 O (0.0)	18 SI(1.0)	0.0
54	297.7295	(AG)			
	(B)	51 O	15 SI(0.0)	55 O (1.0)	0.0
	(B)	16 SI	52 O (0.0)	10 AL(1.0)	0.0
	(B)	53 O	17 SI(0.0)	57 O (1.0)	0.0
	(B)	54 O	18 SI(0.0)	58 O (1.0)	0.0
55	297.9305	(B3G)			
	(B)	5 AL	1 MG(0.0)	39 O (1.0)	-0.1
	(B)	6 AL	1 MG(0.0)	41 O (1.0)	0.0
	(O)	1 MG	23 O (0.1)	17 SI(0.6)	0.0
	(O)	1 MG	25 O (0.1)	15 SI(0.6)	0.0
	(O)	32 O	1 MG(0.3)	39 O (0.4)	0.0
	(O)	34 O	1 MG(0.3)	41 O (0.4)	0.0
	(O)	1 MG	39 O (0.4)	22 SI(0.4)	0.0

(O)	1 MG	41 O (0.4)	20 SI(0.4)	0.0
(B)	5 AL	2 MG(0.0)	40 O (1.0)	0.0
(B)	6 AL	2 MG(0.0)	42 O (1.0)	0.0
(O)	2 MG	24 O (0.1)	18 SI(0.6)	0.0
(O)	2 MG	26 O (0.1)	16 SI(0.6)	0.0
(O)	31 O	2 MG(0.3)	40 O (0.4)	0.0
(O)	33 O	2 MG(0.3)	42 O (0.4)	0.0
(O)	2 MG	40 O (0.4)	21 SI(0.4)	-0.1
(O)	2 MG	42 O (0.4)	19 SI(0.4)	0.0
(B)	7 AL	3 MG(0.0)	43 O (1.0)	0.0
(B)	8 AL	3 MG(0.0)	45 O (1.0)	0.0
(O)	3 MG	27 O (0.1)	18 SI(0.6)	0.0
(O)	3 MG	29 O (0.1)	16 SI(0.6)	0.0
(O)	36 O	3 MG(0.3)	43 O (0.4)	0.0
(O)	38 O	3 MG(0.3)	45 O (0.4)	0.0
(O)	3 MG	43 O (0.4)	21 SI(0.4)	-0.1
(O)	3 MG	45 O (0.4)	19 SI(0.4)	0.0
(B)	7 AL	4 MG(0.0)	44 O (1.0)	0.0
(B)	8 AL	4 MG(0.0)	46 O (1.0)	0.0
(O)	4 MG	28 O (0.1)	17 SI(0.6)	0.0
(O)	4 MG	30 O (0.1)	15 SI(0.6)	0.0
(O)	35 O	4 MG(0.3)	44 O (0.4)	0.0
(O)	37 O	4 MG(0.3)	46 O (0.4)	0.0
(O)	4 MG	44 O (0.4)	22 SI(0.4)	0.0
(O)	4 MG	46 O (0.4)	20 SI(0.4)	0.0

56 298.1540 (B2U)

(B)	33 O	9 AL(0.0)	38 O (1.0)	0.0
(B)	38 O	9 AL(0.0)	33 O (1.0)	0.0
(B)	34 O	10 AL(0.0)	37 O (1.0)	0.0
(B)	37 O	10 AL(0.0)	34 O (1.0)	0.0
(B)	31 O	11 AL(0.0)	36 O (1.0)	0.0
(B)	36 O	11 AL(0.0)	31 O (1.0)	0.0
(B)	32 O	12 AL(0.0)	35 O (1.0)	0.0
(B)	35 O	12 AL(0.0)	32 O (1.0)	0.0
(B)	51 O	15 SI(0.0)	55 O (1.0)	0.0
(B)	16 SI	52 O (0.0)	10 AL(1.0)	0.0
(B)	53 O	17 SI(0.0)	57 O (1.0)	0.0
(B)	54 O	18 SI(0.0)	58 O (1.0)	0.0

57 298.3238 (AU)

(B)	32 O	1 MG(0.0)	39 O (0.9)	0.0
(B)	34 O	1 MG(0.0)	41 O (0.9)	0.0
(B)	31 O	2 MG(0.0)	40 O (0.9)	0.0
(B)	33 O	2 MG(0.0)	42 O (0.9)	0.0
(B)	36 O	3 MG(0.0)	43 O (0.9)	0.0
(B)	38 O	3 MG(0.0)	45 O (0.9)	0.0
(B)	35 O	4 MG(0.0)	44 O (0.9)	0.0
(B)	37 O	4 MG(0.0)	46 O (0.9)	0.0
(O)	31 O	13 SI(0.0)	32 O (0.7)	0.0
(O)	32 O	13 SI(0.0)	31 O (0.7)	0.0
(O)	33 O	13 SI(0.0)	34 O (0.7)	0.0
(O)	34 O	13 SI(0.0)	33 O (0.7)	0.0
(O)	35 O	14 SI(0.0)	36 O (0.7)	0.0
(O)	36 O	14 SI(0.0)	35 O (0.7)	0.0
(O)	37 O	14 SI(0.0)	38 O (0.7)	0.0



(O) 38 O 14 SI(0.0) 37 O (0.7) 0.0

58 302.6463 (B1G)

(B) 32 O 1 MG(0.0) 39 O (0.8) 0.0

(B) 34 O 1 MG(0.0) 41 O (0.8) 0.0

(B) 31 O 2 MG(0.0) 40 O (0.8) 0.0

(B) 33 O 2 MG(0.0) 42 O (0.8) 0.0

(B) 36 O 3 MG(0.0) 43 O (0.8) 0.0

(B) 38 O 3 MG(0.0) 45 O (0.8) 0.0

(B) 35 O 4 MG(0.0) 44 O (0.8) 0.0

(B) 37 O 4 MG(0.0) 46 O (0.8) 0.0

59 306.2413 (B3G)

(O) 48 O 9 AL(0.0) 33 O (0.7) 0.0

(O) 47 O 10 AL(0.0) 34 O (0.7) 0.0

(O) 50 O 11 AL(0.0) 31 O (0.7) 0.0

(O) 49 O 12 AL(0.0) 32 O (0.7) 0.0

60 314.5589 (AG)

(B) 15 SI 55 O (0.1) 19 SI(0.9) 0.0

(B) 16 SI 56 O (0.1) 20 SI(0.9) 0.0

(B) 17 SI 57 O (0.1) 21 SI(0.9) 0.0

(B) 18 SI 58 O (0.1) 22 SI(0.9) 0.0

(B) 47 O 19 SI(0.0) 55 O (1.0) 0.0

(B) 48 O 20 SI(0.0) 56 O (1.0) 0.0

(B) 21 SI 49 O (0.0) 12 AL(1.0) 0.0

(B) 22 SI 50 O (0.0) 11 AL(1.0) 0.0

61 322.1347 (AU)

(B) 5 AL 1 MG(0.3) 6 AL(0.7) 0.0

(B) 6 AL 1 MG(0.3) 5 AL(0.7) 0.0

(B) 39 O 1 MG(0.0) 41 O (1.0) 0.0

(B) 41 O 1 MG(0.0) 39 O (1.0) -0.1

(B) 5 AL 2 MG(0.3) 6 AL(0.7) 0.0

(B) 6 AL 2 MG(0.3) 5 AL(0.7) 0.0

(B) 40 O 2 MG(0.0) 42 O (1.0) 0.0

(B) 42 O 2 MG(0.0) 40 O (1.0) 0.0

(B) 7 AL 3 MG(0.3) 8 AL(0.7) 0.0

(B) 8 AL 3 MG(0.3) 7 AL(0.7) 0.0

(B) 43 O 3 MG(0.0) 45 O (1.0) 0.0

(B) 45 O 3 MG(0.0) 43 O (1.0) 0.0

(B) 7 AL 4 MG(0.3) 8 AL(0.7) 0.0

(B) 8 AL 4 MG(0.3) 7 AL(0.7) 0.0

(B) 44 O 4 MG(0.0) 46 O (1.0) 0.0

(B) 46 O 4 MG(0.0) 44 O (1.0) 0.0

62 326.9807 (B2U)

(S) 5 AL 1 MG(1.0) 0.0

(S) 6 AL 1 MG(1.0) 0.0

(S) 5 AL 2 MG(1.0) 0.0

(S) 6 AL 2 MG(1.0) 0.0

(S) 7 AL 3 MG(1.0) 0.0

(S) 8 AL 3 MG(1.0) 0.0

(S) 7 AL 4 MG(1.0) 0.0

(S) 8 AL 4 MG(1.0) 0.0

(B) 51 O 9 AL(0.0) 48 O (1.0) 0.0

(B) 10 AL 52 O (0.0) 16 SI(1.0) 0.0

(B) 53 O 11 AL(0.0) 50 O (1.0) 0.0

(B) 54 O 12 AL(0.0) 49 O (1.0) 0.0

63 330.0326 (AG )

(B)	42 O	19 SI(0.0)	45 O (1.0)	0.0
(B)	45 O	19 SI(0.0)	42 O (1.0)	0.0
(B)	41 O	20 SI(0.0)	46 O (1.0)	0.0
(B)	46 O	20 SI(0.0)	41 O (1.0)	0.0
(B)	40 O	21 SI(0.0)	43 O (1.0)	-0.1
(B)	43 O	21 SI(0.0)	40 O (1.0)	0.0
(B)	39 O	22 SI(0.0)	44 O (1.0)	0.0
(B)	44 O	22 SI(0.0)	39 O (1.0)	0.0

64 330.1225 (B2G)

(B)	32 O	1 MG(0.4)	25 O (0.6)	0.0
(B)	34 O	1 MG(0.4)	23 O (0.6)	0.0
(B)	31 O	2 MG(0.4)	26 O (0.6)	0.0
(B)	33 O	2 MG(0.4)	24 O (0.6)	0.0
(B)	36 O	3 MG(0.4)	29 O (0.6)	0.0
(B)	38 O	3 MG(0.4)	27 O (0.6)	0.0
(B)	35 O	4 MG(0.4)	30 O (0.6)	0.0
(B)	37 O	4 MG(0.4)	28 O (0.6)	0.0
(O)	51 O	9 AL(0.0)	33 O (0.7)	0.0
(O)	52 O	10 AL(0.0)	34 O (0.7)	0.0
(O)	53 O	11 AL(0.0)	31 O (0.7)	0.0
(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
(O)	49 O	21 SI(0.0)	40 O (0.8)	0.0
(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0

65 331.5545 (B3U)

(S)	5 AL	1 MG(0.6)	34 O (0.4)	0.0
(S)	6 AL	1 MG(0.6)	32 O (0.4)	0.0
(S)	23 O	1 MG(0.6)	39 O (0.4)	0.0
(S)	25 O	1 MG(0.6)	41 O (0.4)	0.0
(S)	5 AL	2 MG(0.6)	33 O (0.4)	0.0
(S)	6 AL	2 MG(0.6)	31 O (0.4)	0.0
(S)	24 O	2 MG(0.6)	40 O (0.4)	0.0
(S)	26 O	2 MG(0.6)	42 O (0.4)	0.0
(S)	7 AL	3 MG(0.6)	38 O (0.4)	0.0
(S)	8 AL	3 MG(0.6)	36 O (0.4)	0.0
(S)	27 O	3 MG(0.6)	43 O (0.4)	0.0
(S)	29 O	3 MG(0.6)	45 O (0.4)	0.0
(S)	7 AL	4 MG(0.6)	37 O (0.4)	0.0
(S)	8 AL	4 MG(0.6)	35 O (0.4)	0.0
(S)	28 O	4 MG(0.6)	44 O (0.4)	0.0
(S)	30 O	4 MG(0.6)	46 O (0.4)	0.0

66 340.4812 (B3U)

(B)	23 O	1 MG(0.0)	32 O (1.0)	0.0
(B)	25 O	1 MG(0.0)	34 O (1.0)	0.0
(B)	24 O	2 MG(0.0)	31 O (1.0)	0.0
(B)	26 O	2 MG(0.0)	33 O (1.0)	0.0
(B)	27 O	3 MG(0.0)	36 O (1.0)	0.0
(B)	29 O	3 MG(0.0)	38 O (1.0)	0.0
(B)	28 O	4 MG(0.0)	35 O (1.0)	0.0
(B)	30 O	4 MG(0.0)	37 O (1.0)	0.0

67 342.1781 (B1U)

(B)	32 O	1 MG(0.3)	5 AL(0.7)	0.0
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	(B)	34 O	1 MG(0.3)	6 AL(0.7)	0.0
	(B)	31 O	2 MG(0.3)	5 AL(0.7)	0.0
	(B)	33 O	2 MG(0.3)	6 AL(0.7)	0.0
	(B)	36 O	3 MG(0.3)	7 AL(0.7)	0.0
	(B)	38 O	3 MG(0.3)	8 AL(0.7)	0.0
	(B)	35 O	4 MG(0.3)	7 AL(0.7)	0.0
	(B)	37 O	4 MG(0.3)	8 AL(0.7)	0.0
68	342.3809	(B1G)			
	(B)	32 O	1 MG(0.1)	5 AL(0.9)	0.0
	(B)	34 O	1 MG(0.1)	6 AL(0.9)	0.0
	(B)	31 O	2 MG(0.1)	5 AL(0.9)	0.0
	(B)	33 O	2 MG(0.1)	6 AL(0.9)	0.0
	(B)	36 O	3 MG(0.1)	7 AL(0.9)	0.0
	(B)	38 O	3 MG(0.1)	8 AL(0.9)	0.0
	(B)	35 O	4 MG(0.1)	7 AL(0.9)	0.0
	(B)	37 O	4 MG(0.1)	8 AL(0.9)	0.0
69	358.6119	(B3U)			
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
	(B)	51 O	15 SI(0.0)	55 O (1.0)	0.0
	(B)	16 SI	52 O (0.0)	10 AL(1.0)	0.0
	(B)	53 O	17 SI(0.0)	57 O (1.0)	0.0
	(B)	54 O	18 SI(0.0)	58 O (1.0)	0.0
70	358.8567	(B1G)			
	(O)	39 O	1 MG(0.1)	23 O (0.7)	0.0
	(O)	41 O	1 MG(0.1)	25 O (0.7)	0.0
	(O)	40 O	2 MG(0.1)	24 O (0.7)	-0.2
	(O)	42 O	2 MG(0.1)	26 O (0.7)	-0.1
	(O)	43 O	3 MG(0.1)	27 O (0.7)	0.0
	(O)	45 O	3 MG(0.1)	29 O (0.7)	0.1
	(O)	44 O	4 MG(0.1)	28 O (0.7)	-0.1
	(O)	46 O	4 MG(0.1)	30 O (0.7)	0.1
71	359.6766	(B2U)			
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
	(B)	15 SI	55 O (0.0)	19 SI(1.0)	0.0
	(B)	16 SI	56 O (0.0)	20 SI(1.0)	0.0
	(B)	17 SI	57 O (0.0)	21 SI(1.0)	0.0
	(B)	18 SI	58 O (0.0)	22 SI(1.0)	0.0
72	363.0313	(AG)			
	(B)	23 O	1 MG(0.4)	32 O (0.6)	0.0
	(B)	25 O	1 MG(0.4)	34 O (0.6)	0.0
	(B)	24 O	2 MG(0.4)	31 O (0.6)	0.0
	(B)	26 O	2 MG(0.4)	33 O (0.6)	0.0
	(B)	27 O	3 MG(0.4)	36 O (0.6)	0.0
	(B)	29 O	3 MG(0.4)	38 O (0.6)	0.0
	(B)	28 O	4 MG(0.4)	35 O (0.6)	0.0
	(B)	30 O	4 MG(0.4)	37 O (0.6)	0.0
73	363.7686	(B2U)			
	(S)	32 O	1 MG(0.6)	25 O (0.3)	0.0

	(S)	34 O	1 MG(0.6)	23 O (0.3)	0.0
	(S)	31 O	2 MG(0.6)	26 O (0.3)	0.0
	(S)	33 O	2 MG(0.6)	24 O (0.3)	0.0
	(S)	36 O	3 MG(0.6)	29 O (0.3)	0.0
	(S)	38 O	3 MG(0.6)	27 O (0.3)	0.0
	(S)	35 O	4 MG(0.6)	30 O (0.3)	0.0
	(S)	37 O	4 MG(0.6)	28 O (0.3)	0.0
74	370.3269 (B1U)				
	(O)	25 O	5 AL(0.0)	26 O (0.8)	0.0
	(O)	26 O	5 AL(0.0)	25 O (0.8)	0.0
	(B)	39 O	5 AL(0.0)	40 O (0.9)	0.0
	(B)	40 O	5 AL(0.0)	39 O (0.9)	0.0
	(O)	23 O	6 AL(0.0)	24 O (0.8)	0.0
	(O)	24 O	6 AL(0.0)	23 O (0.8)	0.0
	(B)	41 O	6 AL(0.0)	42 O (0.9)	0.0
	(B)	42 O	6 AL(0.0)	41 O (0.9)	0.0
	(O)	29 O	7 AL(0.0)	30 O (0.8)	0.0
	(O)	30 O	7 AL(0.0)	29 O (0.8)	0.0
	(B)	43 O	7 AL(0.0)	44 O (0.9)	0.1
	(B)	44 O	7 AL(0.0)	43 O (0.9)	-0.1
	(O)	27 O	8 AL(0.0)	28 O (0.8)	0.0
	(O)	28 O	8 AL(0.0)	27 O (0.8)	0.0
	(B)	45 O	8 AL(0.0)	46 O (0.9)	0.1
	(B)	46 O	8 AL(0.0)	45 O (0.9)	0.0
75	370.4221 (AG )				
	(B)	23 O	1 MG(0.2)	32 O (0.8)	0.0
	(B)	25 O	1 MG(0.2)	34 O (0.8)	0.0
	(B)	24 O	2 MG(0.2)	31 O (0.8)	0.0
	(B)	26 O	2 MG(0.2)	33 O (0.8)	0.0
	(B)	27 O	3 MG(0.2)	36 O (0.8)	0.0
	(B)	29 O	3 MG(0.2)	38 O (0.8)	0.0
	(B)	28 O	4 MG(0.2)	35 O (0.8)	0.0
	(B)	30 O	4 MG(0.2)	37 O (0.8)	0.0
76	371.5579 (AU )				
	(O)	25 O	5 AL(0.0)	26 O (0.8)	0.0
	(O)	26 O	5 AL(0.0)	25 O (0.8)	0.0
	(O)	39 O	5 AL(0.0)	26 O (0.7)	0.0
	(O)	40 O	5 AL(0.0)	25 O (0.7)	0.0
	(O)	23 O	6 AL(0.0)	24 O (0.8)	0.0
	(O)	24 O	6 AL(0.0)	23 O (0.8)	0.0
	(O)	41 O	6 AL(0.0)	24 O (0.7)	0.0
	(O)	42 O	6 AL(0.0)	23 O (0.7)	0.0
	(O)	29 O	7 AL(0.0)	30 O (0.8)	0.0
	(O)	30 O	7 AL(0.0)	29 O (0.8)	0.0
	(O)	43 O	7 AL(0.0)	30 O (0.7)	0.1
	(O)	44 O	7 AL(0.0)	29 O (0.7)	-0.1
	(O)	27 O	8 AL(0.0)	28 O (0.8)	0.0
	(O)	28 O	8 AL(0.0)	27 O (0.8)	0.0
	(O)	45 O	8 AL(0.0)	28 O (0.7)	0.0
	(O)	46 O	8 AL(0.0)	27 O (0.7)	0.0
77	378.3199 (B3G)				
	(S)	5 AL	1 MG(0.9)		0.0
	(S)	6 AL	1 MG(0.9)		-0.1
	(B)	23 O	1 MG(0.3)	5 AL(0.7)	0.0

	(B)	25 O	1 MG(0.3)	6 AL(0.7)	0.0
	(S)	1 MG	39 O (0.7)	22 SI(0.3)	0.0
	(S)	1 MG	41 O (0.7)	20 SI(0.3)	-0.1
	(S)	5 AL	2 MG(0.9)		0.0
	(S)	6 AL	2 MG(0.9)		0.0
	(B)	24 O	2 MG(0.3)	5 AL(0.7)	0.0
	(B)	26 O	2 MG(0.3)	6 AL(0.7)	0.0
	(S)	2 MG	40 O (0.7)	21 SI(0.3)	-0.1
	(S)	2 MG	42 O (0.7)	19 SI(0.3)	-0.1
	(S)	7 AL	3 MG(0.9)		0.0
	(S)	8 AL	3 MG(0.9)		0.0
	(B)	27 O	3 MG(0.3)	7 AL(0.7)	0.0
	(B)	29 O	3 MG(0.3)	8 AL(0.7)	0.0
	(S)	3 MG	43 O (0.7)	21 SI(0.3)	0.0
	(S)	3 MG	45 O (0.7)	19 SI(0.3)	0.0
	(S)	7 AL	4 MG(0.9)		0.0
	(S)	8 AL	4 MG(0.9)		0.0
	(B)	28 O	4 MG(0.3)	7 AL(0.7)	0.0
	(B)	30 O	4 MG(0.3)	8 AL(0.7)	0.0
	(S)	4 MG	44 O (0.7)	22 SI(0.3)	0.0
	(S)	4 MG	46 O (0.7)	20 SI(0.3)	0.0
78	379.7765	(B3U)			
	(B)	32 O	1 MG(0.3)	39 O (0.6)	0.0
	(B)	34 O	1 MG(0.3)	41 O (0.6)	0.0
	(S)	39 O	1 MG(0.8)	23 O (0.2)	0.0
	(S)	41 O	1 MG(0.8)	25 O (0.2)	-0.1
	(B)	31 O	2 MG(0.3)	40 O (0.6)	0.0
	(B)	33 O	2 MG(0.3)	42 O (0.6)	0.0
	(S)	40 O	2 MG(0.8)	24 O (0.2)	0.0
	(S)	42 O	2 MG(0.8)	26 O (0.2)	0.0
	(B)	36 O	3 MG(0.3)	43 O (0.6)	0.0
	(B)	38 O	3 MG(0.3)	45 O (0.6)	0.0
	(S)	43 O	3 MG(0.8)	27 O (0.2)	0.0
	(S)	45 O	3 MG(0.8)	29 O (0.2)	0.0
	(B)	35 O	4 MG(0.3)	44 O (0.6)	0.0
	(B)	37 O	4 MG(0.3)	46 O (0.6)	0.0
	(S)	44 O	4 MG(0.8)	28 O (0.2)	0.0
	(S)	46 O	4 MG(0.8)	30 O (0.2)	0.0
79	385.7357	(B2G)			
	(B)	5 AL	1 MG(0.5)	6 AL(0.5)	0.0
	(B)	6 AL	1 MG(0.5)	5 AL(0.5)	0.0
	(B)	32 O	1 MG(0.5)	25 O (0.5)	0.0
	(B)	34 O	1 MG(0.5)	23 O (0.5)	0.0
	(B)	39 O	1 MG(0.0)	41 O (1.0)	0.0
	(B)	41 O	1 MG(0.0)	39 O (1.0)	-0.1
	(B)	5 AL	2 MG(0.5)	6 AL(0.5)	0.0
	(B)	6 AL	2 MG(0.5)	5 AL(0.5)	0.0
	(B)	31 O	2 MG(0.5)	26 O (0.5)	0.0
	(B)	33 O	2 MG(0.5)	24 O (0.5)	0.0
	(B)	40 O	2 MG(0.0)	42 O (1.0)	0.0
	(B)	42 O	2 MG(0.0)	40 O (1.0)	0.0
	(B)	7 AL	3 MG(0.5)	8 AL(0.5)	0.0
	(B)	8 AL	3 MG(0.5)	7 AL(0.5)	0.0
	(B)	36 O	3 MG(0.5)	29 O (0.5)	0.0

	(B)	38 O	3 MG(0.5)	27 O (0.5)	0.0
	(B)	43 O	3 MG(0.0)	45 O (1.0)	0.0
	(B)	45 O	3 MG(0.0)	43 O (1.0)	0.0
	(B)	7 AL	4 MG(0.5)	8 AL(0.5)	0.0
	(B)	8 AL	4 MG(0.5)	7 AL(0.5)	0.0
	(B)	35 O	4 MG(0.5)	30 O (0.5)	0.0
	(B)	37 O	4 MG(0.5)	28 O (0.5)	0.0
	(B)	44 O	4 MG(0.0)	46 O (1.0)	0.0
	(B)	46 O	4 MG(0.0)	44 O (1.0)	0.0
80	397.7195	(B2G)			
	(S)	32 O	1 MG(0.9)		0.0
	(S)	34 O	1 MG(0.9)		0.0
	(S)	31 O	2 MG(0.9)		0.0
	(S)	33 O	2 MG(0.9)		0.0
	(S)	36 O	3 MG(0.9)		0.0
	(S)	38 O	3 MG(0.9)		0.0
	(S)	35 O	4 MG(0.9)		0.0
	(S)	37 O	4 MG(0.9)		0.0
	(O)	48 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	50 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
81	405.1104	(B2U)			
	(B)	51 O	9 AL(0.0)	48 O (1.0)	0.0
	(B)	10 AL	52 O (0.0)	16 SI(1.0)	0.0
	(B)	53 O	11 AL(0.0)	50 O (1.0)	0.0
	(B)	54 O	12 AL(0.0)	49 O (1.0)	0.0
82	409.8758	(B3U)			
	(B)	25 O	5 AL(0.0)	40 O (0.9)	0.0
	(B)	26 O	5 AL(0.0)	39 O (0.9)	0.0
	(B)	39 O	5 AL(0.0)	26 O (1.0)	0.0
	(B)	40 O	5 AL(0.0)	25 O (1.0)	0.0
	(B)	23 O	6 AL(0.0)	42 O (0.9)	0.0
	(B)	24 O	6 AL(0.0)	41 O (0.9)	0.0
	(B)	41 O	6 AL(0.0)	24 O (1.0)	0.0
	(B)	42 O	6 AL(0.0)	23 O (1.0)	0.0
	(B)	29 O	7 AL(0.0)	44 O (0.9)	0.0
	(B)	30 O	7 AL(0.0)	43 O (0.9)	0.0
	(B)	43 O	7 AL(0.0)	30 O (1.0)	0.0
	(B)	44 O	7 AL(0.0)	29 O (1.0)	-0.1
	(B)	27 O	8 AL(0.0)	46 O (0.9)	0.0
	(B)	28 O	8 AL(0.0)	45 O (0.9)	0.0
	(B)	45 O	8 AL(0.0)	28 O (1.0)	0.0
	(B)	46 O	8 AL(0.0)	27 O (1.0)	-0.1
83	417.1618	(B2U)			
	(S)	5 AL	1 MG(0.5)	6 AL(0.5)	0.0
	(S)	6 AL	1 MG(0.5)	5 AL(0.5)	0.0
	(B)	23 O	1 MG(0.3)	32 O (0.7)	0.0
	(B)	25 O	1 MG(0.3)	34 O (0.7)	0.0
	(S)	32 O	1 MG(0.7)	23 O (0.3)	0.0
	(S)	34 O	1 MG(0.7)	25 O (0.3)	0.0
	(S)	5 AL	2 MG(0.5)	6 AL(0.5)	0.0
	(S)	6 AL	2 MG(0.5)	5 AL(0.5)	0.0
	(B)	24 O	2 MG(0.3)	31 O (0.7)	0.0

	(B)	26 O	2 MG(0.3)	33 O (0.7)	0.0
	(S)	31 O	2 MG(0.7)	24 O (0.3)	0.0
	(S)	33 O	2 MG(0.7)	26 O (0.3)	0.0
	(S)	7 AL	3 MG(0.5)	8 AL(0.5)	0.0
	(S)	8 AL	3 MG(0.5)	7 AL(0.5)	0.0
	(B)	27 O	3 MG(0.3)	36 O (0.7)	0.0
	(B)	29 O	3 MG(0.3)	38 O (0.7)	0.0
	(S)	36 O	3 MG(0.7)	27 O (0.3)	0.0
	(S)	38 O	3 MG(0.7)	29 O (0.3)	0.0
	(S)	7 AL	4 MG(0.5)	8 AL(0.5)	0.0
	(S)	8 AL	4 MG(0.5)	7 AL(0.5)	0.0
	(B)	28 O	4 MG(0.3)	35 O (0.7)	0.0
	(B)	30 O	4 MG(0.3)	37 O (0.7)	0.0
	(S)	35 O	4 MG(0.7)	28 O (0.3)	0.0
	(S)	37 O	4 MG(0.7)	30 O (0.3)	0.0
84	424.3305	(B1G)			
	(B)	39 O	5 AL(0.1)	40 O (0.8)	0.0
	(B)	40 O	5 AL(0.1)	39 O (0.8)	0.0
	(B)	41 O	6 AL(0.1)	42 O (0.8)	0.0
	(B)	42 O	6 AL(0.1)	41 O (0.8)	0.0
	(B)	43 O	7 AL(0.1)	44 O (0.8)	0.1
	(B)	44 O	7 AL(0.1)	43 O (0.8)	0.0
	(B)	45 O	8 AL(0.1)	46 O (0.8)	0.0
	(B)	46 O	8 AL(0.1)	45 O (0.8)	0.0
85	431.4552	(B3U)			
	(B)	23 O	1 MG(0.4)	5 AL(0.6)	0.0
	(B)	25 O	1 MG(0.4)	6 AL(0.6)	0.0
	(B)	24 O	2 MG(0.4)	5 AL(0.6)	0.0
	(B)	26 O	2 MG(0.4)	6 AL(0.6)	0.0
	(B)	27 O	3 MG(0.4)	7 AL(0.6)	0.0
	(B)	29 O	3 MG(0.4)	8 AL(0.6)	0.0
	(B)	28 O	4 MG(0.4)	7 AL(0.6)	0.0
	(B)	30 O	4 MG(0.4)	8 AL(0.6)	0.0
86	435.3946	(AG)			
	(B)	33 O	9 AL(0.1)	38 O (0.9)	0.0
	(B)	38 O	9 AL(0.1)	33 O (0.9)	0.0
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	34 O	10 AL(0.1)	37 O (0.9)	0.0
	(B)	37 O	10 AL(0.1)	34 O (0.9)	0.0
	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(B)	31 O	11 AL(0.1)	36 O (0.9)	0.0
	(B)	36 O	11 AL(0.1)	31 O (0.9)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(B)	32 O	12 AL(0.1)	35 O (0.9)	0.0
	(B)	35 O	12 AL(0.1)	32 O (0.9)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
	(B)	25 O	15 SI(0.0)	30 O (1.0)	0.0
	(B)	30 O	15 SI(0.0)	25 O (1.0)	0.0
	(B)	26 O	16 SI(0.0)	29 O (1.0)	0.0
	(B)	29 O	16 SI(0.0)	26 O (1.0)	0.0
	(B)	23 O	17 SI(0.0)	28 O (1.0)	0.0
	(B)	28 O	17 SI(0.0)	23 O (1.0)	0.0
	(B)	24 O	18 SI(0.0)	27 O (1.0)	0.0
	(B)	27 O	18 SI(0.0)	24 O (1.0)	0.0

87 449.4940 (B2U)

(S)	23 O	1 MG(0.5)	32 O (0.4)	0.0
(S)	25 O	1 MG(0.5)	34 O (0.4)	0.0
(S)	24 O	2 MG(0.5)	31 O (0.4)	0.0
(S)	26 O	2 MG(0.5)	33 O (0.4)	0.0
(S)	27 O	3 MG(0.5)	36 O (0.4)	0.0
(S)	29 O	3 MG(0.5)	38 O (0.4)	0.0
(S)	28 O	4 MG(0.5)	35 O (0.4)	0.0
(S)	30 O	4 MG(0.5)	37 O (0.4)	0.0
(B)	25 O	5 AL(0.0)	40 O (1.0)	0.0
(B)	26 O	5 AL(0.0)	39 O (1.0)	0.0
(B)	39 O	5 AL(0.0)	26 O (0.9)	0.0
(B)	40 O	5 AL(0.0)	25 O (0.9)	0.0
(B)	23 O	6 AL(0.0)	42 O (1.0)	0.0
(B)	24 O	6 AL(0.0)	41 O (1.0)	0.0
(B)	41 O	6 AL(0.0)	24 O (0.9)	0.0
(B)	42 O	6 AL(0.0)	23 O (0.9)	0.0
(B)	29 O	7 AL(0.0)	44 O (1.0)	0.0
(B)	30 O	7 AL(0.0)	43 O (1.0)	0.0
(B)	43 O	7 AL(0.0)	30 O (0.9)	0.1
(B)	44 O	7 AL(0.0)	29 O (0.9)	-0.1
(B)	27 O	8 AL(0.0)	46 O (1.0)	0.0
(B)	28 O	8 AL(0.0)	45 O (1.0)	0.0
(B)	45 O	8 AL(0.0)	28 O (0.9)	0.0
(B)	46 O	8 AL(0.0)	27 O (0.9)	0.0

88 460.7723 (B2G)

(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
(O)	49 O	21 SI(0.0)	40 O (0.8)	-0.1
(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0
(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0

89 462.0409 (B1G)

(B)	42 O	19 SI(0.0)	45 O (1.0)	0.0
(B)	45 O	19 SI(0.0)	42 O (1.0)	0.0
(B)	47 O	19 SI(0.0)	55 O (1.0)	0.0
(B)	41 O	20 SI(0.0)	46 O (1.0)	0.0
(B)	46 O	20 SI(0.0)	41 O (1.0)	0.0
(B)	48 O	20 SI(0.0)	56 O (1.0)	0.0
(B)	40 O	21 SI(0.0)	43 O (1.0)	-0.1
(B)	43 O	21 SI(0.0)	40 O (1.0)	0.0
(B)	21 SI	49 O (0.0)	12 AL(1.0)	0.0
(B)	39 O	22 SI(0.0)	44 O (1.0)	0.0
(B)	44 O	22 SI(0.0)	39 O (1.0)	0.0
(B)	22 SI	50 O (0.0)	11 AL(1.0)	0.0

90 465.6648 (B3G)

(B)	31 O	13 SI(0.0)	34 O (0.8)	0.0
(B)	32 O	13 SI(0.0)	33 O (0.8)	0.0
(B)	33 O	13 SI(0.0)	32 O (0.8)	0.0
(B)	34 O	13 SI(0.0)	31 O (0.8)	0.0
(B)	35 O	14 SI(0.0)	38 O (0.8)	0.0
(B)	36 O	14 SI(0.0)	37 O (0.8)	0.0



	(B)	37 O	14 SI(0.0)	36 O (0.8)	0.0
	(B)	38 O	14 SI(0.0)	35 O (0.8)	0.0
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
91	467.5831 (AU)				
	(O)	48 O	9 AL(0.0)	33 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.0
	(O)	50 O	11 AL(0.0)	31 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
92	475.7624 (AU)				
	(B)	5 AL	39 O (0.1)	22 SI(0.9)	0.0
	(B)	5 AL	40 O (0.1)	21 SI(0.9)	0.0
	(B)	6 AL	41 O (0.1)	20 SI(0.9)	0.0
	(B)	6 AL	42 O (0.1)	19 SI(0.9)	0.0
	(B)	7 AL	43 O (0.1)	21 SI(0.9)	0.0
	(B)	7 AL	44 O (0.1)	22 SI(0.9)	0.0
	(B)	8 AL	45 O (0.1)	19 SI(0.9)	0.0
	(B)	8 AL	46 O (0.1)	20 SI(0.9)	0.0
93	478.4843 (B3G)				
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
94	486.9799 (B1U)				
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
95	489.8360 (AG)				
	(B)	39 O	1 MG(0.1)	41 O (0.8)	0.0
	(B)	41 O	1 MG(0.1)	39 O (0.8)	-0.1
	(B)	40 O	2 MG(0.1)	42 O (0.8)	-0.1
	(B)	42 O	2 MG(0.1)	40 O (0.8)	0.0
	(B)	43 O	3 MG(0.1)	45 O (0.8)	0.0
	(B)	45 O	3 MG(0.1)	43 O (0.8)	0.0
	(B)	44 O	4 MG(0.1)	46 O (0.8)	0.0
	(B)	46 O	4 MG(0.1)	44 O (0.8)	0.0
	(B)	39 O	5 AL(0.0)	40 O (1.0)	0.0
	(B)	40 O	5 AL(0.0)	39 O (1.0)	0.0
	(B)	41 O	6 AL(0.0)	42 O (1.0)	0.0
	(B)	42 O	6 AL(0.0)	41 O (1.0)	0.0
	(B)	43 O	7 AL(0.0)	44 O (1.0)	0.1
	(B)	44 O	7 AL(0.0)	43 O (1.0)	-0.1
	(B)	45 O	8 AL(0.0)	46 O (1.0)	0.1

	(B)	46 O	8 AL(0.0)	45 O (1.0)	0.0
96	494.9119	(B3G)			
	(S)	32 O	1 MG(0.7)	39 O (0.3)	0.0
	(S)	34 O	1 MG(0.7)	41 O (0.3)	0.0
	(S)	31 O	2 MG(0.7)	40 O (0.3)	0.0
	(S)	33 O	2 MG(0.7)	42 O (0.3)	0.0
	(S)	36 O	3 MG(0.7)	43 O (0.3)	0.0
	(S)	38 O	3 MG(0.7)	45 O (0.3)	0.0
	(S)	35 O	4 MG(0.7)	44 O (0.3)	0.0
	(S)	37 O	4 MG(0.7)	46 O (0.3)	0.0
	(O)	31 O	13 SI(0.0)	34 O (0.8)	0.0
	(O)	32 O	13 SI(0.0)	33 O (0.8)	0.0
	(O)	33 O	13 SI(0.0)	32 O (0.8)	0.0
	(O)	34 O	13 SI(0.0)	31 O (0.8)	0.0
	(O)	35 O	14 SI(0.0)	38 O (0.8)	0.0
	(O)	36 O	14 SI(0.0)	37 O (0.8)	0.0
	(O)	37 O	14 SI(0.0)	36 O (0.8)	0.0
	(O)	38 O	14 SI(0.0)	35 O (0.8)	0.0
	(O)	47 O	19 SI(0.0)	42 O (0.8)	-0.1
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	48 O	20 SI(0.0)	41 O (0.8)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	49 O	21 SI(0.0)	40 O (0.8)	-0.1
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	50 O	22 SI(0.0)	39 O (0.8)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
97	497.3200	(B1G)			
	(B)	23 O	1 MG(0.4)	5 AL(0.6)	0.0
	(B)	25 O	1 MG(0.4)	6 AL(0.6)	0.0
	(B)	24 O	2 MG(0.4)	5 AL(0.6)	0.0
	(B)	26 O	2 MG(0.4)	6 AL(0.6)	0.0
	(B)	27 O	3 MG(0.4)	7 AL(0.6)	0.0
	(B)	29 O	3 MG(0.4)	8 AL(0.6)	0.0
	(B)	28 O	4 MG(0.4)	7 AL(0.6)	0.0
	(B)	30 O	4 MG(0.4)	8 AL(0.6)	0.0
98	498.1088	(B1U)			
	(B)	31 O	13 SI(0.0)	32 O (0.9)	0.0
	(B)	32 O	13 SI(0.0)	31 O (0.9)	0.0
	(B)	33 O	13 SI(0.0)	34 O (0.9)	0.0
	(B)	34 O	13 SI(0.0)	33 O (0.9)	0.0
	(B)	35 O	14 SI(0.0)	36 O (0.9)	0.0
	(B)	36 O	14 SI(0.0)	35 O (0.9)	0.0
	(B)	37 O	14 SI(0.0)	38 O (0.9)	0.0
	(B)	38 O	14 SI(0.0)	37 O (0.9)	0.0
99	498.3209	(B3U)			
	(O)	31 O	13 SI(0.0)	32 O (0.7)	0.0
	(O)	32 O	13 SI(0.0)	31 O (0.7)	0.0
	(O)	33 O	13 SI(0.0)	34 O (0.7)	0.0
	(O)	34 O	13 SI(0.0)	33 O (0.7)	0.0
	(O)	35 O	14 SI(0.0)	36 O (0.7)	0.0
	(O)	36 O	14 SI(0.0)	35 O (0.7)	0.0
	(O)	37 O	14 SI(0.0)	38 O (0.7)	0.0
	(O)	38 O	14 SI(0.0)	37 O (0.7)	0.0
100	500.1748	(B2G)			

	(S)	23 O	1 MG(0.8)	32 O (0.2)	0.0
	(S)	25 O	1 MG(0.8)	34 O (0.2)	0.0
	(S)	24 O	2 MG(0.8)	31 O (0.2)	0.0
	(S)	26 O	2 MG(0.8)	33 O (0.2)	0.0
	(S)	27 O	3 MG(0.8)	36 O (0.2)	0.0
	(S)	29 O	3 MG(0.8)	38 O (0.2)	0.0
	(S)	28 O	4 MG(0.8)	35 O (0.2)	0.0
	(S)	30 O	4 MG(0.8)	37 O (0.2)	0.0
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
101	501.3866 (B3U)				
	(B)	31 O	13 SI(0.0)	34 O (0.9)	0.0
	(B)	32 O	13 SI(0.0)	33 O (0.9)	0.0
	(B)	33 O	13 SI(0.0)	32 O (0.9)	0.0
	(B)	34 O	13 SI(0.0)	31 O (0.9)	0.0
	(B)	35 O	14 SI(0.0)	38 O (0.9)	0.0
	(B)	36 O	14 SI(0.0)	37 O (0.9)	0.0
	(B)	37 O	14 SI(0.0)	36 O (0.9)	0.0
	(B)	38 O	14 SI(0.0)	35 O (0.9)	0.0
102	509.2356 (B1U)				
	(S)	39 O	1 MG(0.8)	23 O (0.2)	0.0
	(S)	41 O	1 MG(0.8)	25 O (0.2)	0.0
	(S)	40 O	2 MG(0.8)	24 O (0.2)	-0.1
	(S)	42 O	2 MG(0.8)	26 O (0.2)	0.0
	(S)	43 O	3 MG(0.8)	27 O (0.2)	0.0
	(S)	45 O	3 MG(0.8)	29 O (0.2)	0.0
	(S)	44 O	4 MG(0.8)	28 O (0.2)	0.0
	(S)	46 O	4 MG(0.8)	30 O (0.2)	0.1
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
103	532.7653 (B2U)				
	(B)	25 O	5 AL(0.1)	26 O (0.8)	0.0
	(B)	26 O	5 AL(0.1)	25 O (0.8)	0.0
	(B)	23 O	6 AL(0.1)	24 O (0.8)	0.0
	(B)	24 O	6 AL(0.1)	23 O (0.8)	0.0
	(B)	29 O	7 AL(0.1)	30 O (0.8)	0.0
	(B)	30 O	7 AL(0.1)	29 O (0.8)	0.0
	(B)	27 O	8 AL(0.1)	28 O (0.8)	0.0
	(B)	28 O	8 AL(0.1)	27 O (0.8)	0.0
	(B)	25 O	15 SI(0.0)	55 O (0.9)	0.0
	(B)	30 O	15 SI(0.0)	55 O (0.9)	0.0
	(B)	26 O	16 SI(0.0)	56 O (0.9)	0.0
	(B)	29 O	16 SI(0.0)	56 O (0.9)	0.0
	(B)	23 O	17 SI(0.0)	57 O (0.9)	0.0
	(B)	28 O	17 SI(0.0)	57 O (0.9)	0.0
	(B)	24 O	18 SI(0.0)	58 O (0.9)	0.0
	(B)	27 O	18 SI(0.0)	58 O (0.9)	0.0
104	541.2014 (AU )				
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0

	(O)	52 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	26 O (0.7)	0.0
	(O)	53 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	57 O	17 SI(0.0)	28 O (0.7)	0.0
	(O)	54 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	58 O	18 SI(0.0)	24 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	42 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	41 O (0.7)	0.0
	(O)	57 O	21 SI(0.0)	40 O (0.7)	0.0
	(O)	58 O	22 SI(0.0)	39 O (0.7)	0.0
105		556.1276 (B1G)			
	(S)	32 O	1 MG(0.7)	5 AL(0.3)	0.0
	(S)	34 O	1 MG(0.7)	6 AL(0.3)	0.0
	(S)	31 O	2 MG(0.7)	5 AL(0.3)	0.0
	(S)	33 O	2 MG(0.7)	6 AL(0.3)	0.0
	(S)	36 O	3 MG(0.7)	7 AL(0.3)	0.0
	(S)	38 O	3 MG(0.7)	8 AL(0.3)	0.0
	(S)	35 O	4 MG(0.7)	7 AL(0.3)	0.0
	(S)	37 O	4 MG(0.7)	8 AL(0.3)	0.0
	(B)	33 O	9 AL(0.1)	51 O (0.8)	0.0
	(B)	38 O	9 AL(0.1)	51 O (0.8)	0.0
	(B)	34 O	10 AL(0.1)	52 O (0.8)	0.0
	(B)	37 O	10 AL(0.1)	52 O (0.8)	0.0
	(B)	31 O	11 AL(0.1)	53 O (0.8)	0.0
	(B)	36 O	11 AL(0.1)	53 O (0.8)	0.0
	(B)	32 O	12 AL(0.1)	54 O (0.8)	0.0
	(B)	35 O	12 AL(0.1)	54 O (0.8)	0.0
	(B)	31 O	13 SI(0.1)	32 O (0.8)	0.0
	(B)	32 O	13 SI(0.1)	31 O (0.8)	0.0
	(B)	33 O	13 SI(0.1)	34 O (0.8)	0.0
	(B)	34 O	13 SI(0.1)	33 O (0.8)	0.0
	(B)	35 O	14 SI(0.1)	36 O (0.8)	0.0
	(B)	36 O	14 SI(0.1)	35 O (0.8)	0.0
	(B)	37 O	14 SI(0.1)	38 O (0.8)	0.0
	(B)	38 O	14 SI(0.1)	37 O (0.8)	0.0
106		562.2235 (AG)			
	(S)	23 O	1 MG(0.8)	5 AL(0.2)	0.0
	(S)	25 O	1 MG(0.8)	6 AL(0.2)	0.0
	(S)	24 O	2 MG(0.8)	5 AL(0.2)	0.0
	(S)	26 O	2 MG(0.8)	6 AL(0.2)	0.0
	(S)	27 O	3 MG(0.8)	7 AL(0.2)	0.0
	(S)	29 O	3 MG(0.8)	8 AL(0.2)	0.0
	(S)	28 O	4 MG(0.8)	7 AL(0.2)	0.0
	(S)	30 O	4 MG(0.8)	8 AL(0.2)	0.0
	(B)	5 AL	25 O (0.3)	15 SI(0.6)	0.0
	(B)	5 AL	26 O (0.3)	16 SI(0.6)	0.0
	(B)	6 AL	23 O (0.3)	17 SI(0.6)	0.0
	(B)	6 AL	24 O (0.3)	18 SI(0.6)	0.0
	(B)	7 AL	29 O (0.3)	16 SI(0.6)	0.0
	(B)	7 AL	30 O (0.3)	15 SI(0.6)	0.0
	(B)	8 AL	27 O (0.3)	18 SI(0.6)	0.0
	(B)	8 AL	28 O (0.3)	17 SI(0.6)	0.0
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(S)	51 O	9 AL(0.7)	48 O (0.3)	0.0

	(B)	47 O	10 AL(0.0)	52 O (1.0)	0.0
	(S)	10 AL	52 O (0.7)	16 SI(0.3)	0.0
	(B)	11 AL	50 O (0.0)	22 SI(1.0)	0.0
	(S)	53 O	11 AL(0.7)	50 O (0.3)	0.0
	(B)	12 AL	49 O (0.0)	21 SI(1.0)	0.0
	(S)	54 O	12 AL(0.7)	49 O (0.3)	0.0
107	571.1942	(B2U)			
	(B)	48 O	9 AL(0.5)	51 O (0.5)	0.0
	(B)	47 O	10 AL(0.5)	52 O (0.5)	0.0
	(B)	11 AL	50 O (0.5)	22 SI(0.5)	0.0
	(B)	12 AL	49 O (0.5)	21 SI(0.5)	0.0
108	571.7168	(B1U)			
	(B)	39 O	1 MG(0.4)	32 O (0.6)	0.0
	(B)	41 O	1 MG(0.4)	34 O (0.6)	-0.1
	(B)	40 O	2 MG(0.4)	31 O (0.6)	0.0
	(B)	42 O	2 MG(0.4)	33 O (0.6)	0.0
	(B)	43 O	3 MG(0.4)	36 O (0.6)	0.0
	(B)	45 O	3 MG(0.4)	38 O (0.6)	0.0
	(B)	44 O	4 MG(0.4)	35 O (0.6)	0.0
	(B)	46 O	4 MG(0.4)	37 O (0.6)	0.0
	(B)	25 O	15 SI(0.1)	55 O (0.8)	0.0
	(B)	30 O	15 SI(0.1)	55 O (0.8)	0.0
	(B)	26 O	16 SI(0.1)	56 O (0.8)	0.0
	(B)	29 O	16 SI(0.1)	56 O (0.8)	0.0
	(B)	23 O	17 SI(0.1)	57 O (0.8)	0.0
	(B)	28 O	17 SI(0.1)	57 O (0.8)	0.0
	(B)	24 O	18 SI(0.1)	58 O (0.8)	0.0
	(B)	27 O	18 SI(0.1)	58 O (0.8)	0.0
	(B)	42 O	19 SI(0.1)	47 O (0.9)	0.0
	(B)	45 O	19 SI(0.1)	47 O (0.9)	-0.1
	(B)	41 O	20 SI(0.1)	48 O (0.9)	0.0
	(B)	46 O	20 SI(0.1)	48 O (0.9)	0.0
	(B)	40 O	21 SI(0.1)	49 O (0.9)	0.0
	(B)	43 O	21 SI(0.1)	49 O (0.9)	0.0
	(B)	39 O	22 SI(0.1)	50 O (0.9)	0.0
	(B)	44 O	22 SI(0.1)	50 O (0.9)	0.0
109	573.6112	(B1G)			
	(S)	39 O	1 MG(0.6)	32 O (0.3)	0.0
	(S)	41 O	1 MG(0.6)	34 O (0.3)	-0.1
	(S)	40 O	2 MG(0.6)	31 O (0.3)	0.0
	(S)	42 O	2 MG(0.6)	33 O (0.3)	0.0
	(S)	43 O	3 MG(0.6)	36 O (0.3)	0.0
	(S)	45 O	3 MG(0.6)	38 O (0.3)	0.0
	(S)	44 O	4 MG(0.6)	35 O (0.3)	0.0
	(S)	46 O	4 MG(0.6)	37 O (0.3)	0.0
	(B)	5 AL	39 O (0.4)	22 SI(0.5)	0.0
	(B)	5 AL	40 O (0.4)	21 SI(0.5)	0.0
	(B)	6 AL	41 O (0.4)	20 SI(0.5)	0.0
	(B)	6 AL	42 O (0.4)	19 SI(0.5)	0.0
	(B)	7 AL	43 O (0.4)	21 SI(0.5)	0.0
	(B)	7 AL	44 O (0.4)	22 SI(0.5)	0.0
	(B)	8 AL	45 O (0.4)	19 SI(0.5)	0.0
	(B)	8 AL	46 O (0.4)	20 SI(0.5)	0.0
	(B)	51 O	15 SI(0.0)	55 O (1.0)	0.0

	(B)	16 SI	52 O (0.0)	10 AL(1.0)	0.0
	(B)	53 O	17 SI(0.0)	57 O (1.0)	0.0
	(B)	54 O	18 SI(0.0)	58 O (1.0)	0.0
110	576.3712 (AU )				
	(S)	32 O	1 MG(0.8)	25 O (0.2)	0.0
	(S)	34 O	1 MG(0.8)	23 O (0.2)	0.0
	(S)	31 O	2 MG(0.8)	26 O (0.2)	0.0
	(S)	33 O	2 MG(0.8)	24 O (0.2)	0.0
	(S)	36 O	3 MG(0.8)	29 O (0.2)	0.0
	(S)	38 O	3 MG(0.8)	27 O (0.2)	0.0
	(S)	35 O	4 MG(0.8)	30 O (0.2)	0.0
	(S)	37 O	4 MG(0.8)	28 O (0.2)	0.0
	(B)	33 O	9 AL(0.3)	51 O (0.6)	0.0
	(B)	38 O	9 AL(0.3)	51 O (0.6)	0.0
	(B)	34 O	10 AL(0.3)	52 O (0.6)	0.0
	(B)	37 O	10 AL(0.3)	52 O (0.6)	0.0
	(B)	31 O	11 AL(0.3)	53 O (0.6)	0.0
	(B)	36 O	11 AL(0.3)	53 O (0.6)	0.0
	(B)	32 O	12 AL(0.3)	54 O (0.6)	0.0
	(B)	35 O	12 AL(0.3)	54 O (0.6)	0.0
111	581.0193 (B3U)				
	(B)	25 O	5 AL(0.1)	2 MG(0.9)	0.0
	(B)	26 O	5 AL(0.1)	1 MG(0.9)	0.0
	(B)	23 O	6 AL(0.1)	2 MG(0.9)	0.0
	(B)	24 O	6 AL(0.1)	1 MG(0.9)	0.0
	(B)	29 O	7 AL(0.1)	4 MG(0.9)	0.0
	(B)	30 O	7 AL(0.1)	3 MG(0.9)	0.0
	(B)	27 O	8 AL(0.1)	4 MG(0.9)	0.0
	(B)	28 O	8 AL(0.1)	3 MG(0.9)	0.0
	(B)	51 O	15 SI(0.1)	55 O (0.9)	0.0
	(B)	16 SI	52 O (0.1)	10 AL(0.9)	0.0
	(B)	53 O	17 SI(0.1)	57 O (0.9)	0.0
	(B)	54 O	18 SI(0.1)	58 O (0.9)	0.0
112	585.9221 (AG )				
	(S)	32 O	1 MG(0.9)		0.0
	(S)	34 O	1 MG(0.9)		0.0
	(S)	31 O	2 MG(0.9)		0.0
	(S)	33 O	2 MG(0.9)		0.0
	(S)	36 O	3 MG(0.9)		0.0
	(S)	38 O	3 MG(0.9)		0.0
	(S)	35 O	4 MG(0.9)		0.0
	(S)	37 O	4 MG(0.9)		0.0
113	601.1202 (B3U)				
	(S)	33 O	9 AL(0.6)	38 O (0.4)	0.0
	(S)	38 O	9 AL(0.6)	33 O (0.4)	0.0
	(S)	34 O	10 AL(0.6)	37 O (0.4)	0.0
	(S)	37 O	10 AL(0.6)	34 O (0.4)	0.0
	(S)	31 O	11 AL(0.6)	36 O (0.4)	0.0
	(S)	36 O	11 AL(0.6)	31 O (0.4)	0.0
	(S)	32 O	12 AL(0.6)	35 O (0.4)	0.0
	(S)	35 O	12 AL(0.6)	32 O (0.4)	0.0
114	602.6717 (B1G)				
	(S)	33 O	9 AL(0.5)	38 O (0.4)	0.0
	(S)	38 O	9 AL(0.5)	33 O (0.4)	0.0

	(S)	34 O	10 AL(0.5)	37 O (0.4)	0.0
	(S)	37 O	10 AL(0.5)	34 O (0.4)	0.0
	(S)	31 O	11 AL(0.5)	36 O (0.4)	0.0
	(S)	36 O	11 AL(0.5)	31 O (0.4)	0.0
	(S)	32 O	12 AL(0.5)	35 O (0.4)	0.0
	(S)	35 O	12 AL(0.5)	32 O (0.4)	0.0
115	621.9862 (AU)				
	(B)	33 O	9 AL(0.3)	51 O (0.7)	0.0
	(B)	38 O	9 AL(0.3)	51 O (0.7)	0.0
	(B)	34 O	10 AL(0.3)	52 O (0.7)	0.0
	(B)	37 O	10 AL(0.3)	52 O (0.7)	0.0
	(B)	31 O	11 AL(0.3)	53 O (0.7)	0.0
	(B)	36 O	11 AL(0.3)	53 O (0.7)	0.0
	(B)	32 O	12 AL(0.3)	54 O (0.7)	0.0
	(B)	35 O	12 AL(0.3)	54 O (0.7)	0.0
116	625.8584 (B1U)				
	(S)	33 O	9 AL(0.8)	38 O (0.1)	0.1
	(S)	38 O	9 AL(0.8)	33 O (0.1)	0.0
	(S)	34 O	10 AL(0.8)	37 O (0.1)	0.0
	(S)	37 O	10 AL(0.8)	34 O (0.1)	0.0
	(S)	31 O	11 AL(0.8)	36 O (0.1)	0.0
	(S)	36 O	11 AL(0.8)	31 O (0.1)	0.0
	(S)	32 O	12 AL(0.8)	35 O (0.1)	0.0
	(S)	35 O	12 AL(0.8)	32 O (0.1)	0.0
117	630.9981 (B3G)				
	(S)	33 O	9 AL(0.7)	38 O (0.3)	0.0
	(S)	38 O	9 AL(0.7)	33 O (0.3)	0.0
	(S)	34 O	10 AL(0.7)	37 O (0.3)	0.0
	(S)	37 O	10 AL(0.7)	34 O (0.3)	0.0
	(S)	31 O	11 AL(0.7)	36 O (0.3)	0.0
	(S)	36 O	11 AL(0.7)	31 O (0.3)	0.0
	(S)	32 O	12 AL(0.7)	35 O (0.3)	0.0
	(S)	35 O	12 AL(0.7)	32 O (0.3)	0.0
118	636.2483 (AG)				
	(S)	39 O	1 MG(0.8)	41 O (0.2)	0.0
	(S)	41 O	1 MG(0.8)	39 O (0.2)	-0.1
	(S)	40 O	2 MG(0.8)	42 O (0.2)	0.0
	(S)	42 O	2 MG(0.8)	40 O (0.2)	0.0
	(S)	43 O	3 MG(0.8)	45 O (0.2)	0.0
	(S)	45 O	3 MG(0.8)	43 O (0.2)	0.0
	(S)	44 O	4 MG(0.8)	46 O (0.2)	0.0
	(S)	46 O	4 MG(0.8)	44 O (0.2)	0.0
	(B)	51 O	15 SI(0.1)	55 O (0.9)	0.0
	(B)	16 SI	52 O (0.1)	10 AL(0.9)	0.0
	(B)	53 O	17 SI(0.1)	57 O (0.9)	0.0
	(B)	54 O	18 SI(0.1)	58 O (0.9)	0.0
	(B)	19 SI	42 O (0.3)	6 AL(0.7)	0.0
	(B)	19 SI	45 O (0.3)	8 AL(0.7)	0.0
	(B)	20 SI	41 O (0.3)	6 AL(0.7)	-0.1
	(B)	20 SI	46 O (0.3)	8 AL(0.7)	0.0
	(B)	21 SI	40 O (0.3)	5 AL(0.7)	0.0
	(B)	21 SI	43 O (0.3)	7 AL(0.7)	0.0
	(B)	22 SI	39 O (0.3)	5 AL(0.7)	0.0
	(B)	22 SI	44 O (0.3)	7 AL(0.7)	0.0

119 663.9417 (B3G)

(S)	25 O	5 AL(0.7)	26 O (0.2)	0.0
(S)	26 O	5 AL(0.7)	25 O (0.2)	0.0
(S)	23 O	6 AL(0.7)	24 O (0.2)	0.0
(S)	24 O	6 AL(0.7)	23 O (0.2)	0.0
(S)	29 O	7 AL(0.7)	30 O (0.2)	0.0
(S)	30 O	7 AL(0.7)	29 O (0.2)	0.0
(S)	27 O	8 AL(0.7)	28 O (0.2)	0.0
(S)	28 O	8 AL(0.7)	27 O (0.2)	0.0

120 671.8840 (B2G)

(S)	39 O	5 AL(0.6)	26 O (0.3)	0.0
(S)	40 O	5 AL(0.6)	25 O (0.3)	0.0
(S)	41 O	6 AL(0.6)	24 O (0.3)	0.0
(S)	42 O	6 AL(0.6)	23 O (0.3)	0.0
(S)	43 O	7 AL(0.6)	30 O (0.3)	0.0
(S)	44 O	7 AL(0.6)	29 O (0.3)	-0.1
(S)	45 O	8 AL(0.6)	28 O (0.3)	0.0
(S)	46 O	8 AL(0.6)	27 O (0.3)	0.0

121 672.8022 (B3U)

(S)	48 O	9 AL(0.7)	51 O (0.3)	0.0
(S)	47 O	10 AL(0.7)	52 O (0.3)	0.0
(S)	11 AL	50 O (0.7)	22 SI(0.3)	-0.1
(S)	12 AL	49 O (0.7)	21 SI(0.3)	0.0

122 688.4036 (AG )

(S)	48 O	9 AL(0.5)	51 O (0.5)	0.0
(S)	47 O	10 AL(0.5)	52 O (0.5)	0.0
(S)	11 AL	50 O (0.5)	22 SI(0.5)	0.0
(S)	12 AL	49 O (0.5)	21 SI(0.5)	0.0

123 690.3724 (B2U)

(S)	39 O	5 AL(0.9)		0.0
(S)	40 O	5 AL(0.9)		0.0
(S)	41 O	6 AL(0.9)		0.0
(S)	42 O	6 AL(0.9)		0.0
(S)	43 O	7 AL(0.9)		0.0
(S)	44 O	7 AL(0.9)		0.0
(S)	45 O	8 AL(0.9)		0.0
(S)	46 O	8 AL(0.9)		0.0
(O)	42 O	19 SI(0.1)	55 O (0.7)	0.0
(O)	45 O	19 SI(0.1)	55 O (0.7)	0.0
(B)	47 O	19 SI(0.1)	55 O (0.9)	0.0
(O)	41 O	20 SI(0.1)	56 O (0.7)	0.0
(O)	46 O	20 SI(0.1)	56 O (0.7)	0.0
(B)	48 O	20 SI(0.1)	56 O (0.9)	0.0
(O)	40 O	21 SI(0.1)	57 O (0.7)	-0.1
(O)	43 O	21 SI(0.1)	57 O (0.7)	0.0
(B)	21 SI	49 O (0.1)	12 AL(0.9)	0.0
(O)	39 O	22 SI(0.1)	58 O (0.7)	0.0
(O)	44 O	22 SI(0.1)	58 O (0.7)	0.0
(B)	22 SI	50 O (0.1)	11 AL(0.9)	0.0

124 705.3465 (B1G)

(B)	9 AL	33 O (0.1)	2 MG(0.9)	0.0
(B)	9 AL	38 O (0.1)	3 MG(0.9)	0.0
(S)	48 O	9 AL(1.0)		0.0
(B)	10 AL	34 O (0.1)	1 MG(0.9)	0.0



	(B)	10 AL	37 O (0.1)	4 MG(0.9)	0.0
	(S)	47 O	10 AL(1.0)		0.1
	(B)	11 AL	31 O (0.1)	2 MG(0.9)	0.0
	(B)	11 AL	36 O (0.1)	3 MG(0.9)	0.0
	(S)	50 O	11 AL(1.0)		-0.2
	(B)	12 AL	32 O (0.1)	1 MG(0.9)	0.0
	(B)	12 AL	35 O (0.1)	4 MG(0.9)	0.0
	(S)	49 O	12 AL(1.0)		0.1
125	706.7811 (AU)				
	(S)	25 O	5 AL(0.8)	26 O (0.2)	0.0
	(S)	26 O	5 AL(0.8)	25 O (0.2)	0.0
	(S)	39 O	5 AL(0.8)	40 O (0.2)	0.0
	(S)	40 O	5 AL(0.8)	39 O (0.2)	0.0
	(S)	23 O	6 AL(0.8)	24 O (0.2)	0.0
	(S)	24 O	6 AL(0.8)	23 O (0.2)	0.0
	(S)	41 O	6 AL(0.8)	42 O (0.2)	0.0
	(S)	42 O	6 AL(0.8)	41 O (0.2)	0.0
	(S)	29 O	7 AL(0.8)	30 O (0.2)	0.0
	(S)	30 O	7 AL(0.8)	29 O (0.2)	0.0
	(S)	43 O	7 AL(0.8)	44 O (0.2)	0.0
	(S)	44 O	7 AL(0.8)	43 O (0.2)	0.0
	(S)	27 O	8 AL(0.8)	28 O (0.2)	0.0
	(S)	28 O	8 AL(0.8)	27 O (0.2)	0.0
	(S)	45 O	8 AL(0.8)	46 O (0.2)	0.0
	(S)	46 O	8 AL(0.8)	45 O (0.2)	-0.1
126	711.8569 (B2U)				
	(S)	5 AL	25 O (0.6)	15 SI(0.4)	0.0
	(S)	5 AL	26 O (0.6)	16 SI(0.4)	0.0
	(S)	6 AL	23 O (0.6)	17 SI(0.4)	0.0
	(S)	6 AL	24 O (0.6)	18 SI(0.4)	0.0
	(S)	7 AL	29 O (0.6)	16 SI(0.4)	0.0
	(S)	7 AL	30 O (0.6)	15 SI(0.4)	0.0
	(S)	8 AL	27 O (0.6)	18 SI(0.4)	0.0
	(S)	8 AL	28 O (0.6)	17 SI(0.4)	0.0
	(S)	48 O	9 AL(0.9)		0.0
	(S)	47 O	10 AL(0.9)		0.0
	(S)	50 O	11 AL(0.9)		-0.1
	(S)	49 O	12 AL(0.9)		0.0
	(S)	19 SI	55 O (0.8)	15 SI(0.2)	0.0
	(S)	20 SI	56 O (0.8)	16 SI(0.2)	0.0
	(S)	21 SI	57 O (0.8)	17 SI(0.2)	0.0
	(S)	22 SI	58 O (0.8)	18 SI(0.2)	0.0
127	716.9671 (B1U)				
	(S)	25 O	5 AL(0.7)	26 O (0.2)	0.0
	(S)	26 O	5 AL(0.7)	25 O (0.2)	0.0
	(S)	39 O	5 AL(0.7)	40 O (0.2)	0.0
	(S)	40 O	5 AL(0.7)	39 O (0.2)	0.0
	(S)	23 O	6 AL(0.7)	24 O (0.2)	0.0
	(S)	24 O	6 AL(0.7)	23 O (0.2)	0.0
	(S)	41 O	6 AL(0.7)	42 O (0.2)	0.0
	(S)	42 O	6 AL(0.7)	41 O (0.2)	0.0
	(S)	29 O	7 AL(0.7)	30 O (0.2)	0.0
	(S)	30 O	7 AL(0.7)	29 O (0.2)	0.0
	(S)	43 O	7 AL(0.7)	44 O (0.2)	0.0

	(S)	44 O	7 AL(0.7)	43 O (0.2)	0.0
	(S)	27 O	8 AL(0.7)	28 O (0.2)	0.0
	(S)	28 O	8 AL(0.7)	27 O (0.2)	0.0
	(S)	45 O	8 AL(0.7)	46 O (0.2)	0.0
	(S)	46 O	8 AL(0.7)	45 O (0.2)	-0.1
128	728.3854	(AG )			
	(S)	48 O	9 AL(0.9)		0.0
	(S)	47 O	10 AL(0.9)		0.1
	(S)	50 O	11 AL(0.9)		-0.1
	(S)	49 O	12 AL(0.9)		0.1
	(B)	25 O	15 SI(0.0)	51 O (0.9)	0.0
	(B)	30 O	15 SI(0.0)	51 O (0.9)	0.0
	(B)	26 O	16 SI(0.0)	52 O (0.9)	0.0
	(B)	29 O	16 SI(0.0)	52 O (0.9)	0.0
	(B)	23 O	17 SI(0.0)	53 O (0.9)	0.0
	(B)	28 O	17 SI(0.0)	53 O (0.9)	0.0
	(B)	24 O	18 SI(0.0)	54 O (0.9)	0.0
	(B)	27 O	18 SI(0.0)	54 O (0.9)	0.0
129	737.0089	(B1G)			
	(B)	15 SI	25 O (0.1)	1 MG(0.9)	0.0
	(B)	15 SI	30 O (0.1)	4 MG(0.9)	0.0
	(B)	16 SI	26 O (0.1)	2 MG(0.9)	0.0
	(B)	16 SI	29 O (0.1)	3 MG(0.9)	0.0
	(B)	17 SI	23 O (0.1)	1 MG(0.9)	0.0
	(B)	17 SI	28 O (0.1)	4 MG(0.9)	0.0
	(B)	18 SI	24 O (0.1)	2 MG(0.9)	0.0
	(B)	18 SI	27 O (0.1)	3 MG(0.9)	0.0
130	741.9026	(AG )			
	(B)	25 O	15 SI(0.0)	55 O (0.9)	0.0
	(B)	30 O	15 SI(0.0)	55 O (0.9)	0.0
	(B)	26 O	16 SI(0.0)	56 O (0.9)	0.0
	(B)	29 O	16 SI(0.0)	56 O (0.9)	0.0
	(B)	23 O	17 SI(0.0)	57 O (0.9)	0.0
	(B)	28 O	17 SI(0.0)	57 O (0.9)	0.0
	(B)	24 O	18 SI(0.0)	58 O (0.9)	0.0
	(B)	27 O	18 SI(0.0)	58 O (0.9)	0.0
	(B)	19 SI	42 O (0.0)	2 MG(1.0)	-0.1
	(B)	19 SI	45 O (0.0)	3 MG(1.0)	0.0
	(B)	20 SI	41 O (0.0)	1 MG(1.0)	-0.1
	(B)	20 SI	46 O (0.0)	4 MG(1.0)	0.0
	(B)	21 SI	40 O (0.0)	2 MG(1.0)	0.0
	(B)	21 SI	43 O (0.0)	3 MG(1.0)	0.0
	(B)	22 SI	39 O (0.0)	1 MG(1.0)	0.0
	(B)	22 SI	44 O (0.0)	4 MG(1.0)	0.0
131	755.6839	(B3G)			
	(B)	25 O	5 AL(0.4)	39 O (0.6)	0.0
	(B)	26 O	5 AL(0.4)	40 O (0.6)	0.0
	(S)	5 AL	39 O (0.6)	22 SI(0.4)	0.0
	(S)	5 AL	40 O (0.6)	21 SI(0.4)	0.0
	(B)	23 O	6 AL(0.4)	41 O (0.6)	0.0
	(B)	24 O	6 AL(0.4)	42 O (0.6)	0.0
	(S)	6 AL	41 O (0.6)	20 SI(0.4)	0.0
	(S)	6 AL	42 O (0.6)	19 SI(0.4)	-0.1
	(B)	29 O	7 AL(0.4)	43 O (0.6)	0.0

	(B)	30 O	7 AL(0.4)	44 O (0.6)	0.0
	(S)	7 AL	43 O (0.6)	21 SI(0.4)	0.1
	(S)	7 AL	44 O (0.6)	22 SI(0.4)	-0.1
	(B)	27 O	8 AL(0.4)	45 O (0.6)	0.0
	(B)	28 O	8 AL(0.4)	46 O (0.6)	0.0
	(S)	8 AL	45 O (0.6)	19 SI(0.4)	0.0
	(S)	8 AL	46 O (0.6)	20 SI(0.4)	-0.1
132	759.7064	(B1G)			
	(B)	42 O	19 SI(0.1)	55 O (0.9)	-0.1
	(B)	45 O	19 SI(0.1)	55 O (0.9)	0.0
	(B)	41 O	20 SI(0.1)	56 O (0.9)	-0.1
	(B)	46 O	20 SI(0.1)	56 O (0.9)	0.0
	(B)	40 O	21 SI(0.1)	57 O (0.9)	0.0
	(B)	43 O	21 SI(0.1)	57 O (0.9)	0.0
	(B)	39 O	22 SI(0.1)	58 O (0.9)	0.0
	(B)	44 O	22 SI(0.1)	58 O (0.9)	0.0
133	761.9336	(B3U)			
	(B)	15 SI	25 O (0.0)	1 MG(0.9)	0.0
	(B)	15 SI	30 O (0.0)	4 MG(0.9)	0.0
	(B)	16 SI	26 O (0.0)	2 MG(0.9)	0.0
	(B)	16 SI	29 O (0.0)	3 MG(0.9)	0.0
	(B)	17 SI	23 O (0.0)	1 MG(0.9)	0.0
	(B)	17 SI	28 O (0.0)	4 MG(0.9)	0.0
	(B)	18 SI	24 O (0.0)	2 MG(0.9)	0.0
	(B)	18 SI	27 O (0.0)	3 MG(0.9)	0.0
134	770.2159	(B2G)			
	(S)	5 AL	25 O (0.7)	15 SI(0.3)	0.0
	(S)	5 AL	26 O (0.7)	16 SI(0.3)	0.0
	(S)	6 AL	23 O (0.7)	17 SI(0.3)	0.0
	(S)	6 AL	24 O (0.7)	18 SI(0.3)	0.0
	(S)	7 AL	29 O (0.7)	16 SI(0.3)	0.0
	(S)	7 AL	30 O (0.7)	15 SI(0.3)	0.0
	(S)	8 AL	27 O (0.7)	18 SI(0.3)	0.0
	(S)	8 AL	28 O (0.7)	17 SI(0.3)	0.0
	(B)	31 O	13 SI(0.1)	33 O (0.9)	0.0
	(B)	13 SI	32 O (0.1)	1 MG(0.9)	0.0
	(B)	33 O	13 SI(0.1)	31 O (0.9)	0.0
	(B)	34 O	13 SI(0.1)	32 O (0.9)	0.0
	(B)	35 O	14 SI(0.1)	37 O (0.9)	0.0
	(B)	36 O	14 SI(0.1)	38 O (0.9)	0.0
	(B)	37 O	14 SI(0.1)	35 O (0.9)	0.0
	(B)	14 SI	38 O (0.1)	3 MG(0.9)	0.0
135	778.4303	(B2U)			
	(B)	31 O	13 SI(0.1)	33 O (0.9)	0.0
	(B)	13 SI	32 O (0.1)	1 MG(0.9)	0.0
	(B)	33 O	13 SI(0.1)	31 O (0.9)	0.0
	(B)	13 SI	34 O (0.1)	1 MG(0.9)	0.0
	(B)	14 SI	35 O (0.1)	4 MG(0.9)	0.0
	(B)	36 O	14 SI(0.1)	38 O (0.9)	0.0
	(B)	37 O	14 SI(0.1)	35 O (0.9)	0.0
	(B)	14 SI	38 O (0.1)	3 MG(0.9)	0.0
136	783.8259	(B3U)			
	(B)	39 O	5 AL(0.4)	2 MG(0.6)	0.0
	(B)	40 O	5 AL(0.4)	1 MG(0.6)	0.0

(B)	41 O	6 AL(0.4)	2 MG(0.6)	0.0
(B)	42 O	6 AL(0.4)	1 MG(0.6)	-0.1
(B)	43 O	7 AL(0.4)	4 MG(0.6)	0.1
(B)	44 O	7 AL(0.4)	3 MG(0.6)	-0.1
(B)	45 O	8 AL(0.4)	4 MG(0.6)	0.0
(B)	46 O	8 AL(0.4)	3 MG(0.6)	-0.1
(B)	42 O	19 SI(0.1)	55 O (0.9)	-0.1
(B)	45 O	19 SI(0.1)	55 O (0.9)	0.0
(B)	41 O	20 SI(0.1)	56 O (0.9)	-0.1
(B)	46 O	20 SI(0.1)	56 O (0.9)	0.1
(B)	40 O	21 SI(0.1)	57 O (0.9)	0.0
(B)	43 O	21 SI(0.1)	57 O (0.9)	0.0
(B)	39 O	22 SI(0.1)	58 O (0.9)	0.0
(B)	44 O	22 SI(0.1)	58 O (0.9)	0.0

137 816.8635 (B2G)

(S)	5 AL	25 O (0.6)	15 SI(0.4)	0.0
(S)	5 AL	26 O (0.6)	16 SI(0.4)	0.0
(S)	5 AL	39 O (0.6)	22 SI(0.4)	0.0
(S)	5 AL	40 O (0.6)	21 SI(0.4)	0.0
(S)	6 AL	23 O (0.6)	17 SI(0.4)	0.0
(S)	6 AL	24 O (0.6)	18 SI(0.4)	0.0
(S)	6 AL	41 O (0.6)	20 SI(0.4)	0.0
(S)	6 AL	42 O (0.6)	19 SI(0.4)	-0.1
(S)	7 AL	29 O (0.6)	16 SI(0.4)	0.0
(S)	7 AL	30 O (0.6)	15 SI(0.4)	0.0
(S)	7 AL	43 O (0.6)	21 SI(0.4)	0.0
(S)	7 AL	44 O (0.6)	22 SI(0.4)	0.0
(S)	8 AL	27 O (0.6)	18 SI(0.4)	0.0
(S)	8 AL	28 O (0.6)	17 SI(0.4)	0.0
(S)	8 AL	45 O (0.6)	19 SI(0.4)	0.0
(S)	8 AL	46 O (0.6)	20 SI(0.4)	-0.1
(B)	13 SI	31 O (0.0)	11 AL(1.0)	0.0
(B)	13 SI	32 O (0.0)	12 AL(1.0)	0.0
(B)	13 SI	33 O (0.0)	9 AL(1.0)	0.0
(B)	13 SI	34 O (0.0)	10 AL(1.0)	0.0
(B)	14 SI	35 O (0.0)	12 AL(1.0)	0.0
(B)	14 SI	36 O (0.0)	11 AL(1.0)	0.0
(B)	14 SI	37 O (0.0)	10 AL(1.0)	0.0
(B)	14 SI	38 O (0.0)	9 AL(1.0)	0.0

138 846.2795 (B2U)

(B)	25 O	5 AL(0.3)	39 O (0.7)	0.0
(B)	26 O	5 AL(0.3)	40 O (0.7)	0.0
(B)	39 O	5 AL(0.3)	2 MG(0.7)	0.0
(B)	40 O	5 AL(0.3)	1 MG(0.7)	0.0
(B)	23 O	6 AL(0.3)	41 O (0.7)	0.0
(B)	24 O	6 AL(0.3)	42 O (0.7)	0.0
(B)	41 O	6 AL(0.3)	2 MG(0.7)	0.0
(B)	42 O	6 AL(0.3)	1 MG(0.7)	0.0
(B)	29 O	7 AL(0.3)	43 O (0.7)	0.0
(B)	30 O	7 AL(0.3)	44 O (0.7)	0.0
(B)	43 O	7 AL(0.3)	4 MG(0.7)	0.0
(B)	44 O	7 AL(0.3)	3 MG(0.7)	0.0
(B)	27 O	8 AL(0.3)	45 O (0.7)	0.0
(B)	28 O	8 AL(0.3)	46 O (0.7)	0.0

	(B) 45 O	8 AL(0.3)	4 MG(0.7)	0.0
	(B) 46 O	8 AL(0.3)	3 MG(0.7)	-0.1
139	902.1617 (B3G)			
	(S) 25 O	15 SI(0.9)		0.0
	(S) 30 O	15 SI(0.9)		0.0
	(S) 26 O	16 SI(0.9)		0.0
	(S) 29 O	16 SI(0.9)		0.0
	(S) 23 O	17 SI(0.9)		0.0
	(S) 28 O	17 SI(0.9)		0.0
	(S) 24 O	18 SI(0.9)		0.0
	(S) 27 O	18 SI(0.9)		0.0
	(S) 42 O	19 SI(0.9)		-0.1
	(S) 45 O	19 SI(0.9)		-0.1
	(S) 41 O	20 SI(0.9)		-0.1
	(S) 46 O	20 SI(0.9)		0.0
	(S) 40 O	21 SI(0.9)		-0.1
	(S) 43 O	21 SI(0.9)		-0.1
	(S) 39 O	22 SI(0.9)		-0.1
	(S) 44 O	22 SI(0.9)		-0.1
140	906.2879 (B2G)			
	(S) 25 O	15 SI(0.9)		0.0
	(S) 30 O	15 SI(0.9)		0.0
	(S) 26 O	16 SI(0.9)		0.0
	(S) 29 O	16 SI(0.9)		0.0
	(S) 23 O	17 SI(0.9)		0.0
	(S) 28 O	17 SI(0.9)		0.0
	(S) 24 O	18 SI(0.9)		0.0
	(S) 27 O	18 SI(0.9)		0.0
	(S) 42 O	19 SI(0.9)		-0.1
	(S) 45 O	19 SI(0.9)		-0.1
	(S) 41 O	20 SI(0.9)		-0.1
	(S) 46 O	20 SI(0.9)		0.0
	(S) 40 O	21 SI(0.9)		-0.1
	(S) 43 O	21 SI(0.9)		-0.1
	(S) 39 O	22 SI(0.9)		-0.1
	(S) 44 O	22 SI(0.9)		-0.1
141	908.8577 (B1U)			
	(S) 25 O	15 SI(0.9)		0.0
	(S) 30 O	15 SI(0.9)		0.0
	(S) 26 O	16 SI(0.9)		0.0
	(S) 29 O	16 SI(0.9)		0.0
	(S) 23 O	17 SI(0.9)		0.0
	(S) 28 O	17 SI(0.9)		0.0
	(S) 24 O	18 SI(0.9)		0.0
	(S) 27 O	18 SI(0.9)		0.0
	(S) 42 O	19 SI(0.9)		-0.1
	(S) 45 O	19 SI(0.9)		-0.1
	(S) 41 O	20 SI(0.9)		0.0
	(S) 46 O	20 SI(0.9)		0.0
	(S) 40 O	21 SI(0.9)		0.0
	(S) 43 O	21 SI(0.9)		-0.1
	(S) 39 O	22 SI(0.9)		-0.1
	(S) 44 O	22 SI(0.9)		-0.1
142	909.3702 (B3G)			

(S)	31 O	13 SI(0.7)	34 O (0.3)	0.0
(S)	32 O	13 SI(0.7)	33 O (0.3)	0.0
(S)	33 O	13 SI(0.7)	32 O (0.3)	0.0
(S)	34 O	13 SI(0.7)	31 O (0.3)	0.0
(S)	35 O	14 SI(0.7)	38 O (0.3)	0.0
(S)	36 O	14 SI(0.7)	37 O (0.3)	0.0
(S)	37 O	14 SI(0.7)	36 O (0.3)	0.0
(S)	38 O	14 SI(0.7)	35 O (0.3)	0.0
143	910.1619 (AU)			
(S)	25 O	15 SI(0.9)		0.0
(S)	30 O	15 SI(0.9)		0.0
(S)	26 O	16 SI(0.9)		0.0
(S)	29 O	16 SI(0.9)		0.0
(S)	23 O	17 SI(0.9)		0.0
(S)	28 O	17 SI(0.9)		0.0
(S)	24 O	18 SI(0.9)		0.0
(S)	27 O	18 SI(0.9)		0.0
(S)	42 O	19 SI(0.9)		-0.1
(S)	45 O	19 SI(0.9)		-0.1
(S)	41 O	20 SI(0.9)		0.0
(S)	46 O	20 SI(0.9)		0.0
(S)	40 O	21 SI(0.9)		-0.1
(S)	43 O	21 SI(0.9)		-0.1
(S)	39 O	22 SI(0.9)		-0.1
(S)	44 O	22 SI(0.9)		-0.1
144	915.1047 (B3U)			
(S)	25 O	5 AL(0.5)	39 O (0.4)	0.0
(S)	26 O	5 AL(0.5)	40 O (0.4)	0.0
(S)	39 O	5 AL(0.7)	2 MG(0.2)	0.0
(S)	40 O	5 AL(0.7)	1 MG(0.2)	0.0
(S)	23 O	6 AL(0.5)	41 O (0.4)	0.0
(S)	24 O	6 AL(0.5)	42 O (0.4)	0.0
(S)	41 O	6 AL(0.7)	2 MG(0.2)	0.0
(S)	42 O	6 AL(0.7)	1 MG(0.2)	0.0
(S)	29 O	7 AL(0.5)	43 O (0.4)	0.0
(S)	30 O	7 AL(0.5)	44 O (0.4)	0.0
(S)	43 O	7 AL(0.7)	4 MG(0.2)	-0.1
(S)	44 O	7 AL(0.7)	3 MG(0.2)	0.0
(S)	27 O	8 AL(0.5)	45 O (0.4)	0.0
(S)	28 O	8 AL(0.5)	46 O (0.4)	0.0
(S)	45 O	8 AL(0.7)	4 MG(0.2)	0.0
(S)	46 O	8 AL(0.7)	3 MG(0.2)	0.0
(S)	25 O	15 SI(0.9)		0.0
(S)	30 O	15 SI(0.9)		0.0
(S)	26 O	16 SI(0.9)		0.0
(S)	29 O	16 SI(0.9)		0.0
(S)	23 O	17 SI(0.9)		0.0
(S)	28 O	17 SI(0.9)		0.0
(S)	24 O	18 SI(0.9)		0.0
(S)	27 O	18 SI(0.9)		0.0
(S)	42 O	19 SI(0.8)	47 O (0.2)	0.0
(S)	45 O	19 SI(0.8)	47 O (0.2)	-0.1
(S)	41 O	20 SI(0.8)	48 O (0.2)	0.0
(S)	46 O	20 SI(0.8)	48 O (0.2)	0.0

	(S)	40 O	21 SI(0.8)	49 O (0.2)	0.0
	(S)	43 O	21 SI(0.8)	49 O (0.2)	-0.1
	(S)	39 O	22 SI(0.8)	50 O (0.2)	-0.1
	(S)	44 O	22 SI(0.8)	50 O (0.2)	0.0
145	931.1252 (AG )				
	(S)	5 AL	25 O (0.5)	15 SI(0.4)	0.0
	(S)	5 AL	26 O (0.5)	16 SI(0.4)	0.0
	(S)	5 AL	39 O (0.7)	22 SI(0.3)	0.0
	(S)	5 AL	40 O (0.7)	21 SI(0.3)	0.0
	(S)	6 AL	23 O (0.5)	17 SI(0.4)	0.0
	(S)	6 AL	24 O (0.5)	18 SI(0.4)	0.0
	(S)	6 AL	41 O (0.7)	20 SI(0.3)	0.0
	(S)	6 AL	42 O (0.7)	19 SI(0.3)	0.0
	(S)	7 AL	29 O (0.5)	16 SI(0.4)	0.0
	(S)	7 AL	30 O (0.5)	15 SI(0.4)	0.0
	(S)	7 AL	43 O (0.7)	21 SI(0.3)	-0.1
	(S)	7 AL	44 O (0.7)	22 SI(0.3)	0.0
	(S)	8 AL	27 O (0.5)	18 SI(0.4)	0.0
	(S)	8 AL	28 O (0.5)	17 SI(0.4)	0.0
	(S)	8 AL	45 O (0.7)	19 SI(0.3)	0.0
	(S)	8 AL	46 O (0.7)	20 SI(0.3)	0.0
	(S)	25 O	15 SI(0.9)		0.0
	(S)	30 O	15 SI(0.9)		0.0
	(S)	26 O	16 SI(0.9)		0.0
	(S)	29 O	16 SI(0.9)		0.0
	(S)	23 O	17 SI(0.9)		0.0
	(S)	28 O	17 SI(0.9)		0.0
	(S)	24 O	18 SI(0.9)		0.0
	(S)	27 O	18 SI(0.9)		0.0
146	945.1382 (B1U)				
	(S)	31 O	13 SI(0.7)	32 O (0.3)	0.1
	(S)	32 O	13 SI(0.7)	31 O (0.3)	0.0
	(S)	33 O	13 SI(0.7)	34 O (0.3)	0.1
	(S)	34 O	13 SI(0.7)	33 O (0.3)	0.0
	(S)	35 O	14 SI(0.7)	36 O (0.3)	0.0
	(S)	36 O	14 SI(0.7)	35 O (0.3)	0.0
	(S)	37 O	14 SI(0.7)	38 O (0.3)	0.0
	(S)	38 O	14 SI(0.7)	37 O (0.3)	0.0
147	963.5452 (B1G)				
	(S)	31 O	13 SI(0.7)	32 O (0.3)	0.0
	(S)	32 O	13 SI(0.7)	31 O (0.3)	0.0
	(S)	33 O	13 SI(0.7)	34 O (0.3)	0.0
	(S)	34 O	13 SI(0.7)	33 O (0.3)	0.0
	(S)	35 O	14 SI(0.7)	36 O (0.3)	0.0
	(S)	36 O	14 SI(0.7)	35 O (0.3)	0.0
	(S)	37 O	14 SI(0.7)	38 O (0.3)	0.0
	(S)	38 O	14 SI(0.7)	37 O (0.3)	0.0
	(S)	42 O	19 SI(0.9)		0.0
	(S)	45 O	19 SI(0.9)		-0.1
	(S)	41 O	20 SI(0.9)		0.0
	(S)	46 O	20 SI(0.9)		0.1
	(S)	40 O	21 SI(0.9)		0.0
	(S)	43 O	21 SI(0.9)		-0.1
	(S)	39 O	22 SI(0.9)		-0.1

	(S)	44 O	22 SI(0.9)	0.0
148	964.7716	(B3U)		
	(S)	31 O	13 SI(0.7) 34 O (0.3)	0.0
	(S)	32 O	13 SI(0.7) 33 O (0.3)	0.0
	(S)	33 O	13 SI(0.7) 32 O (0.3)	0.0
	(S)	34 O	13 SI(0.7) 31 O (0.3)	0.0
	(S)	35 O	14 SI(0.7) 38 O (0.3)	0.0
	(S)	36 O	14 SI(0.7) 37 O (0.3)	0.0
	(S)	37 O	14 SI(0.7) 36 O (0.3)	0.0
	(S)	38 O	14 SI(0.7) 35 O (0.3)	0.0
149	970.3805	(B2U)		
	(S)	25 O	15 SI(0.8) 30 O (0.1)	0.0
	(S)	30 O	15 SI(0.8) 25 O (0.1)	0.0
	(S)	26 O	16 SI(0.8) 29 O (0.1)	0.0
	(S)	29 O	16 SI(0.8) 26 O (0.1)	0.0
	(S)	23 O	17 SI(0.8) 28 O (0.1)	0.0
	(S)	28 O	17 SI(0.8) 23 O (0.1)	0.0
	(S)	24 O	18 SI(0.8) 27 O (0.1)	0.0
	(S)	27 O	18 SI(0.8) 24 O (0.1)	0.0
	(S)	42 O	19 SI(0.8) 45 O (0.1)	0.0
	(S)	45 O	19 SI(0.8) 42 O (0.1)	-0.1
	(S)	41 O	20 SI(0.8) 46 O (0.1)	0.0
	(S)	46 O	20 SI(0.8) 41 O (0.1)	0.1
	(S)	40 O	21 SI(0.8) 43 O (0.1)	0.0
	(S)	43 O	21 SI(0.8) 40 O (0.1)	-0.1
	(S)	39 O	22 SI(0.8) 44 O (0.1)	-0.1
	(S)	44 O	22 SI(0.8) 39 O (0.1)	0.0
150	977.5961	(B3G)		
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	-0.1
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	-0.1
	(S)	46 O	20 SI(0.9)	0.0
	(S)	40 O	21 SI(0.9)	-0.1
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	-0.1
151	979.1124	(B2U)		
	(S)	39 O	5 AL(1.0)	0.0
	(S)	40 O	5 AL(1.0)	0.0
	(S)	41 O	6 AL(1.0)	0.0
	(S)	42 O	6 AL(1.0)	0.0
	(S)	43 O	7 AL(1.0)	0.0
	(S)	44 O	7 AL(1.0)	0.0
	(S)	45 O	8 AL(1.0)	0.0
	(S)	46 O	8 AL(1.0)	0.0
	(S)	25 O	15 SI(0.9)	0.0



	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	0.0
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	0.0
	(S)	46 O	20 SI(0.9)	0.1
	(S)	40 O	21 SI(0.9)	0.0
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	0.0
152	984.4347 (AU )			
	(S)	33 O	9 AL(0.9)	0.0
	(S)	38 O	9 AL(0.9)	0.0
	(S)	34 O	10 AL(0.9)	0.0
	(S)	37 O	10 AL(0.9)	0.0
	(S)	31 O	11 AL(0.9)	0.1
	(S)	36 O	11 AL(0.9)	0.0
	(S)	32 O	12 AL(0.9)	0.0
	(S)	35 O	12 AL(0.9)	0.1
153	987.8548 (AG )			
	(S)	33 O	9 AL(0.8) 51 O (0.2)	0.0
	(S)	38 O	9 AL(0.8) 51 O (0.2)	0.0
	(S)	34 O	10 AL(0.8) 52 O (0.2)	0.0
	(S)	37 O	10 AL(0.8) 52 O (0.2)	0.0
	(S)	31 O	11 AL(0.8) 53 O (0.2)	0.1
	(S)	36 O	11 AL(0.8) 53 O (0.2)	0.0
	(S)	32 O	12 AL(0.8) 54 O (0.2)	0.0
	(S)	35 O	12 AL(0.8) 54 O (0.2)	0.1
154	987.8705 (B2G)			
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	-0.1
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	0.0
	(S)	46 O	20 SI(0.9)	0.0
	(S)	40 O	21 SI(0.9)	0.0
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	0.0
155	988.6330 (B1G)			
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0

	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
156	1014.8141	(AG )		
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	0.0
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	0.0
	(S)	46 O	20 SI(0.9)	0.1
	(S)	40 O	21 SI(0.9)	0.0
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	0.0
157	1015.1952	(B2G)		
	(S)	31 O	13 SI(0.9)	0.1
	(S)	32 O	13 SI(0.9)	0.0
	(S)	33 O	13 SI(0.9)	0.0
	(S)	34 O	13 SI(0.9)	0.0
	(S)	35 O	14 SI(0.9)	0.0
	(S)	36 O	14 SI(0.9)	0.0
	(S)	37 O	14 SI(0.9)	0.0
	(S)	38 O	14 SI(0.9)	0.0
158	1015.2143	(B3U)		
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	0.0
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	0.0
	(S)	46 O	20 SI(0.9)	0.1
	(S)	40 O	21 SI(0.9)	0.0
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	0.0
159	1025.0226	(B1U)		
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0

	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	-0.1
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	-0.1
	(S)	46 O	20 SI(0.9)	0.0
	(S)	40 O	21 SI(0.9)	-0.1
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	-0.1
160	1035.9359	(B1G)		
	(S)	31 O	13 SI(0.6) 32 O (0.4)	0.0
	(S)	32 O	13 SI(0.6) 31 O (0.4)	0.0
	(S)	33 O	13 SI(0.6) 34 O (0.4)	0.0
	(S)	34 O	13 SI(0.6) 33 O (0.4)	0.0
	(S)	35 O	14 SI(0.6) 36 O (0.4)	0.0
	(S)	36 O	14 SI(0.6) 35 O (0.4)	0.0
	(S)	37 O	14 SI(0.6) 38 O (0.4)	0.0
	(S)	38 O	14 SI(0.6) 37 O (0.4)	0.0
161	1047.9539	(B2U)		
	(S)	31 O	13 SI(0.9)	0.1
	(S)	32 O	13 SI(0.9)	0.0
	(S)	33 O	13 SI(0.9)	0.0
	(S)	34 O	13 SI(0.9)	0.0
	(S)	35 O	14 SI(0.9)	0.0
	(S)	36 O	14 SI(0.9)	0.0
	(S)	37 O	14 SI(0.9)	0.0
	(S)	38 O	14 SI(0.9)	0.0
162	1071.3151	(AU )		
	(S)	25 O	15 SI(0.9)	0.0
	(S)	30 O	15 SI(0.9)	0.0
	(S)	26 O	16 SI(0.9)	0.0
	(S)	29 O	16 SI(0.9)	0.0
	(S)	23 O	17 SI(0.9)	0.0
	(S)	28 O	17 SI(0.9)	0.0
	(S)	24 O	18 SI(0.9)	0.0
	(S)	27 O	18 SI(0.9)	0.0
	(S)	42 O	19 SI(0.9)	-0.1
	(S)	45 O	19 SI(0.9)	-0.1
	(S)	41 O	20 SI(0.9)	-0.1
	(S)	46 O	20 SI(0.9)	0.0
	(S)	40 O	21 SI(0.9)	-0.1
	(S)	43 O	21 SI(0.9)	-0.1
	(S)	39 O	22 SI(0.9)	-0.1
	(S)	44 O	22 SI(0.9)	-0.1
163	1128.9554	(AG )		
	(S)	51 O	15 SI(1.0)	0.0
	(S)	52 O	16 SI(1.0)	0.0
	(S)	53 O	17 SI(1.0)	0.0
	(S)	54 O	18 SI(1.0)	0.0
164	1130.7386	(B1G)		
	(S)	51 O	15 SI(1.0)	0.0
	(S)	52 O	16 SI(1.0)	0.0

	(S) 53 O	17 SI(1.0)	0.0
	(S) 54 O	18 SI(1.0)	0.0
165	1149.6359 (B3U)		
	(S) 51 O	9 AL(1.0)	0.0
	(S) 52 O	10 AL(1.0)	0.0
	(S) 53 O	11 AL(1.0)	0.1
	(S) 54 O	12 AL(1.0)	0.1
	(S) 51 O	15 SI(1.0)	0.0
	(S) 52 O	16 SI(1.0)	0.0
	(S) 53 O	17 SI(1.0)	0.0
	(S) 54 O	18 SI(1.0)	0.0
166	1156.6356 (B2U)		
	(S) 51 O	15 SI(1.0)	0.0
	(S) 52 O	16 SI(1.0)	0.0
	(S) 53 O	17 SI(1.0)	0.0
	(S) 54 O	18 SI(1.0)	0.0
167	1170.0097 (B3U)		
	(S) 55 O	15 SI(1.0)	0.0
	(S) 56 O	16 SI(1.0)	0.0
	(S) 57 O	17 SI(1.0)	0.0
	(S) 58 O	18 SI(1.0)	0.0
168	1175.5552 (B2U)		
	(S) 55 O	15 SI(1.0)	0.0
	(S) 56 O	16 SI(1.0)	0.0
	(S) 57 O	17 SI(1.0)	0.0
	(S) 58 O	18 SI(1.0)	0.0
	(S) 55 O	19 SI(1.0)	0.0
	(S) 56 O	20 SI(1.0)	0.0
	(S) 57 O	21 SI(1.0)	0.0
	(S) 58 O	22 SI(1.0)	0.0
169	1176.1336 (B1G)		
	(S) 55 O	15 SI(1.0)	0.0
	(S) 56 O	16 SI(1.0)	0.0
	(S) 57 O	17 SI(1.0)	0.0
	(S) 58 O	18 SI(1.0)	0.0
	(S) 55 O	19 SI(1.0)	0.0
	(S) 56 O	20 SI(1.0)	0.0
	(S) 57 O	21 SI(1.0)	0.0
	(S) 58 O	22 SI(1.0)	0.0
170	1176.7623 (AG )		
	(S) 55 O	15 SI(1.0)	0.0
	(S) 56 O	16 SI(1.0)	0.0
	(S) 57 O	17 SI(1.0)	0.0
	(S) 58 O	18 SI(1.0)	0.0
	(S) 55 O	19 SI(1.0)	0.0
	(S) 56 O	20 SI(1.0)	0.0
	(S) 57 O	21 SI(1.0)	0.0
	(S) 58 O	22 SI(1.0)	0.0
171	1190.9563 (B3U)		
	(S) 47 O	19 SI(1.0)	0.1
	(S) 48 O	20 SI(1.0)	-0.2
	(S) 49 O	21 SI(1.0)	0.1
	(S) 50 O	22 SI(1.0)	0.0
172	1194.9448 (B2U)		

	(S)	47 O	19 SI(1.0)	0.2
	(S)	48 O	20 SI(1.0)	-0.2
	(S)	49 O	21 SI(1.0)	0.2
	(S)	50 O	22 SI(1.0)	0.0
173	1209.8635 (AG )			
	(S)	47 O	19 SI(1.0)	0.2
	(S)	48 O	20 SI(1.0)	-0.2
	(S)	49 O	21 SI(1.0)	0.2
	(S)	50 O	22 SI(1.0)	0.0
174	1212.6108 (B1G)			
	(S)	47 O	19 SI(1.0)	0.2
	(S)	48 O	20 SI(1.0)	-0.2
	(S)	49 O	21 SI(1.0)	0.2
	(S)	50 O	22 SI(1.0)	0.0

# NORMAL MODES NORMALIZED TO CLASSICAL AMPLITUDES

FREQ(CM\*\*-1)   -2.66   -2.37   -1.60   94.41   99.18   113.78

AT. 1	MG X	0.0000	0.2087	0.0000	-0.0082	0.0000	0.0000
	Y	0.1955	0.0000	-0.0004	0.0000	-0.0118	0.0013
	Z	-0.0007	0.0000	0.2531	0.0000	0.0019	0.0018
AT. 2	MG X	0.0000	0.2087	0.0000	-0.0082	0.0000	0.0000
	Y	0.1955	0.0000	0.0004	0.0000	-0.0118	-0.0013
	Z	0.0007	0.0000	0.2531	0.0000	-0.0019	0.0018
AT. 3	MG X	0.0000	0.2087	0.0000	0.0082	0.0000	0.0000
	Y	0.1955	0.0000	-0.0004	0.0000	0.0118	0.0013
	Z	-0.0007	0.0000	0.2531	0.0000	-0.0019	0.0018
AT. 4	MG X	0.0000	0.2087	0.0000	0.0082	0.0000	0.0000
	Y	0.1955	0.0000	0.0004	0.0000	0.0118	-0.0013
	Z	0.0007	0.0000	0.2531	0.0000	0.0019	0.0018
AT. 5	AL X	0.0011	0.2086	0.0000	0.0293	0.0326	0.0000
	Y	0.1965	0.0003	0.0000	0.0288	-0.0012	0.0000
	Z	0.0000	0.0000	0.2543	0.0000	0.0000	-0.0278
AT. 6	AL X	-0.0011	0.2086	0.0000	0.0293	-0.0326	0.0000
	Y	0.1965	-0.0003	0.0000	-0.0288	-0.0012	0.0000
	Z	0.0000	0.0000	0.2543	0.0000	0.0000	-0.0278
AT. 7	AL X	0.0011	0.2086	0.0000	-0.0293	-0.0326	0.0000
	Y	0.1965	0.0003	0.0000	-0.0288	0.0012	0.0000
	Z	0.0000	0.0000	0.2543	0.0000	0.0000	-0.0278
AT. 8	AL X	-0.0011	0.2086	0.0000	-0.0293	0.0326	0.0000
	Y	0.1965	-0.0003	0.0000	0.0288	0.0012	0.0000
	Z	0.0000	0.0000	0.2543	0.0000	0.0000	-0.0278
AT. 9	AL X	-0.0006	0.2083	0.0000	0.0000	0.0000	0.0000
	Y	0.1975	0.0003	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2543	-0.0008	0.0290	0.0333
AT. 10	AL X	-0.0006	0.2083	0.0000	0.0000	0.0000	0.0000
	Y	0.1975	0.0003	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2543	0.0008	-0.0290	0.0333
AT. 11	AL X	0.0006	0.2083	0.0000	0.0000	0.0000	0.0000
	Y	0.1975	-0.0003	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2543	0.0008	0.0290	0.0333
AT. 12	AL X	0.0006	0.2083	0.0000	0.0000	0.0000	0.0000
	Y	0.1975	-0.0003	0.0000	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.2543	-0.0008	-0.0290	0.0333
AT. 13	SI X	0.0000	0.2074	0.0000	-0.0164	0.0000	0.0000
	Y	0.1973	0.0000	0.0000	0.0000	0.0374	0.0000
	Z	0.0000	0.0000	0.2540	0.0000	0.0000	0.0514
AT. 14	SI X	0.0000	0.2074	0.0000	0.0164	0.0000	0.0000
	Y	0.1973	0.0000	0.0000	0.0000	-0.0374	0.0000
	Z	0.0000	0.0000	0.2540	0.0000	0.0000	0.0514
AT. 15	SI X	0.0013	0.2089	0.0000	0.0000	0.0000	0.0000
	Y	0.1981	-0.0006	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2546	0.0290	0.0180	-0.0129
AT. 16	SI X	0.0013	0.2089	0.0000	0.0000	0.0000	0.0000
	Y	0.1981	-0.0006	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2546	-0.0290	-0.0180	-0.0129
AT. 17	SI X	-0.0013	0.2089	0.0000	0.0000	0.0000	0.0000
	Y	0.1981	0.0006	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2546	-0.0290	0.0180	-0.0129
AT. 18	SI X	-0.0013	0.2089	0.0000	0.0000	0.0000	0.0000
	Y	0.1981	0.0006	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2546	0.0290	-0.0180	-0.0129
AT. 19	SI X	-0.0012	0.2101	0.0000	0.0000	0.0000	0.0000
	Y	0.1957	-0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2544	0.0324	-0.0146	-0.0184
AT. 20	SI X	-0.0012	0.2101	0.0000	0.0000	0.0000	0.0000
	Y	0.1957	-0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2544	-0.0324	0.0146	-0.0184
AT. 21	SI X	0.0012	0.2101	0.0000	0.0000	0.0000	0.0000
	Y	0.1957	0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2544	-0.0324	-0.0146	-0.0184
AT. 22	SI X	0.0012	0.2101	0.0000	0.0000	0.0000	0.0000
	Y	0.1957	0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2544	0.0324	0.0146	-0.0184
AT. 23	O X	-0.0011	0.2079	0.0013	0.0182	-0.0359	-0.0224
	Y	0.1967	0.0000	0.0000	-0.0200	0.0028	-0.0013
	Z	0.0004	-0.0011	0.2545	-0.0122	-0.0075	-0.0281
AT. 24	O X	-0.0011	0.2079	-0.0013	0.0182	-0.0359	0.0224
	Y	0.1967	0.0000	0.0000	-0.0200	0.0028	0.0013
	Z	-0.0004	0.0011	0.2545	0.0122	0.0075	-0.0281
AT. 25	O X	0.0011	0.2079	-0.0013	0.0182	0.0359	0.0224
	Y	0.1967	0.0000	0.0000	0.0200	0.0028	-0.0013
	Z	0.0004	0.0011	0.2545	0.0122	-0.0075	-0.0281
AT. 26	O X	0.0011	0.2079	0.0013	0.0182	0.0359	-0.0224
	Y	0.1967	0.0000	0.0000	0.0200	0.0028	0.0013
	Z	-0.0004	-0.0011	0.2545	-0.0122	0.0075	-0.0281
AT. 27	O X	-0.0011	0.2079	0.0013	-0.0182	0.0359	-0.0224
	Y	0.1967	0.0000	0.0000	0.0200	-0.0028	-0.0013
	Z	0.0004	-0.0011	0.2545	0.0122	0.0075	-0.0281
AT. 28	O X	-0.0011	0.2079	-0.0013	-0.0182	0.0359	0.0224
	Y	0.1967	0.0000	0.0000	0.0200	-0.0028	0.0013
	Z	-0.0004	0.0011	0.2545	-0.0122	-0.0075	-0.0281
AT. 29	O X	0.0011	0.2079	-0.0013	-0.0182	-0.0359	0.0224
	Y	0.1967	0.0000	0.0000	-0.0200	-0.0028	-0.0013
	Z	0.0004	0.0011	0.2545	-0.0122	0.0075	-0.0281
AT. 30	O X	0.0011	0.2079	0.0013	-0.0182	-0.0359	-0.0224
	Y	0.1967	0.0000	0.0000	-0.0200	-0.0028	0.0013

	Z	-0.0004	-0.0011	0.2545	0.0122	-0.0075	-0.0281
AT. 31	O X	0.0002	0.2078	0.0008	-0.0175	-0.0014	0.0183
	Y	0.1977	-0.0002	-0.0011	0.0055	0.0296	-0.0175
	Z	-0.0003	0.0003	0.2543	-0.0047	0.0063	0.0463
AT. 32	O X	0.0002	0.2078	-0.0008	-0.0175	-0.0014	-0.0183
	Y	0.1977	-0.0002	0.0011	0.0055	0.0296	0.0175
	Z	0.0003	-0.0003	0.2543	0.0047	-0.0063	0.0463
AT. 33	O X	-0.0002	0.2078	-0.0008	-0.0175	0.0014	-0.0183
	Y	0.1977	0.0002	-0.0011	-0.0055	0.0296	-0.0175
	Z	-0.0003	-0.0003	0.2543	0.0047	0.0063	0.0463
AT. 34	O X	-0.0002	0.2078	0.0008	-0.0175	0.0014	0.0183
	Y	0.1977	0.0002	0.0011	-0.0055	0.0296	0.0175
	Z	0.0003	0.0003	0.2543	-0.0047	-0.0063	0.0463
AT. 35	O X	0.0002	0.2078	0.0008	0.0175	0.0014	0.0183
	Y	0.1977	-0.0002	-0.0011	-0.0055	-0.0296	-0.0175
	Z	-0.0003	0.0003	0.2543	0.0047	-0.0063	0.0463
AT. 36	O X	0.0002	0.2078	-0.0008	0.0175	0.0014	-0.0183
	Y	0.1977	-0.0002	0.0011	-0.0055	-0.0296	0.0175
	Z	0.0003	-0.0003	0.2543	-0.0047	0.0063	0.0463
AT. 37	O X	-0.0002	0.2078	-0.0008	0.0175	-0.0014	-0.0183
	Y	0.1977	0.0002	-0.0011	0.0055	-0.0296	-0.0175
	Z	-0.0003	-0.0003	0.2543	-0.0047	-0.0063	0.0463
AT. 38	O X	-0.0002	0.2078	0.0008	0.0175	-0.0014	0.0183
	Y	0.1977	0.0002	0.0011	0.0055	-0.0296	0.0175
	Z	0.0003	0.0003	0.2543	0.0047	0.0063	0.0463
AT. 39	O X	0.0002	0.2099	0.0006	0.0188	0.0144	-0.0069
	Y	0.1953	0.0011	-0.0013	0.0258	-0.0165	0.0049
	Z	0.0003	0.0000	0.2539	0.0095	0.0155	-0.0159
AT. 40	O X	0.0002	0.2099	-0.0006	0.0188	0.0144	0.0069
	Y	0.1953	0.0011	0.0013	0.0258	-0.0165	-0.0049
	Z	-0.0003	0.0000	0.2539	-0.0095	-0.0155	-0.0159
AT. 41	O X	-0.0002	0.2099	-0.0006	0.0188	-0.0144	0.0069
	Y	0.1953	-0.0011	-0.0013	-0.0258	-0.0165	0.0049
	Z	0.0003	0.0000	0.2539	-0.0095	0.0155	-0.0159
AT. 42	O X	-0.0002	0.2099	0.0006	0.0188	-0.0144	-0.0069
	Y	0.1953	-0.0011	0.0013	-0.0258	-0.0165	-0.0049
	Z	-0.0003	0.0000	0.2539	0.0095	-0.0155	-0.0159
AT. 43	O X	0.0002	0.2099	0.0006	-0.0188	-0.0144	-0.0069
	Y	0.1953	0.0011	-0.0013	-0.0258	0.0165	0.0049
	Z	0.0003	0.0000	0.2539	-0.0095	-0.0155	-0.0159
AT. 44	O X	0.0002	0.2099	-0.0006	-0.0188	-0.0144	0.0069
	Y	0.1953	0.0011	0.0013	-0.0258	0.0165	-0.0049
	Z	-0.0003	0.0000	0.2539	0.0095	0.0155	-0.0159
AT. 45	O X	-0.0002	0.2099	-0.0006	-0.0188	0.0144	0.0069
	Y	0.1953	-0.0011	-0.0013	0.0258	0.0165	0.0049
	Z	0.0003	0.0000	0.2539	0.0095	-0.0155	-0.0159
AT. 46	O X	-0.0002	0.2099	0.0006	-0.0188	0.0144	-0.0069
	Y	0.1953	-0.0011	0.0013	0.0258	0.0165	-0.0049
	Z	-0.0003	0.0000	0.2539	-0.0095	0.0155	-0.0159
AT. 47	O X	-0.0005	0.2085	0.0000	0.0000	0.0000	0.0000
	Y	0.1955	-0.0016	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2542	0.0526	-0.0474	-0.0234
AT. 48	O X	-0.0005	0.2085	0.0000	0.0000	0.0000	0.0000
	Y	0.1955	-0.0016	0.0000	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.2542	-0.0526	0.0474	-0.0234
AT. 49	O X	0.0005	0.2085	0.0000	0.0000	0.0000	0.0000
	Y	0.1955	0.0016	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2542	-0.0526	-0.0474	-0.0234
AT. 50	O X	0.0005	0.2085	0.0000	0.0000	0.0000	0.0000
	Y	0.1955	0.0016	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2542	0.0526	0.0474	-0.0234
AT. 51	O X	0.0010	0.2081	0.0000	0.0000	0.0000	0.0000
	Y	0.1984	-0.0005	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2541	0.0254	0.0628	0.0267
AT. 52	O X	0.0010	0.2081	0.0000	0.0000	0.0000	0.0000
	Y	0.1984	-0.0005	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2541	-0.0254	-0.0628	0.0267
AT. 53	O X	-0.0010	0.2081	0.0000	0.0000	0.0000	0.0000
	Y	0.1984	0.0005	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2541	-0.0254	0.0628	0.0267
AT. 54	O X	-0.0010	0.2081	0.0000	0.0000	0.0000	0.0000
	Y	0.1984	0.0005	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2541	0.0254	-0.0628	0.0267
AT. 55	O X	-0.0003	0.2097	0.0000	0.0000	0.0000	0.0000
	Y	0.1970	-0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2520	0.0729	0.0349	-0.0098
AT. 56	O X	-0.0003	0.2097	0.0000	0.0000	0.0000	0.0000
	Y	0.1970	-0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2520	-0.0729	-0.0349	-0.0098
AT. 57	O X	0.0003	0.2097	0.0000	0.0000	0.0000	0.0000
	Y	0.1970	0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2520	-0.0729	0.0349	-0.0098
AT. 58	O X	0.0003	0.2097	0.0000	0.0000	0.0000	0.0000
	Y	0.1970	0.0011	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.2520	0.0729	-0.0349	-0.0098

FREQ(CM\*\*-1) 117.22 118.76 127.95 130.77 132.88 133.17

AT. 1	MG X	0.0000	0.0000	0.0000	0.0000	-0.0117	0.0128
	Y	0.0000	-0.0021	0.0121	0.0075	0.0000	0.0000
	Z	0.0000	-0.0260	-0.0034	0.0060	0.0000	0.0000
AT. 2	MG X	0.0000	0.0000	0.0000	0.0000	-0.0117	-0.0128
	Y	0.0000	-0.0021	-0.0121	0.0075	0.0000	0.0000
	Z	0.0000	0.0260	-0.0034	-0.0060	0.0000	0.0000
AT. 3	MG X	0.0000	0.0000	0.0000	0.0000	0.0117	-0.0128
	Y	0.0000	0.0021	-0.0121	0.0075	0.0000	0.0000
	Z	0.0000	0.0260	0.0034	0.0060	0.0000	0.0000
AT. 4	MG X	0.0000	0.0000	0.0000	0.0000	0.0117	0.0128
	Y	0.0000	0.0021	0.0121	0.0075	0.0000	0.0000
	Z	0.0000	-0.0260	0.0034	-0.0060	0.0000	0.0000
AT. 5	AL X	0.0000	0.0221	0.0000	-0.0348	-0.0007	0.0000
	Y	0.0000	0.0122	0.0000	-0.0124	0.0065	0.0000
	Z	-0.0474	0.0000	0.0052	0.0000	0.0000	0.0102
AT. 6	AL X	0.0000	-0.0221	0.0000	0.0348	-0.0007	0.0000
	Y	0.0000	0.0122	0.0000	-0.0124	-0.0065	0.0000
	Z	0.0474	0.0000	0.0052	0.0000	0.0000	-0.0102
AT. 7	AL X	0.0000	-0.0221	0.0000	-0.0348	0.0007	0.0000
	Y	0.0000	-0.0122	0.0000	-0.0124	-0.0065	0.0000



	Z	-0.0474	0.0000	-0.0052	0.0000	0.0000	-0.0102
AT. 8	AL X	0.0000	0.0221	0.0000	0.0348	0.0007	0.0000
	Y	0.0000	-0.0122	0.0000	-0.0124	0.0065	0.0000
	Z	0.0474	0.0000	-0.0052	0.0000	0.0000	0.0102
AT. 9	AL X	0.0000	0.0000	-0.0144	-0.0041	0.0000	0.0079
	Y	0.0000	0.0000	-0.0364	0.0107	0.0000	-0.0079
	Z	0.0027	-0.0022	0.0000	0.0000	0.0058	0.0000
AT. 10	AL X	0.0000	0.0000	0.0144	-0.0041	0.0000	-0.0079
	Y	0.0000	0.0000	0.0364	0.0107	0.0000	0.0079
	Z	0.0027	0.0022	0.0000	0.0000	-0.0058	0.0000
AT. 11	AL X	0.0000	0.0000	0.0144	0.0041	0.0000	0.0079
	Y	0.0000	0.0000	-0.0364	0.0107	0.0000	0.0079
	Z	-0.0027	-0.0022	0.0000	0.0000	-0.0058	0.0000
AT. 12	AL X	0.0000	0.0000	-0.0144	0.0041	0.0000	-0.0079
	Y	0.0000	0.0000	0.0364	0.0107	0.0000	-0.0079
	Z	-0.0027	0.0022	0.0000	0.0000	0.0058	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	-0.0117	0.0000
	Y	0.0000	-0.0314	0.0000	0.0272	0.0000	0.0000
	Z	0.0000	0.0000	-0.0128	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0117	0.0000
	Y	0.0000	0.0314	0.0000	0.0272	0.0000	0.0000
	Z	0.0000	0.0000	0.0128	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0141	-0.0144	0.0000	0.0306
	Y	0.0000	0.0000	-0.0079	-0.0037	0.0000	0.0133
	Z	-0.0294	-0.0105	0.0000	0.0000	-0.0079	0.0000
AT. 16	SI X	0.0000	0.0000	-0.0141	-0.0144	0.0000	-0.0306
	Y	0.0000	0.0000	0.0079	-0.0037	0.0000	-0.0133
	Z	-0.0294	0.0105	0.0000	0.0000	0.0079	0.0000
AT. 17	SI X	0.0000	0.0000	-0.0141	0.0144	0.0000	0.0306
	Y	0.0000	0.0000	-0.0079	-0.0037	0.0000	-0.0133
	Z	0.0294	-0.0105	0.0000	0.0000	0.0079	0.0000
AT. 18	SI X	0.0000	0.0000	0.0141	0.0144	0.0000	-0.0306
	Y	0.0000	0.0000	0.0079	-0.0037	0.0000	0.0133
	Z	0.0294	0.0105	0.0000	0.0000	-0.0079	0.0000
AT. 19	SI X	0.0000	0.0000	0.0186	0.0154	0.0000	-0.0155
	Y	0.0000	0.0000	-0.0053	-0.0112	0.0000	0.0274
	Z	0.0252	0.0083	0.0000	0.0000	-0.0087	0.0000
AT. 20	SI X	0.0000	0.0000	-0.0186	0.0154	0.0000	0.0155
	Y	0.0000	0.0000	0.0053	-0.0112	0.0000	-0.0274
	Z	0.0252	-0.0083	0.0000	0.0000	0.0087	0.0000
AT. 21	SI X	0.0000	0.0000	-0.0186	-0.0154	0.0000	-0.0155
	Y	0.0000	0.0000	-0.0053	-0.0112	0.0000	-0.0274
	Z	-0.0252	0.0083	0.0000	0.0000	0.0087	0.0000
AT. 22	SI X	0.0000	0.0000	0.0186	-0.0154	0.0000	0.0155
	Y	0.0000	0.0000	0.0053	-0.0112	0.0000	0.0274
	Z	-0.0252	-0.0083	0.0000	0.0000	-0.0087	0.0000
AT. 23	O X	0.0122	-0.0128	-0.0116	0.0149	-0.0245	0.0269
	Y	0.0102	0.0307	0.0080	-0.0150	-0.0013	-0.0004
	Z	0.0336	-0.0253	-0.0017	0.0022	-0.0085	-0.0032
AT. 24	O X	-0.0122	-0.0128	0.0116	0.0149	-0.0245	-0.0269
	Y	-0.0102	0.0307	-0.0080	-0.0150	-0.0013	0.0004
	Z	0.0336	0.0253	-0.0017	-0.0022	0.0085	-0.0032
AT. 25	O X	0.0122	0.0128	0.0116	-0.0149	-0.0245	0.0269
	Y	-0.0102	0.0307	0.0080	-0.0150	0.0013	0.0004

	Z	-0.0336	-0.0253	-0.0017	0.0022	0.0085	0.0032
AT. 26	O X	-0.0122	0.0128	-0.0116	-0.0149	-0.0245	-0.0269
	Y	0.0102	0.0307	-0.0080	-0.0150	0.0013	-0.0004
	Z	-0.0336	0.0253	-0.0017	-0.0022	-0.0085	0.0032
AT. 27	O X	0.0122	0.0128	0.0116	0.0149	0.0245	-0.0269
	Y	0.0102	-0.0307	-0.0080	-0.0150	0.0013	0.0004
	Z	0.0336	0.0253	0.0017	0.0022	0.0085	0.0032
AT. 28	O X	-0.0122	0.0128	-0.0116	0.0149	0.0245	0.0269
	Y	-0.0102	-0.0307	0.0080	-0.0150	0.0013	-0.0004
	Z	0.0336	-0.0253	0.0017	-0.0022	-0.0085	0.0032
AT. 29	O X	0.0122	-0.0128	-0.0116	-0.0149	0.0245	-0.0269
	Y	-0.0102	-0.0307	-0.0080	-0.0150	-0.0013	-0.0004
	Z	-0.0336	0.0253	0.0017	0.0022	-0.0085	-0.0032
AT. 30	O X	-0.0122	-0.0128	0.0116	-0.0149	0.0245	0.0269
	Y	0.0102	-0.0307	0.0080	-0.0150	-0.0013	0.0004
	Z	-0.0336	-0.0253	0.0017	-0.0022	0.0085	-0.0032
AT. 31	O X	0.0023	-0.0151	0.0142	0.0122	-0.0103	-0.0048
	Y	-0.0072	-0.0284	-0.0248	0.0206	0.0444	-0.0002
	Z	0.0040	0.0163	-0.0063	-0.0069	-0.0398	0.0019
AT. 32	O X	-0.0023	-0.0151	-0.0142	0.0122	-0.0103	0.0048
	Y	0.0072	-0.0284	0.0248	0.0206	0.0444	0.0002
	Z	0.0040	-0.0163	-0.0063	0.0069	0.0398	0.0019
AT. 33	O X	0.0023	0.0151	-0.0142	-0.0122	-0.0103	-0.0048
	Y	0.0072	-0.0284	-0.0248	0.0206	-0.0444	0.0002
	Z	-0.0040	0.0163	-0.0063	-0.0069	0.0398	-0.0019
AT. 34	O X	-0.0023	0.0151	0.0142	-0.0122	-0.0103	0.0048
	Y	-0.0072	-0.0284	0.0248	0.0206	-0.0444	-0.0002
	Z	-0.0040	-0.0163	-0.0063	0.0069	-0.0398	-0.0019
AT. 35	O X	0.0023	0.0151	-0.0142	0.0122	0.0103	0.0048
	Y	-0.0072	0.0284	0.0248	0.0206	-0.0444	0.0002
	Z	0.0040	-0.0163	0.0063	-0.0069	0.0398	-0.0019
AT. 36	O X	-0.0023	0.0151	0.0142	0.0122	0.0103	-0.0048
	Y	0.0072	0.0284	-0.0248	0.0206	-0.0444	-0.0002
	Z	0.0040	0.0163	0.0063	0.0069	-0.0398	-0.0019
AT. 37	O X	0.0023	-0.0151	0.0142	-0.0122	0.0103	0.0048
	Y	0.0072	0.0284	0.0248	0.0206	0.0444	-0.0002
	Z	-0.0040	-0.0163	0.0063	-0.0069	-0.0398	0.0019
AT. 38	O X	-0.0023	-0.0151	-0.0142	-0.0122	0.0103	-0.0048
	Y	-0.0072	0.0284	-0.0248	0.0206	0.0444	0.0002
	Z	-0.0040	0.0163	0.0063	0.0069	0.0398	0.0019
AT. 39	O X	0.0045	0.0218	0.0031	-0.0305	0.0185	0.0176
	Y	0.0267	-0.0106	0.0134	0.0018	0.0082	0.0206
	Z	-0.0401	-0.0136	0.0031	0.0018	-0.0230	0.0016
AT. 40	O X	-0.0045	0.0218	-0.0031	-0.0305	0.0185	-0.0176
	Y	-0.0267	-0.0106	-0.0134	0.0018	0.0082	-0.0206
	Z	-0.0401	0.0136	0.0031	-0.0018	0.0230	0.0016
AT. 41	O X	0.0045	-0.0218	-0.0031	0.0305	0.0185	0.0176
	Y	-0.0267	-0.0106	0.0134	0.0018	-0.0082	-0.0206
	Z	0.0401	-0.0136	0.0031	0.0018	0.0230	-0.0016
AT. 42	O X	-0.0045	-0.0218	0.0031	0.0305	0.0185	-0.0176
	Y	0.0267	-0.0106	-0.0134	0.0018	-0.0082	0.0206
	Z	0.0401	0.0136	0.0031	-0.0018	-0.0230	-0.0016
AT. 43	O X	0.0045	-0.0218	-0.0031	-0.0305	-0.0185	-0.0176
	Y	0.0267	0.0106	-0.0134	0.0018	-0.0082	-0.0206

	Z	-0.0401	0.0136	-0.0031	0.0018	0.0230	-0.0016
AT. 44	O X	-0.0045	-0.0218	0.0031	-0.0305	-0.0185	0.0176
	Y	-0.0267	0.0106	0.0134	0.0018	-0.0082	0.0206
	Z	-0.0401	-0.0136	-0.0031	-0.0018	-0.0230	-0.0016
AT. 45	O X	0.0045	0.0218	0.0031	0.0305	-0.0185	-0.0176
	Y	-0.0267	0.0106	-0.0134	0.0018	0.0082	0.0206
	Z	0.0401	0.0136	-0.0031	0.0018	-0.0230	0.0016
AT. 46	O X	-0.0045	0.0218	-0.0031	0.0305	-0.0185	0.0176
	Y	0.0267	0.0106	0.0134	0.0018	0.0082	-0.0206
	Z	0.0401	-0.0136	-0.0031	-0.0018	0.0230	0.0016
AT. 47	O X	0.0000	0.0000	0.0149	0.0185	0.0000	-0.0198
	Y	0.0000	0.0000	0.0382	-0.0545	0.0000	0.0511
	Z	0.0287	-0.0218	0.0000	0.0000	0.0243	0.0000
AT. 48	O X	0.0000	0.0000	-0.0149	0.0185	0.0000	0.0198
	Y	0.0000	0.0000	-0.0382	-0.0545	0.0000	-0.0511
	Z	0.0287	0.0218	0.0000	0.0000	-0.0243	0.0000
AT. 49	O X	0.0000	0.0000	-0.0149	-0.0185	0.0000	-0.0198
	Y	0.0000	0.0000	0.0382	-0.0545	0.0000	-0.0511
	Z	-0.0287	-0.0218	0.0000	0.0000	-0.0243	0.0000
AT. 50	O X	0.0000	0.0000	0.0149	-0.0185	0.0000	0.0198
	Y	0.0000	0.0000	-0.0382	-0.0545	0.0000	0.0511
	Z	-0.0287	0.0218	0.0000	0.0000	0.0243	0.0000
AT. 51	O X	0.0000	0.0000	-0.0150	0.0125	0.0000	0.0473
	Y	0.0000	0.0000	-0.0407	0.0272	0.0000	0.0330
	Z	-0.0030	-0.0449	0.0000	0.0000	-0.0461	0.0000
AT. 52	O X	0.0000	0.0000	0.0150	0.0125	0.0000	-0.0473
	Y	0.0000	0.0000	0.0407	0.0272	0.0000	-0.0330
	Z	-0.0030	0.0449	0.0000	0.0000	0.0461	0.0000
AT. 53	O X	0.0000	0.0000	0.0150	-0.0125	0.0000	0.0473
	Y	0.0000	0.0000	-0.0407	0.0272	0.0000	-0.0330
	Z	0.0030	-0.0449	0.0000	0.0000	0.0461	0.0000
AT. 54	O X	0.0000	0.0000	-0.0150	-0.0125	0.0000	-0.0473
	Y	0.0000	0.0000	0.0407	0.0272	0.0000	0.0330
	Z	0.0030	0.0449	0.0000	0.0000	-0.0461	0.0000
AT. 55	O X	0.0000	0.0000	0.0638	-0.0423	0.0000	0.0050
	Y	0.0000	0.0000	-0.0213	0.0066	0.0000	0.0219
	Z	-0.0348	0.0493	0.0000	0.0000	-0.0146	0.0000
AT. 56	O X	0.0000	0.0000	-0.0638	-0.0423	0.0000	-0.0050
	Y	0.0000	0.0000	0.0213	0.0066	0.0000	-0.0219
	Z	-0.0348	-0.0493	0.0000	0.0000	0.0146	0.0000
AT. 57	O X	0.0000	0.0000	-0.0638	0.0423	0.0000	0.0050
	Y	0.0000	0.0000	-0.0213	0.0066	0.0000	-0.0219
	Z	0.0348	0.0493	0.0000	0.0000	0.0146	0.0000
AT. 58	O X	0.0000	0.0000	0.0638	0.0423	0.0000	-0.0050
	Y	0.0000	0.0000	0.0213	0.0066	0.0000	0.0219
	Z	0.0348	-0.0493	0.0000	0.0000	-0.0146	0.0000

FREQ(CM\*\*-1) 134.41 157.39 161.52 162.20 167.81 169.55

AT. 1 MG	X	0.0000	0.0055	0.0395	0.0033	0.0000	0.0000
	Y	-0.0102	0.0000	0.0000	0.0000	-0.0100	-0.0025
	Z	0.0055	0.0000	0.0000	0.0000	0.0089	-0.0046
AT. 2 MG	X	0.0000	0.0055	0.0395	-0.0033	0.0000	0.0000
	Y	-0.0102	0.0000	0.0000	0.0000	-0.0100	0.0025

	Z	-0.0055	0.0000	0.0000	0.0000	-0.0089	-0.0046
AT. 3	MG X	0.0000	0.0055	-0.0395	-0.0033	0.0000	0.0000
	Y	0.0102	0.0000	0.0000	0.0000	-0.0100	0.0025
	Z	-0.0055	0.0000	0.0000	0.0000	0.0089	0.0046
AT. 4	MG X	0.0000	0.0055	-0.0395	0.0033	0.0000	0.0000
	Y	0.0102	0.0000	0.0000	0.0000	-0.0100	-0.0025
	Z	0.0055	0.0000	0.0000	0.0000	-0.0089	0.0046
AT. 5	AL X	-0.0064	-0.0141	0.0189	0.0000	0.0153	0.0000
	Y	-0.0126	0.0031	-0.0188	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	0.0099	0.0000	-0.0015
AT. 6	AL X	0.0064	-0.0141	0.0189	0.0000	-0.0153	0.0000
	Y	-0.0126	-0.0031	0.0188	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	-0.0099	0.0000	-0.0015
AT. 7	AL X	0.0064	-0.0141	-0.0189	0.0000	0.0153	0.0000
	Y	0.0126	0.0031	0.0188	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	-0.0099	0.0000	0.0015
AT. 8	AL X	-0.0064	-0.0141	-0.0189	0.0000	-0.0153	0.0000
	Y	0.0126	-0.0031	-0.0188	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	0.0099	0.0000	0.0015
AT. 9	AL X	0.0000	0.0071	0.0000	-0.0085	-0.0296	-0.0020
	Y	0.0000	-0.0021	0.0000	-0.0233	-0.0081	-0.0061
	Z	-0.0177	0.0000	0.0041	0.0000	0.0000	0.0000
AT. 10	AL X	0.0000	0.0071	0.0000	0.0085	-0.0296	0.0020
	Y	0.0000	-0.0021	0.0000	0.0233	-0.0081	0.0061
	Z	0.0177	0.0000	-0.0041	0.0000	0.0000	0.0000
AT. 11	AL X	0.0000	0.0071	0.0000	-0.0085	0.0296	0.0020
	Y	0.0000	0.0021	0.0000	0.0233	-0.0081	-0.0061
	Z	-0.0177	0.0000	-0.0041	0.0000	0.0000	0.0000
AT. 12	AL X	0.0000	0.0071	0.0000	0.0085	0.0296	-0.0020
	Y	0.0000	0.0021	0.0000	-0.0233	-0.0081	0.0061
	Z	0.0177	0.0000	0.0041	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0182	0.0287	0.0000	0.0000	0.0000
	Y	-0.0043	0.0000	0.0000	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0055
AT. 14	SI X	0.0000	0.0182	-0.0287	0.0000	0.0000	0.0000
	Y	0.0043	0.0000	0.0000	0.0000	-0.0012	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0055
AT. 15	SI X	0.0000	-0.0049	0.0000	0.0101	-0.0208	0.0181
	Y	0.0000	-0.0130	0.0000	-0.0054	0.0055	0.0135
	Z	-0.0085	0.0000	0.0017	0.0000	0.0000	0.0000
AT. 16	SI X	0.0000	-0.0049	0.0000	-0.0101	-0.0208	-0.0181
	Y	0.0000	-0.0130	0.0000	0.0054	0.0055	-0.0135
	Z	0.0085	0.0000	-0.0017	0.0000	0.0000	0.0000
AT. 17	SI X	0.0000	-0.0049	0.0000	0.0101	0.0208	-0.0181
	Y	0.0000	0.0130	0.0000	0.0054	0.0055	0.0135
	Z	-0.0085	0.0000	-0.0017	0.0000	0.0000	0.0000
AT. 18	SI X	0.0000	-0.0049	0.0000	-0.0101	0.0208	0.0181
	Y	0.0000	0.0130	0.0000	-0.0054	0.0055	-0.0135
	Z	0.0085	0.0000	0.0017	0.0000	0.0000	0.0000
AT. 19	SI X	0.0000	-0.0014	0.0000	0.0080	-0.0305	-0.0102
	Y	0.0000	-0.0093	0.0000	-0.0022	0.0068	0.0264
	Z	0.0061	0.0000	0.0009	0.0000	0.0000	0.0000
AT. 20	SI X	0.0000	-0.0014	0.0000	-0.0080	-0.0305	0.0102
	Y	0.0000	-0.0093	0.0000	0.0022	0.0068	-0.0264

	Z	-0.0061	0.0000	-0.0009	0.0000	0.0000	0.0000
AT. 21	SI X	0.0000	-0.0014	0.0000	0.0080	0.0305	0.0102
	Y	0.0000	0.0093	0.0000	0.0022	0.0068	0.0264
	Z	0.0061	0.0000	-0.0009	0.0000	0.0000	0.0000
AT. 22	SI X	0.0000	-0.0014	0.0000	-0.0080	0.0305	-0.0102
	Y	0.0000	0.0093	0.0000	-0.0022	0.0068	-0.0264
	Z	-0.0061	0.0000	0.0009	0.0000	0.0000	0.0000
AT. 23	O X	-0.0265	-0.0126	0.0193	0.0045	0.0140	-0.0163
	Y	0.0080	-0.0025	0.0140	-0.0082	-0.0013	-0.0007
	Z	-0.0290	-0.0032	0.0078	-0.0006	0.0011	-0.0002
AT. 24	O X	-0.0265	-0.0126	0.0193	-0.0045	0.0140	0.0163
	Y	0.0080	-0.0025	0.0140	0.0082	-0.0013	0.0007
	Z	0.0290	0.0032	-0.0078	-0.0006	-0.0011	-0.0002
AT. 25	O X	0.0265	-0.0126	0.0193	0.0045	-0.0140	0.0163
	Y	0.0080	0.0025	-0.0140	0.0082	-0.0013	-0.0007
	Z	-0.0290	0.0032	-0.0078	0.0006	0.0011	-0.0002
AT. 26	O X	0.0265	-0.0126	0.0193	-0.0045	-0.0140	-0.0163
	Y	0.0080	0.0025	-0.0140	-0.0082	-0.0013	0.0007
	Z	0.0290	-0.0032	0.0078	0.0006	-0.0011	-0.0002
AT. 27	O X	0.0265	-0.0126	-0.0193	-0.0045	0.0140	0.0163
	Y	-0.0080	-0.0025	-0.0140	0.0082	-0.0013	0.0007
	Z	0.0290	-0.0032	-0.0078	0.0006	0.0011	0.0002
AT. 28	O X	0.0265	-0.0126	-0.0193	0.0045	0.0140	-0.0163
	Y	-0.0080	-0.0025	-0.0140	-0.0082	-0.0013	-0.0007
	Z	-0.0290	0.0032	0.0078	0.0006	-0.0011	0.0002
AT. 29	O X	-0.0265	-0.0126	-0.0193	-0.0045	-0.0140	-0.0163
	Y	-0.0080	0.0025	0.0140	-0.0082	-0.0013	0.0007
	Z	0.0290	0.0032	0.0078	-0.0006	0.0011	0.0002
AT. 30	O X	-0.0265	-0.0126	-0.0193	0.0045	-0.0140	0.0163
	Y	-0.0080	0.0025	0.0140	0.0082	-0.0013	-0.0007
	Z	-0.0290	-0.0032	-0.0078	-0.0006	-0.0011	0.0002
AT. 31	O X	0.0122	0.0179	0.0247	-0.0076	0.0111	0.0103
	Y	-0.0031	-0.0009	0.0111	0.0104	-0.0080	-0.0066
	Z	-0.0140	0.0025	-0.0082	0.0015	-0.0033	0.0012
AT. 32	O X	0.0122	0.0179	0.0247	0.0076	0.0111	-0.0103
	Y	-0.0031	-0.0009	0.0111	-0.0104	-0.0080	0.0066
	Z	0.0140	-0.0025	0.0082	0.0015	0.0033	0.0012
AT. 33	O X	-0.0122	0.0179	0.0247	-0.0076	-0.0111	-0.0103
	Y	-0.0031	0.0009	-0.0111	-0.0104	-0.0080	-0.0066
	Z	-0.0140	-0.0025	0.0082	-0.0015	-0.0033	0.0012
AT. 34	O X	-0.0122	0.0179	0.0247	0.0076	-0.0111	0.0103
	Y	-0.0031	0.0009	-0.0111	0.0104	-0.0080	0.0066
	Z	0.0140	0.0025	-0.0082	-0.0015	0.0033	0.0012
AT. 35	O X	-0.0122	0.0179	-0.0247	0.0076	0.0111	-0.0103
	Y	0.0031	-0.0009	-0.0111	-0.0104	-0.0080	0.0066
	Z	0.0140	0.0025	0.0082	-0.0015	-0.0033	-0.0012
AT. 36	O X	-0.0122	0.0179	-0.0247	-0.0076	0.0111	0.0103
	Y	0.0031	-0.0009	-0.0111	0.0104	-0.0080	-0.0066
	Z	-0.0140	-0.0025	-0.0082	-0.0015	0.0033	-0.0012
AT. 37	O X	0.0122	0.0179	-0.0247	0.0076	-0.0111	0.0103
	Y	0.0031	0.0009	0.0111	0.0104	-0.0080	0.0066
	Z	0.0140	-0.0025	-0.0082	0.0015	-0.0033	-0.0012
AT. 38	O X	0.0122	0.0179	-0.0247	-0.0076	-0.0111	-0.0103
	Y	0.0031	0.0009	0.0111	-0.0104	-0.0080	-0.0066

	Z	-0.0140	0.0025	0.0082	0.0015	0.0033	-0.0012
AT. 39	O X	-0.0326	-0.0095	0.0312	0.0049	0.0234	-0.0118
	Y	-0.0274	0.0177	-0.0081	-0.0113	0.0111	-0.0172
	Z	0.0245	-0.0012	-0.0108	-0.0008	-0.0030	-0.0001
AT. 40	O X	-0.0326	-0.0095	0.0312	-0.0049	0.0234	0.0118
	Y	-0.0274	0.0177	-0.0081	0.0113	0.0111	0.0172
	Z	-0.0245	0.0012	0.0108	-0.0008	0.0030	-0.0001
AT. 41	O X	0.0326	-0.0095	0.0312	0.0049	-0.0234	0.0118
	Y	-0.0274	-0.0177	0.0081	0.0113	0.0111	-0.0172
	Z	0.0245	0.0012	0.0108	0.0008	-0.0030	-0.0001
AT. 42	O X	0.0326	-0.0095	0.0312	-0.0049	-0.0234	-0.0118
	Y	-0.0274	-0.0177	0.0081	-0.0113	0.0111	0.0172
	Z	-0.0245	-0.0012	-0.0108	0.0008	0.0030	-0.0001
AT. 43	O X	0.0326	-0.0095	-0.0312	-0.0049	0.0234	0.0118
	Y	0.0274	0.0177	0.0081	0.0113	0.0111	0.0172
	Z	-0.0245	-0.0012	0.0108	0.0008	-0.0030	0.0001
AT. 44	O X	0.0326	-0.0095	-0.0312	0.0049	0.0234	-0.0118
	Y	0.0274	0.0177	0.0081	-0.0113	0.0111	-0.0172
	Z	0.0245	0.0012	-0.0108	0.0008	0.0030	0.0001
AT. 45	O X	-0.0326	-0.0095	-0.0312	-0.0049	-0.0234	-0.0118
	Y	0.0274	-0.0177	-0.0081	-0.0113	0.0111	0.0172
	Z	-0.0245	0.0012	-0.0108	-0.0008	-0.0030	0.0001
AT. 46	O X	-0.0326	-0.0095	-0.0312	0.0049	-0.0234	0.0118
	Y	0.0274	-0.0177	-0.0081	0.0113	0.0111	-0.0172
	Z	0.0245	-0.0012	0.0108	-0.0008	0.0030	0.0001
AT. 47	O X	0.0000	-0.0061	0.0000	0.0047	-0.0286	-0.0144
	Y	0.0000	0.0408	0.0000	0.0417	-0.0121	0.0574
	Z	0.0560	0.0000	0.0307	0.0000	0.0000	0.0000
AT. 48	O X	0.0000	-0.0061	0.0000	-0.0047	-0.0286	0.0144
	Y	0.0000	0.0408	0.0000	-0.0417	-0.0121	-0.0574
	Z	-0.0560	0.0000	-0.0307	0.0000	0.0000	0.0000
AT. 49	O X	0.0000	-0.0061	0.0000	0.0047	0.0286	0.0144
	Y	0.0000	-0.0408	0.0000	-0.0417	-0.0121	0.0574
	Z	0.0560	0.0000	-0.0307	0.0000	0.0000	0.0000
AT. 50	O X	0.0000	-0.0061	0.0000	-0.0047	0.0286	-0.0144
	Y	0.0000	-0.0408	0.0000	0.0417	-0.0121	-0.0574
	Z	-0.0560	0.0000	0.0307	0.0000	0.0000	0.0000
AT. 51	O X	0.0000	-0.0373	0.0000	-0.0224	-0.0197	0.0403
	Y	0.0000	-0.0494	0.0000	-0.0416	0.0047	0.0374
	Z	0.0084	0.0000	0.0294	0.0000	0.0000	0.0000
AT. 52	O X	0.0000	-0.0373	0.0000	0.0224	-0.0197	-0.0403
	Y	0.0000	-0.0494	0.0000	0.0416	0.0047	-0.0374
	Z	-0.0084	0.0000	-0.0294	0.0000	0.0000	0.0000
AT. 53	O X	0.0000	-0.0373	0.0000	-0.0224	0.0197	-0.0403
	Y	0.0000	0.0494	0.0000	0.0416	0.0047	0.0374
	Z	0.0084	0.0000	-0.0294	0.0000	0.0000	0.0000
AT. 54	O X	0.0000	-0.0373	0.0000	0.0224	0.0197	0.0403
	Y	0.0000	0.0494	0.0000	-0.0416	0.0047	-0.0374
	Z	-0.0084	0.0000	0.0294	0.0000	0.0000	0.0000
AT. 55	O X	0.0000	0.0503	0.0000	0.0685	-0.0520	0.0023
	Y	0.0000	-0.0284	0.0000	-0.0231	0.0138	0.0205
	Z	0.0279	0.0000	-0.0199	0.0000	0.0000	0.0000
AT. 56	O X	0.0000	0.0503	0.0000	-0.0685	-0.0520	-0.0023
	Y	0.0000	-0.0284	0.0000	0.0231	0.0138	-0.0205

	Z	-0.0279	0.0000	0.0199	0.0000	0.0000	0.0000
AT. 57	O X	0.0000	0.0503	0.0000	0.0685	0.0520	-0.0023
	Y	0.0000	0.0284	0.0000	0.0231	0.0138	0.0205
	Z	0.0279	0.0000	0.0199	0.0000	0.0000	0.0000
AT. 58	O X	0.0000	0.0503	0.0000	-0.0685	0.0520	0.0023
	Y	0.0000	0.0284	0.0000	-0.0231	0.0138	-0.0205
	Z	-0.0279	0.0000	-0.0199	0.0000	0.0000	0.0000

FREQ(CM\*\*-1) 173.24 174.42 175.44 177.04 184.39 185.53

AT. 1	MG X	-0.0042	0.0000	0.0000	0.0000	0.0000	0.0124
	Y	0.0000	-0.0036	0.0062	0.0362	0.0280	0.0000
	Z	0.0000	0.0255	-0.0200	-0.0302	0.0384	0.0000
AT. 2	MG X	-0.0042	0.0000	0.0000	0.0000	0.0000	-0.0124
	Y	0.0000	-0.0036	-0.0062	0.0362	0.0280	0.0000
	Z	0.0000	-0.0255	-0.0200	0.0302	-0.0384	0.0000
AT. 3	MG X	-0.0042	0.0000	0.0000	0.0000	0.0000	0.0124
	Y	0.0000	-0.0036	0.0062	-0.0362	-0.0280	0.0000
	Z	0.0000	0.0255	-0.0200	0.0302	-0.0384	0.0000
AT. 4	MG X	-0.0042	0.0000	0.0000	0.0000	0.0000	-0.0124
	Y	0.0000	-0.0036	-0.0062	-0.0362	-0.0280	0.0000
	Z	0.0000	-0.0255	-0.0200	-0.0302	0.0384	0.0000
AT. 5	AL X	-0.0025	0.0063	0.0000	-0.0222	0.0085	0.0000
	Y	0.0098	0.0018	0.0000	0.0156	0.0298	0.0000
	Z	0.0000	0.0000	-0.0072	0.0000	0.0000	-0.0018
AT. 6	AL X	-0.0025	-0.0063	0.0000	0.0222	-0.0085	0.0000
	Y	-0.0098	0.0018	0.0000	0.0156	0.0298	0.0000
	Z	0.0000	0.0000	-0.0072	0.0000	0.0000	0.0018
AT. 7	AL X	-0.0025	0.0063	0.0000	0.0222	-0.0085	0.0000
	Y	0.0098	0.0018	0.0000	-0.0156	-0.0298	0.0000
	Z	0.0000	0.0000	-0.0072	0.0000	0.0000	-0.0018
AT. 8	AL X	-0.0025	-0.0063	0.0000	-0.0222	0.0085	0.0000
	Y	-0.0098	0.0018	0.0000	-0.0156	-0.0298	0.0000
	Z	0.0000	0.0000	-0.0072	0.0000	0.0000	0.0018
AT. 9	AL X	0.0049	0.0036	0.0000	0.0000	0.0000	0.0000
	Y	0.0224	-0.0164	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0016	0.0168	-0.0120	0.0008
AT. 10	AL X	0.0049	0.0036	0.0000	0.0000	0.0000	0.0000
	Y	0.0224	-0.0164	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0016	-0.0168	0.0120	0.0008
AT. 11	AL X	0.0049	-0.0036	0.0000	0.0000	0.0000	0.0000
	Y	-0.0224	-0.0164	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0016	0.0168	-0.0120	-0.0008
AT. 12	AL X	0.0049	-0.0036	0.0000	0.0000	0.0000	0.0000
	Y	-0.0224	-0.0164	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0016	-0.0168	0.0120	-0.0008
AT. 13	SI X	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	-0.0156	0.0000	0.0276	0.0025	0.0000
	Z	0.0000	0.0000	-0.0095	0.0000	0.0000	0.0000
AT. 14	SI X	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	-0.0156	0.0000	-0.0276	-0.0025	0.0000
	Z	0.0000	0.0000	-0.0095	0.0000	0.0000	0.0000
AT. 15	SI X	0.0034	0.0295	0.0000	0.0000	0.0000	0.0000
	Y	0.0222	0.0050	0.0000	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.0050	-0.0111	0.0134	0.0160
AT. 16	SI X	0.0034	0.0295	0.0000	0.0000	0.0000	0.0000
	Y	0.0222	0.0050	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0050	0.0111	-0.0134	0.0160
AT. 17	SI X	0.0034	-0.0295	0.0000	0.0000	0.0000	0.0000
	Y	-0.0222	0.0050	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0050	-0.0111	0.0134	-0.0160
AT. 18	SI X	0.0034	-0.0295	0.0000	0.0000	0.0000	0.0000
	Y	-0.0222	0.0050	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0050	0.0111	-0.0134	-0.0160
AT. 19	SI X	-0.0061	-0.0023	0.0000	0.0000	0.0000	0.0000
	Y	0.0293	0.0110	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0103	0.0124	-0.0107	-0.0067
AT. 20	SI X	-0.0061	-0.0023	0.0000	0.0000	0.0000	0.0000
	Y	0.0293	0.0110	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0103	-0.0124	0.0107	-0.0067
AT. 21	SI X	-0.0061	0.0023	0.0000	0.0000	0.0000	0.0000
	Y	-0.0293	0.0110	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0103	0.0124	-0.0107	0.0067
AT. 22	SI X	-0.0061	0.0023	0.0000	0.0000	0.0000	0.0000
	Y	-0.0293	0.0110	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0103	-0.0124	0.0107	0.0067
AT. 23	O X	0.0043	-0.0290	-0.0310	-0.0051	0.0066	0.0227
	Y	-0.0153	-0.0019	0.0112	0.0241	0.0210	0.0069
	Z	0.0026	0.0001	-0.0195	-0.0186	0.0124	-0.0009
AT. 24	O X	0.0043	-0.0290	0.0310	-0.0051	0.0066	-0.0227
	Y	-0.0153	-0.0019	-0.0112	0.0241	0.0210	-0.0069
	Z	-0.0026	-0.0001	-0.0195	0.0186	-0.0124	-0.0009
AT. 25	O X	0.0043	0.0290	0.0310	0.0051	-0.0066	0.0227
	Y	0.0153	-0.0019	0.0112	0.0241	0.0210	-0.0069
	Z	-0.0026	0.0001	-0.0195	-0.0186	0.0124	0.0009
AT. 26	O X	0.0043	0.0290	-0.0310	0.0051	-0.0066	-0.0227
	Y	0.0153	-0.0019	-0.0112	0.0241	0.0210	0.0069
	Z	0.0026	-0.0001	-0.0195	0.0186	-0.0124	0.0009
AT. 27	O X	0.0043	-0.0290	-0.0310	0.0051	-0.0066	0.0227
	Y	-0.0153	-0.0019	0.0112	-0.0241	-0.0210	0.0069
	Z	0.0026	0.0001	-0.0195	0.0186	-0.0124	-0.0009
AT. 28	O X	0.0043	-0.0290	0.0310	0.0051	-0.0066	-0.0227
	Y	-0.0153	-0.0019	-0.0112	-0.0241	-0.0210	-0.0069
	Z	-0.0026	-0.0001	-0.0195	-0.0186	0.0124	-0.0009
AT. 29	O X	0.0043	0.0290	0.0310	-0.0051	0.0066	0.0227
	Y	0.0153	-0.0019	0.0112	-0.0241	-0.0210	-0.0069
	Z	-0.0026	0.0001	-0.0195	0.0186	-0.0124	0.0009
AT. 30	O X	0.0043	0.0290	-0.0310	-0.0051	0.0066	-0.0227
	Y	0.0153	-0.0019	-0.0112	-0.0241	-0.0210	0.0069
	Z	0.0026	-0.0001	-0.0195	-0.0186	0.0124	0.0009
AT. 31	O X	0.0106	0.0011	-0.0053	0.0013	0.0072	-0.0053
	Y	-0.0176	-0.0156	0.0112	0.0230	0.0122	-0.0029
	Z	0.0057	-0.0009	-0.0117	0.0007	-0.0182	0.0030
AT. 32	O X	0.0106	0.0011	0.0053	0.0013	0.0072	0.0053
	Y	-0.0176	-0.0156	-0.0112	0.0230	0.0122	0.0029
	Z	-0.0057	0.0009	-0.0117	-0.0007	0.0182	0.0030
AT. 33	O X	0.0106	-0.0011	0.0053	-0.0013	-0.0072	-0.0053
	Y	0.0176	-0.0156	0.0112	0.0230	0.0122	0.0029



	Z	-0.0057	-0.0009	-0.0117	0.0007	-0.0182	-0.0030
AT. 34	O X	0.0106	-0.0011	-0.0053	-0.0013	-0.0072	0.0053
	Y	0.0176	-0.0156	-0.0112	0.0230	0.0122	-0.0029
	Z	0.0057	0.0009	-0.0117	-0.0007	0.0182	-0.0030
AT. 35	O X	0.0106	0.0011	-0.0053	-0.0013	-0.0072	-0.0053
	Y	-0.0176	-0.0156	0.0112	-0.0230	-0.0122	-0.0029
	Z	0.0057	-0.0009	-0.0117	-0.0007	0.0182	0.0030
AT. 36	O X	0.0106	0.0011	0.0053	-0.0013	-0.0072	0.0053
	Y	-0.0176	-0.0156	-0.0112	-0.0230	-0.0122	0.0029
	Z	-0.0057	0.0009	-0.0117	0.0007	-0.0182	0.0030
AT. 37	O X	0.0106	-0.0011	0.0053	0.0013	0.0072	-0.0053
	Y	0.0176	-0.0156	0.0112	-0.0230	-0.0122	0.0029
	Z	-0.0057	-0.0009	-0.0117	-0.0007	0.0182	-0.0030
AT. 38	O X	0.0106	-0.0011	-0.0053	0.0013	0.0072	0.0053
	Y	0.0176	-0.0156	-0.0112	-0.0230	-0.0122	-0.0029
	Z	0.0057	0.0009	-0.0117	0.0007	-0.0182	-0.0030
AT. 39	O X	-0.0131	0.0021	0.0113	-0.0092	-0.0079	0.0127
	Y	-0.0159	0.0077	0.0242	0.0169	0.0055	0.0142
	Z	0.0001	0.0038	-0.0086	-0.0146	0.0111	-0.0059
AT. 40	O X	-0.0131	0.0021	-0.0113	-0.0092	-0.0079	-0.0127
	Y	-0.0159	0.0077	-0.0242	0.0169	0.0055	-0.0142
	Z	-0.0001	-0.0038	-0.0086	0.0146	-0.0111	-0.0059
AT. 41	O X	-0.0131	-0.0021	-0.0113	0.0092	0.0079	0.0127
	Y	0.0159	0.0077	0.0242	0.0169	0.0055	-0.0142
	Z	-0.0001	0.0038	-0.0086	-0.0146	0.0111	0.0059
AT. 42	O X	-0.0131	-0.0021	0.0113	0.0092	0.0079	-0.0127
	Y	0.0159	0.0077	-0.0242	0.0169	0.0055	0.0142
	Z	0.0001	-0.0038	-0.0086	0.0146	-0.0111	0.0059
AT. 43	O X	-0.0131	0.0021	0.0113	0.0092	0.0079	0.0127
	Y	-0.0159	0.0077	0.0242	-0.0169	-0.0055	0.0142
	Z	0.0001	0.0038	-0.0086	0.0146	-0.0111	-0.0059
AT. 44	O X	-0.0131	0.0021	-0.0113	0.0092	0.0079	-0.0127
	Y	-0.0159	0.0077	-0.0242	-0.0169	-0.0055	-0.0142
	Z	-0.0001	-0.0038	-0.0086	-0.0146	0.0111	-0.0059
AT. 45	O X	-0.0131	-0.0021	-0.0113	-0.0092	-0.0079	0.0127
	Y	0.0159	0.0077	0.0242	-0.0169	-0.0055	-0.0142
	Z	-0.0001	0.0038	-0.0086	0.0146	-0.0111	0.0059
AT. 46	O X	-0.0131	-0.0021	0.0113	-0.0092	-0.0079	-0.0127
	Y	0.0159	0.0077	-0.0242	-0.0169	-0.0055	0.0142
	Z	0.0001	-0.0038	-0.0086	-0.0146	0.0111	0.0059
AT. 47	O X	-0.0090	0.0022	0.0000	0.0000	0.0000	0.0000
	Y	0.0614	-0.0178	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0240	0.0117	-0.0088	-0.0418
AT. 48	O X	-0.0090	0.0022	0.0000	0.0000	0.0000	0.0000
	Y	0.0614	-0.0178	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0240	-0.0117	0.0088	-0.0418
AT. 49	O X	-0.0090	-0.0022	0.0000	0.0000	0.0000	0.0000
	Y	-0.0614	-0.0178	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0240	0.0117	-0.0088	0.0418
AT. 50	O X	-0.0090	-0.0022	0.0000	0.0000	0.0000	0.0000
	Y	-0.0614	-0.0178	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0240	-0.0117	0.0088	0.0418
AT. 51	O X	0.0050	0.0527	0.0000	0.0000	0.0000	0.0000
	Y	0.0243	0.0342	0.0000	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.0247	0.0119	-0.0251	0.0742
AT. 52	O X	0.0050	0.0527	0.0000	0.0000	0.0000	0.0000
	Y	0.0243	0.0342	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0247	-0.0119	0.0251	0.0742
AT. 53	O X	0.0050	-0.0527	0.0000	0.0000	0.0000	0.0000
	Y	-0.0243	0.0342	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0247	0.0119	-0.0251	-0.0742
AT. 54	O X	0.0050	-0.0527	0.0000	0.0000	0.0000	0.0000
	Y	-0.0243	0.0342	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0247	-0.0119	0.0251	-0.0742
AT. 55	O X	0.0057	-0.0176	0.0000	0.0000	0.0000	0.0000
	Y	0.0232	0.0180	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0583	-0.0041	0.0311	-0.0105
AT. 56	O X	0.0057	-0.0176	0.0000	0.0000	0.0000	0.0000
	Y	0.0232	0.0180	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0583	0.0041	-0.0311	-0.0105
AT. 57	O X	0.0057	0.0176	0.0000	0.0000	0.0000	0.0000
	Y	-0.0232	0.0180	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0583	-0.0041	0.0311	0.0105
AT. 58	O X	0.0057	0.0176	0.0000	0.0000	0.0000	0.0000
	Y	-0.0232	0.0180	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0583	0.0041	-0.0311	0.0105

FREQ(CM\*\*-1) 188.51 189.51 191.69 193.00 193.52 195.59

AT. 1	MG X	0.0000	0.0207	0.0000	0.0000	0.0341	0.0008
	Y	0.0010	0.0000	-0.0327	-0.0153	0.0000	0.0000
	Z	-0.0363	0.0000	-0.0046	-0.0082	0.0000	0.0000
AT. 2	MG X	0.0000	0.0207	0.0000	0.0000	0.0341	-0.0008
	Y	-0.0010	0.0000	-0.0327	0.0153	0.0000	0.0000
	Z	-0.0363	0.0000	0.0046	-0.0082	0.0000	0.0000
AT. 3	MG X	0.0000	-0.0207	0.0000	0.0000	0.0341	0.0008
	Y	-0.0010	0.0000	-0.0327	-0.0153	0.0000	0.0000
	Z	0.0363	0.0000	-0.0046	-0.0082	0.0000	0.0000
AT. 4	MG X	0.0000	-0.0207	0.0000	0.0000	0.0341	-0.0008
	Y	0.0010	0.0000	-0.0327	0.0153	0.0000	0.0000
	Z	0.0363	0.0000	0.0046	-0.0082	0.0000	0.0000
AT. 5	AL X	0.0000	-0.0041	0.0184	0.0000	-0.0189	0.0000
	Y	0.0000	0.0103	-0.0210	0.0000	-0.0303	0.0000
	Z	0.0216	0.0000	0.0000	-0.0052	0.0000	-0.0042
AT. 6	AL X	0.0000	-0.0041	-0.0184	0.0000	-0.0189	0.0000
	Y	0.0000	-0.0103	-0.0210	0.0000	0.0303	0.0000
	Z	0.0216	0.0000	0.0000	-0.0052	0.0000	0.0042
AT. 7	AL X	0.0000	0.0041	0.0184	0.0000	-0.0189	0.0000
	Y	0.0000	-0.0103	-0.0210	0.0000	-0.0303	0.0000
	Z	-0.0216	0.0000	0.0000	-0.0052	0.0000	-0.0042
AT. 8	AL X	0.0000	0.0041	-0.0184	0.0000	-0.0189	0.0000
	Y	0.0000	0.0103	-0.0210	0.0000	0.0303	0.0000
	Z	-0.0216	0.0000	0.0000	-0.0052	0.0000	0.0042
AT. 9	AL X	-0.0277	0.0000	0.0026	0.0000	-0.0005	0.0000
	Y	0.0047	0.0000	0.0205	0.0000	-0.0038	0.0000
	Z	0.0000	0.0003	0.0000	0.0169	0.0000	0.0124
AT. 10	AL X	0.0277	0.0000	0.0026	0.0000	-0.0005	0.0000
	Y	-0.0047	0.0000	0.0205	0.0000	-0.0038	0.0000

	Z	0.0000	-0.0003	0.0000	0.0169	0.0000	0.0124
AT. 11	AL X	0.0277	0.0000	-0.0026	0.0000	-0.0005	0.0000
	Y	0.0047	0.0000	0.0205	0.0000	0.0038	0.0000
	Z	0.0000	-0.0003	0.0000	0.0169	0.0000	-0.0124
AT. 12	AL X	-0.0277	0.0000	-0.0026	0.0000	-0.0005	0.0000
	Y	-0.0047	0.0000	0.0205	0.0000	0.0038	0.0000
	Z	0.0000	0.0003	0.0000	0.0169	0.0000	-0.0124
AT. 13	SI X	0.0000	0.0358	0.0000	0.0000	0.0299	0.0000
	Y	0.0000	0.0000	0.0346	0.0000	0.0000	0.0000
	Z	0.0095	0.0000	0.0000	0.0014	0.0000	0.0000
AT. 14	SI X	0.0000	-0.0358	0.0000	0.0000	0.0299	0.0000
	Y	0.0000	0.0000	0.0346	0.0000	0.0000	0.0000
	Z	-0.0095	0.0000	0.0000	0.0014	0.0000	0.0000
AT. 15	SI X	-0.0162	0.0000	0.0011	0.0000	-0.0039	0.0000
	Y	0.0247	0.0000	-0.0028	0.0000	-0.0112	0.0000
	Z	0.0000	0.0011	0.0000	0.0015	0.0000	0.0109
AT. 16	SI X	0.0162	0.0000	0.0011	0.0000	-0.0039	0.0000
	Y	-0.0247	0.0000	-0.0028	0.0000	-0.0112	0.0000
	Z	0.0000	-0.0011	0.0000	0.0015	0.0000	0.0109
AT. 17	SI X	0.0162	0.0000	-0.0011	0.0000	-0.0039	0.0000
	Y	0.0247	0.0000	-0.0028	0.0000	0.0112	0.0000
	Z	0.0000	-0.0011	0.0000	0.0015	0.0000	-0.0109
AT. 18	SI X	-0.0162	0.0000	-0.0011	0.0000	-0.0039	0.0000
	Y	-0.0247	0.0000	-0.0028	0.0000	0.0112	0.0000
	Z	0.0000	0.0011	0.0000	0.0015	0.0000	-0.0109
AT. 19	SI X	0.0190	0.0000	-0.0052	0.0000	-0.0155	0.0000
	Y	0.0174	0.0000	-0.0038	0.0000	0.0011	0.0000
	Z	0.0000	-0.0024	0.0000	-0.0102	0.0000	0.0203
AT. 20	SI X	-0.0190	0.0000	-0.0052	0.0000	-0.0155	0.0000
	Y	-0.0174	0.0000	-0.0038	0.0000	0.0011	0.0000
	Z	0.0000	0.0024	0.0000	-0.0102	0.0000	0.0203
AT. 21	SI X	-0.0190	0.0000	0.0052	0.0000	-0.0155	0.0000
	Y	0.0174	0.0000	-0.0038	0.0000	-0.0011	0.0000
	Z	0.0000	0.0024	0.0000	-0.0102	0.0000	-0.0203
AT. 22	SI X	0.0190	0.0000	0.0052	0.0000	-0.0155	0.0000
	Y	-0.0174	0.0000	-0.0038	0.0000	-0.0011	0.0000
	Z	0.0000	-0.0024	0.0000	-0.0102	0.0000	-0.0203
AT. 23	O X	0.0139	0.0022	-0.0080	0.0025	0.0019	0.0230
	Y	0.0154	-0.0147	-0.0187	-0.0116	0.0251	-0.0065
	Z	0.0004	0.0033	-0.0009	0.0049	0.0028	0.0105
AT. 24	O X	-0.0139	0.0022	-0.0080	-0.0025	0.0019	-0.0230
	Y	-0.0154	-0.0147	-0.0187	0.0116	0.0251	0.0065
	Z	0.0004	-0.0033	0.0009	0.0049	-0.0028	0.0105
AT. 25	O X	-0.0139	0.0022	0.0080	-0.0025	0.0019	0.0230
	Y	0.0154	0.0147	-0.0187	-0.0116	-0.0251	0.0065
	Z	0.0004	-0.0033	-0.0009	0.0049	-0.0028	-0.0105
AT. 26	O X	0.0139	0.0022	0.0080	0.0025	0.0019	-0.0230
	Y	-0.0154	0.0147	-0.0187	0.0116	-0.0251	-0.0065
	Z	0.0004	0.0033	0.0009	0.0049	0.0028	-0.0105
AT. 27	O X	-0.0139	-0.0022	-0.0080	0.0025	0.0019	0.0230
	Y	-0.0154	0.0147	-0.0187	-0.0116	0.0251	-0.0065
	Z	-0.0004	-0.0033	-0.0009	0.0049	0.0028	0.0105
AT. 28	O X	0.0139	-0.0022	-0.0080	-0.0025	0.0019	-0.0230
	Y	0.0154	0.0147	-0.0187	0.0116	0.0251	0.0065

	Z	-0.0004	0.0033	0.0009	0.0049	-0.0028	0.0105
AT. 29	O X	0.0139	-0.0022	0.0080	-0.0025	0.0019	0.0230
	Y	-0.0154	-0.0147	-0.0187	-0.0116	-0.0251	0.0065
	Z	-0.0004	0.0033	-0.0009	0.0049	-0.0028	-0.0105
AT. 30	O X	-0.0139	-0.0022	0.0080	0.0025	0.0019	-0.0230
	Y	0.0154	-0.0147	-0.0187	0.0116	-0.0251	-0.0065
	Z	-0.0004	-0.0033	0.0009	0.0049	0.0028	-0.0105
AT. 31	O X	0.0078	0.0326	0.0034	-0.0135	0.0235	0.0035
	Y	0.0009	0.0066	0.0247	0.0247	0.0014	-0.0073
	Z	-0.0013	-0.0022	-0.0002	-0.0047	0.0031	0.0000
AT. 32	O X	-0.0078	0.0326	0.0034	0.0135	0.0235	-0.0035
	Y	-0.0009	0.0066	0.0247	-0.0247	0.0014	0.0073
	Z	-0.0013	0.0022	0.0002	-0.0047	-0.0031	0.0000
AT. 33	O X	-0.0078	0.0326	-0.0034	0.0135	0.0235	0.0035
	Y	0.0009	-0.0066	0.0247	0.0247	-0.0014	0.0073
	Z	-0.0013	0.0022	-0.0002	-0.0047	-0.0031	0.0000
AT. 34	O X	0.0078	0.0326	-0.0034	-0.0135	0.0235	-0.0035
	Y	-0.0009	-0.0066	0.0247	-0.0247	-0.0014	-0.0073
	Z	-0.0013	-0.0022	0.0002	-0.0047	0.0031	0.0000
AT. 35	O X	-0.0078	-0.0326	0.0034	-0.0135	0.0235	0.0035
	Y	-0.0009	-0.0066	0.0247	0.0247	0.0014	-0.0073
	Z	0.0013	0.0022	-0.0002	-0.0047	0.0031	0.0000
AT. 36	O X	0.0078	-0.0326	0.0034	0.0135	0.0235	-0.0035
	Y	0.0009	-0.0066	0.0247	-0.0247	0.0014	0.0073
	Z	0.0013	-0.0022	0.0002	-0.0047	-0.0031	0.0000
AT. 37	O X	0.0078	-0.0326	-0.0034	0.0135	0.0235	0.0035
	Y	-0.0009	0.0066	0.0247	0.0247	-0.0014	0.0073
	Z	0.0013	-0.0022	-0.0002	-0.0047	-0.0031	0.0000
AT. 38	O X	-0.0078	-0.0326	-0.0034	-0.0135	0.0235	-0.0035
	Y	0.0009	0.0066	0.0247	-0.0247	-0.0014	-0.0073
	Z	0.0013	0.0022	0.0002	-0.0047	0.0031	0.0000
AT. 39	O X	0.0119	-0.0005	0.0119	0.0139	-0.0099	-0.0124
	Y	-0.0114	0.0130	-0.0180	-0.0016	-0.0103	-0.0191
	Z	-0.0003	-0.0077	0.0045	-0.0160	0.0012	-0.0002
AT. 40	O X	-0.0119	-0.0005	0.0119	-0.0139	-0.0099	0.0124
	Y	0.0114	0.0130	-0.0180	0.0016	-0.0103	0.0191
	Z	-0.0003	0.0077	-0.0045	-0.0160	-0.0012	-0.0002
AT. 41	O X	-0.0119	-0.0005	-0.0119	-0.0139	-0.0099	-0.0124
	Y	-0.0114	-0.0130	-0.0180	-0.0016	0.0103	0.0191
	Z	-0.0003	0.0077	0.0045	-0.0160	-0.0012	0.0002
AT. 42	O X	0.0119	-0.0005	-0.0119	0.0139	-0.0099	0.0124
	Y	0.0114	-0.0130	-0.0180	0.0016	0.0103	-0.0191
	Z	-0.0003	-0.0077	-0.0045	-0.0160	0.0012	0.0002
AT. 43	O X	-0.0119	0.0005	0.0119	0.0139	-0.0099	-0.0124
	Y	0.0114	-0.0130	-0.0180	-0.0016	-0.0103	-0.0191
	Z	0.0003	0.0077	0.0045	-0.0160	0.0012	-0.0002
AT. 44	O X	0.0119	0.0005	0.0119	-0.0139	-0.0099	0.0124
	Y	-0.0114	-0.0130	-0.0180	0.0016	-0.0103	0.0191
	Z	0.0003	-0.0077	-0.0045	-0.0160	-0.0012	-0.0002
AT. 45	O X	0.0119	0.0005	-0.0119	-0.0139	-0.0099	-0.0124
	Y	0.0114	0.0130	-0.0180	-0.0016	0.0103	0.0191
	Z	0.0003	-0.0077	0.0045	-0.0160	-0.0012	0.0002
AT. 46	O X	-0.0119	0.0005	-0.0119	0.0139	-0.0099	0.0124
	Y	-0.0114	0.0130	-0.0180	0.0016	0.0103	-0.0191

	Z	0.0003	0.0077	-0.0045	-0.0160	0.0012	0.0002
AT. 47 O	X	0.0206	0.0000	-0.0055	0.0000	-0.0118	0.0000
	Y	0.0000	0.0000	0.0304	0.0000	0.0085	0.0000
	Z	0.0000	-0.0373	0.0000	0.0469	0.0000	0.0420
AT. 48 O	X	-0.0206	0.0000	-0.0055	0.0000	-0.0118	0.0000
	Y	0.0000	0.0000	0.0304	0.0000	0.0085	0.0000
	Z	0.0000	0.0373	0.0000	0.0469	0.0000	0.0420
AT. 49 O	X	-0.0206	0.0000	0.0055	0.0000	-0.0118	0.0000
	Y	0.0000	0.0000	0.0304	0.0000	-0.0085	0.0000
	Z	0.0000	0.0373	0.0000	0.0469	0.0000	-0.0420
AT. 50 O	X	0.0206	0.0000	0.0055	0.0000	-0.0118	0.0000
	Y	0.0000	0.0000	0.0304	0.0000	-0.0085	0.0000
	Z	0.0000	-0.0373	0.0000	0.0469	0.0000	-0.0420
AT. 51 O	X	-0.0259	0.0000	0.0189	0.0000	0.0069	0.0000
	Y	0.0090	0.0000	0.0252	0.0000	0.0022	0.0000
	Z	0.0000	-0.0359	0.0000	0.0371	0.0000	0.0290
AT. 52 O	X	0.0259	0.0000	0.0189	0.0000	0.0069	0.0000
	Y	-0.0090	0.0000	0.0252	0.0000	0.0022	0.0000
	Z	0.0000	0.0359	0.0000	0.0371	0.0000	0.0290
AT. 53 O	X	0.0259	0.0000	-0.0189	0.0000	0.0069	0.0000
	Y	0.0090	0.0000	0.0252	0.0000	-0.0022	0.0000
	Z	0.0000	0.0359	0.0000	0.0371	0.0000	-0.0290
AT. 54 O	X	-0.0259	0.0000	-0.0189	0.0000	0.0069	0.0000
	Y	-0.0090	0.0000	0.0252	0.0000	-0.0022	0.0000
	Z	0.0000	-0.0359	0.0000	0.0371	0.0000	-0.0290
AT. 55 O	X	-0.0025	0.0000	-0.0036	0.0000	-0.0356	0.0000
	Y	0.0202	0.0000	-0.0022	0.0000	0.0036	0.0000
	Z	0.0000	0.0462	0.0000	-0.0463	0.0000	0.0571
AT. 56 O	X	0.0025	0.0000	-0.0036	0.0000	-0.0356	0.0000
	Y	-0.0202	0.0000	-0.0022	0.0000	0.0036	0.0000
	Z	0.0000	-0.0462	0.0000	-0.0463	0.0000	0.0571
AT. 57 O	X	0.0025	0.0000	0.0036	0.0000	-0.0356	0.0000
	Y	0.0202	0.0000	-0.0022	0.0000	-0.0036	0.0000
	Z	0.0000	-0.0462	0.0000	-0.0463	0.0000	-0.0571
AT. 58 O	X	-0.0025	0.0000	0.0036	0.0000	-0.0356	0.0000
	Y	-0.0202	0.0000	-0.0022	0.0000	-0.0036	0.0000
	Z	0.0000	0.0462	0.0000	-0.0463	0.0000	-0.0571

FREQ(CM\*\*-1) 200.29 202.80 213.06 216.02 221.03 243.98

AT. 1 MG	X	0.0000	-0.0045	0.0000	0.0041	-0.0032	0.0000
	Y	-0.0019	0.0000	-0.0014	0.0000	0.0000	-0.0157
	Z	0.0039	0.0000	0.0006	0.0000	0.0000	-0.0228
AT. 2 MG	X	0.0000	-0.0045	0.0000	-0.0041	-0.0032	0.0000
	Y	0.0019	0.0000	-0.0014	0.0000	0.0000	-0.0157
	Z	0.0039	0.0000	-0.0006	0.0000	0.0000	0.0228
AT. 3 MG	X	0.0000	0.0045	0.0000	0.0041	0.0032	0.0000
	Y	-0.0019	0.0000	0.0014	0.0000	0.0000	0.0157
	Z	0.0039	0.0000	-0.0006	0.0000	0.0000	0.0228
AT. 4 MG	X	0.0000	0.0045	0.0000	-0.0041	0.0032	0.0000
	Y	0.0019	0.0000	0.0014	0.0000	0.0000	0.0157
	Z	0.0039	0.0000	0.0006	0.0000	0.0000	-0.0228
AT. 5 AL	X	0.0000	-0.0173	0.0049	0.0000	-0.0136	0.0025
	Y	0.0000	-0.0044	-0.0094	0.0000	0.0065	-0.0071

	Z	-0.0004	0.0000	0.0000	-0.0028	0.0000	0.0000
AT. 6	AL X	0.0000	-0.0173	-0.0049	0.0000	-0.0136	-0.0025
	Y	0.0000	0.0044	-0.0094	0.0000	-0.0065	-0.0071
	Z	-0.0004	0.0000	0.0000	0.0028	0.0000	0.0000
AT. 7	AL X	0.0000	0.0173	-0.0049	0.0000	0.0136	-0.0025
	Y	0.0000	0.0044	0.0094	0.0000	-0.0065	0.0071
	Z	-0.0004	0.0000	0.0000	-0.0028	0.0000	0.0000
AT. 8	AL X	0.0000	0.0173	0.0049	0.0000	0.0136	0.0025
	Y	0.0000	-0.0044	0.0094	0.0000	0.0065	0.0071
	Z	-0.0004	0.0000	0.0000	0.0028	0.0000	0.0000
AT. 9	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0102	0.0218	0.0005	-0.0130	-0.0046	0.0108
AT. 10	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0102	-0.0218	-0.0005	-0.0130	0.0046	-0.0108
AT. 11	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0102	-0.0218	0.0005	0.0130	0.0046	0.0108
AT. 12	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0102	0.0218	-0.0005	0.0130	-0.0046	-0.0108
AT. 13	SI X	0.0000	-0.0105	0.0000	0.0000	0.0017	0.0000
	Y	0.0000	0.0000	0.0058	0.0000	0.0000	0.0325
	Z	-0.0142	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0105	0.0000	0.0000	-0.0017	0.0000
	Y	0.0000	0.0000	-0.0058	0.0000	0.0000	-0.0325
	Z	-0.0142	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0135	0.0073	-0.0240	-0.0032	0.0128	-0.0023
AT. 16	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0135	-0.0073	0.0240	-0.0032	-0.0128	0.0023
AT. 17	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0135	-0.0073	-0.0240	0.0032	-0.0128	-0.0023
AT. 18	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0135	0.0073	0.0240	0.0032	0.0128	0.0023
AT. 19	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0051	-0.0095	-0.0238	0.0078	-0.0192	0.0090
AT. 20	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0051	0.0095	0.0238	0.0078	0.0192	-0.0090
AT. 21	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0051	0.0095	-0.0238	-0.0078	0.0192	0.0090
AT. 22	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0051	-0.0095	0.0238	-0.0078	-0.0192	-0.0090
AT. 23	O X	-0.0142	0.0138	-0.0037	0.0083	-0.0167	0.0198
	Y	-0.0067	0.0033	0.0048	-0.0081	0.0084	-0.0103

	Z	0.0041	0.0029	-0.0227	0.0110	-0.0223	0.0120
AT. 24	O X	0.0142	0.0138	-0.0037	-0.0083	-0.0167	0.0198
	Y	0.0067	0.0033	0.0048	0.0081	0.0084	-0.0103
	Z	0.0041	-0.0029	0.0227	0.0110	0.0223	-0.0120
AT. 25	O X	0.0142	0.0138	0.0037	0.0083	-0.0167	-0.0198
	Y	-0.0067	-0.0033	0.0048	0.0081	-0.0084	-0.0103
	Z	0.0041	-0.0029	-0.0227	-0.0110	0.0223	0.0120
AT. 26	O X	-0.0142	0.0138	0.0037	-0.0083	-0.0167	-0.0198
	Y	0.0067	-0.0033	0.0048	-0.0081	-0.0084	-0.0103
	Z	0.0041	0.0029	0.0227	-0.0110	-0.0223	-0.0120
AT. 27	O X	-0.0142	-0.0138	0.0037	0.0083	0.0167	-0.0198
	Y	-0.0067	-0.0033	-0.0048	-0.0081	-0.0084	0.0103
	Z	0.0041	-0.0029	0.0227	0.0110	0.0223	-0.0120
AT. 28	O X	0.0142	-0.0138	0.0037	-0.0083	0.0167	-0.0198
	Y	0.0067	-0.0033	-0.0048	0.0081	-0.0084	0.0103
	Z	0.0041	0.0029	-0.0227	0.0110	-0.0223	0.0120
AT. 29	O X	0.0142	-0.0138	-0.0037	0.0083	0.0167	0.0198
	Y	-0.0067	0.0033	-0.0048	0.0081	0.0084	0.0103
	Z	0.0041	0.0029	0.0227	-0.0110	-0.0223	-0.0120
AT. 30	O X	-0.0142	-0.0138	-0.0037	-0.0083	0.0167	0.0198
	Y	0.0067	0.0033	-0.0048	-0.0081	0.0084	0.0103
	Z	0.0041	-0.0029	-0.0227	-0.0110	0.0223	0.0120
AT. 31	O X	0.0001	-0.0046	0.0002	-0.0073	0.0021	0.0073
	Y	0.0062	0.0198	0.0105	0.0074	-0.0169	0.0210
	Z	-0.0158	-0.0279	-0.0063	0.0020	0.0154	-0.0031
AT. 32	O X	-0.0001	-0.0046	0.0002	0.0073	0.0021	0.0073
	Y	-0.0062	0.0198	0.0105	-0.0074	-0.0169	0.0210
	Z	-0.0158	0.0279	0.0063	0.0020	-0.0154	0.0031
AT. 33	O X	-0.0001	-0.0046	-0.0002	-0.0073	0.0021	-0.0073
	Y	0.0062	-0.0198	0.0105	-0.0074	0.0169	0.0210
	Z	-0.0158	0.0279	-0.0063	-0.0020	-0.0154	-0.0031
AT. 34	O X	0.0001	-0.0046	-0.0002	0.0073	0.0021	-0.0073
	Y	-0.0062	-0.0198	0.0105	0.0074	0.0169	0.0210
	Z	-0.0158	-0.0279	0.0063	-0.0020	0.0154	0.0031
AT. 35	O X	0.0001	0.0046	-0.0002	-0.0073	-0.0021	-0.0073
	Y	0.0062	-0.0198	-0.0105	0.0074	0.0169	-0.0210
	Z	-0.0158	0.0279	0.0063	0.0020	-0.0154	0.0031
AT. 36	O X	-0.0001	0.0046	-0.0002	0.0073	-0.0021	-0.0073
	Y	-0.0062	-0.0198	-0.0105	-0.0074	0.0169	-0.0210
	Z	-0.0158	-0.0279	-0.0063	0.0020	0.0154	-0.0031
AT. 37	O X	-0.0001	0.0046	0.0002	-0.0073	-0.0021	0.0073
	Y	0.0062	0.0198	-0.0105	-0.0074	-0.0169	-0.0210
	Z	-0.0158	-0.0279	0.0063	-0.0020	0.0154	0.0031
AT. 38	O X	0.0001	0.0046	0.0002	0.0073	-0.0021	0.0073
	Y	-0.0062	0.0198	-0.0105	0.0074	-0.0169	-0.0210
	Z	-0.0158	0.0279	-0.0063	-0.0020	-0.0154	-0.0031
AT. 39	O X	-0.0155	-0.0115	-0.0061	0.0176	0.0175	-0.0049
	Y	-0.0139	0.0045	0.0005	0.0025	0.0210	-0.0154
	Z	0.0115	-0.0038	0.0219	-0.0189	-0.0342	0.0028
AT. 40	O X	0.0155	-0.0115	-0.0061	-0.0176	0.0175	-0.0049
	Y	0.0139	0.0045	0.0005	-0.0025	0.0210	-0.0154
	Z	0.0115	0.0038	-0.0219	-0.0189	0.0342	-0.0028
AT. 41	O X	0.0155	-0.0115	0.0061	0.0176	0.0175	0.0049
	Y	-0.0139	-0.0045	0.0005	-0.0025	-0.0210	-0.0154

	Z	0.0115	0.0038	0.0219	0.0189	0.0342	0.0028
AT. 42	O X	-0.0155	-0.0115	0.0061	-0.0176	0.0175	0.0049
	Y	0.0139	-0.0045	0.0005	0.0025	-0.0210	-0.0154
	Z	0.0115	-0.0038	-0.0219	0.0189	-0.0342	-0.0028
AT. 43	O X	-0.0155	0.0115	0.0061	0.0176	-0.0175	0.0049
	Y	-0.0139	-0.0045	-0.0005	0.0025	-0.0210	0.0154
	Z	0.0115	0.0038	-0.0219	-0.0189	0.0342	-0.0028
AT. 44	O X	0.0155	0.0115	0.0061	-0.0176	-0.0175	0.0049
	Y	0.0139	-0.0045	-0.0005	-0.0025	-0.0210	0.0154
	Z	0.0115	-0.0038	0.0219	-0.0189	-0.0342	0.0028
AT. 45	O X	0.0155	0.0115	-0.0061	0.0176	-0.0175	-0.0049
	Y	-0.0139	0.0045	-0.0005	-0.0025	0.0210	0.0154
	Z	0.0115	-0.0038	-0.0219	0.0189	-0.0342	-0.0028
AT. 46	O X	-0.0155	0.0115	-0.0061	-0.0176	-0.0175	-0.0049
	Y	0.0139	0.0045	-0.0005	0.0025	0.0210	0.0154
	Z	0.0115	0.0038	0.0219	0.0189	0.0342	0.0028
AT. 47	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0481	-0.0372	-0.0343	-0.0488	-0.0029	0.0029
AT. 48	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0481	0.0372	0.0343	-0.0488	0.0029	-0.0029
AT. 49	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0481	0.0372	-0.0343	0.0488	0.0029	0.0029
AT. 50	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0481	-0.0372	0.0343	0.0488	-0.0029	-0.0029
AT. 51	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0638	0.0534	-0.0350	-0.0325	0.0234	-0.0395
AT. 52	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0638	-0.0534	0.0350	-0.0325	-0.0234	0.0395
AT. 53	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0638	-0.0534	-0.0350	0.0325	-0.0234	-0.0395
AT. 54	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0638	0.0534	0.0350	0.0325	0.0234	0.0395
AT. 55	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0054	0.0137	-0.0420	0.0524	0.0007	0.0281
AT. 56	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0054	-0.0137	0.0420	0.0524	-0.0007	-0.0281
AT. 57	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0054	-0.0137	-0.0420	-0.0524	-0.0007	0.0281
AT. 58	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0054	0.0137	0.0420	-0.0524	0.0007	-0.0281

FREQ(CM\*\*-1) 244.64 244.96 245.67 247.53 249.76 252.64



AT. 1 MG X	-0.0184	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0025	0.0223	0.0038	-0.0064	-0.0049
Z	0.0000	-0.0555	0.0228	0.0616	-0.0222	0.0134
AT. 2 MG X	0.0184	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0025	-0.0223	-0.0038	0.0064	0.0049
Z	0.0000	0.0555	0.0228	0.0616	-0.0222	0.0134
AT. 3 MG X	0.0184	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0025	-0.0223	0.0038	0.0064	-0.0049
Z	0.0000	-0.0555	-0.0228	0.0616	0.0222	0.0134
AT. 4 MG X	-0.0184	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0025	0.0223	-0.0038	-0.0064	0.0049
Z	0.0000	0.0555	-0.0228	0.0616	0.0222	0.0134
AT. 5 AL X	0.0000	-0.0017	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
Z	0.0126	0.0000	0.0034	-0.0194	0.0147	0.0003
AT. 6 AL X	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
Z	-0.0126	0.0000	0.0034	-0.0194	0.0147	0.0003
AT. 7 AL X	0.0000	-0.0017	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
Z	-0.0126	0.0000	-0.0034	-0.0194	-0.0147	0.0003
AT. 8 AL X	0.0000	0.0017	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
Z	0.0126	0.0000	-0.0034	-0.0194	-0.0147	0.0003
AT. 9 AL X	-0.0178	0.0061	-0.0107	0.0000	0.0100	0.0000
Y	0.0111	0.0090	-0.0002	0.0000	-0.0085	0.0000
Z	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0023
AT. 10 AL X	0.0178	0.0061	0.0107	0.0000	-0.0100	0.0000
Y	-0.0111	0.0090	0.0002	0.0000	0.0085	0.0000
Z	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0023
AT. 11 AL X	-0.0178	-0.0061	0.0107	0.0000	-0.0100	0.0000
Y	-0.0111	0.0090	-0.0002	0.0000	-0.0085	0.0000
Z	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0023
AT. 12 AL X	0.0178	-0.0061	-0.0107	0.0000	0.0100	0.0000
Y	0.0111	0.0090	0.0002	0.0000	0.0085	0.0000
Z	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0023
AT. 13 SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0164	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	0.0164	-0.0150	-0.0197	-0.0052
AT. 14 SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	-0.0164	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0164	-0.0150	0.0197	-0.0052
AT. 15 SI X	-0.0235	-0.0066	0.0042	0.0000	0.0252	0.0000
Y	0.0200	0.0026	0.0029	0.0000	0.0013	0.0000
Z	0.0000	0.0000	0.0000	0.0005	0.0000	-0.0149
AT. 16 SI X	0.0235	-0.0066	-0.0042	0.0000	-0.0252	0.0000
Y	-0.0200	0.0026	-0.0029	0.0000	-0.0013	0.0000
Z	0.0000	0.0000	0.0000	0.0005	0.0000	-0.0149
AT. 17 SI X	-0.0235	0.0066	-0.0042	0.0000	-0.0252	0.0000
Y	-0.0200	0.0026	0.0029	0.0000	0.0013	0.0000
Z	0.0000	0.0000	0.0000	0.0005	0.0000	-0.0149
AT. 18 SI X	0.0235	0.0066	0.0042	0.0000	0.0252	0.0000
Y	0.0200	0.0026	-0.0029	0.0000	-0.0013	0.0000

	Z	0.0000	0.0000	0.0000	0.0005	0.0000	-0.0149
AT. 19	SI X	-0.0038	0.0037	0.0156	0.0000	0.0117	0.0000
	Y	0.0172	-0.0023	-0.0090	0.0000	-0.0020	0.0000
	Z	0.0000	0.0000	0.0000	-0.0031	0.0000	0.0129
AT. 20	SI X	0.0038	0.0037	-0.0156	0.0000	-0.0117	0.0000
	Y	-0.0172	-0.0023	0.0090	0.0000	0.0020	0.0000
	Z	0.0000	0.0000	0.0000	-0.0031	0.0000	0.0129
AT. 21	SI X	-0.0038	-0.0037	-0.0156	0.0000	-0.0117	0.0000
	Y	-0.0172	-0.0023	-0.0090	0.0000	-0.0020	0.0000
	Z	0.0000	0.0000	0.0000	-0.0031	0.0000	0.0129
AT. 22	SI X	0.0038	-0.0037	0.0156	0.0000	0.0117	0.0000
	Y	0.0172	-0.0023	0.0090	0.0000	0.0020	0.0000
	Z	0.0000	0.0000	0.0000	-0.0031	0.0000	0.0129
AT. 23	O X	-0.0256	-0.0020	-0.0017	-0.0020	-0.0244	-0.0193
	Y	-0.0092	0.0005	-0.0020	-0.0066	0.0040	0.0123
	Z	-0.0054	-0.0054	0.0051	-0.0012	-0.0011	-0.0275
AT. 24	O X	0.0256	-0.0020	0.0017	0.0020	0.0244	0.0193
	Y	0.0092	0.0005	0.0020	0.0066	-0.0040	-0.0123
	Z	-0.0054	0.0054	0.0051	-0.0012	-0.0011	-0.0275
AT. 25	O X	-0.0256	0.0020	0.0017	0.0020	0.0244	0.0193
	Y	0.0092	0.0005	-0.0020	-0.0066	0.0040	0.0123
	Z	0.0054	-0.0054	0.0051	-0.0012	-0.0011	-0.0275
AT. 26	O X	0.0256	0.0020	-0.0017	-0.0020	-0.0244	-0.0193
	Y	-0.0092	0.0005	0.0020	0.0066	-0.0040	-0.0123
	Z	0.0054	0.0054	0.0051	-0.0012	-0.0011	-0.0275
AT. 27	O X	0.0256	-0.0020	0.0017	-0.0020	0.0244	-0.0193
	Y	0.0092	0.0005	0.0020	-0.0066	-0.0040	0.0123
	Z	0.0054	-0.0054	-0.0051	-0.0012	0.0011	-0.0275
AT. 28	O X	-0.0256	-0.0020	-0.0017	0.0020	-0.0244	0.0193
	Y	-0.0092	0.0005	-0.0020	0.0066	0.0040	-0.0123
	Z	0.0054	0.0054	-0.0051	-0.0012	0.0011	-0.0275
AT. 29	O X	0.0256	0.0020	-0.0017	0.0020	-0.0244	0.0193
	Y	-0.0092	0.0005	0.0020	-0.0066	-0.0040	0.0123
	Z	-0.0054	-0.0054	-0.0051	-0.0012	0.0011	-0.0275
AT. 30	O X	-0.0256	0.0020	0.0017	-0.0020	0.0244	-0.0193
	Y	0.0092	0.0005	-0.0020	0.0066	0.0040	-0.0123
	Z	-0.0054	0.0054	-0.0051	-0.0012	0.0011	-0.0275
AT. 31	O X	-0.0001	-0.0099	0.0169	-0.0066	-0.0100	-0.0088
	Y	-0.0072	-0.0162	-0.0233	0.0038	0.0082	0.0075
	Z	0.0037	0.0152	0.0199	-0.0062	-0.0131	-0.0028
AT. 32	O X	0.0001	-0.0099	-0.0169	0.0066	0.0100	0.0088
	Y	0.0072	-0.0162	0.0233	-0.0038	-0.0082	-0.0075
	Z	0.0037	-0.0152	0.0199	-0.0062	-0.0131	-0.0028
AT. 33	O X	-0.0001	0.0099	-0.0169	0.0066	0.0100	0.0088
	Y	0.0072	-0.0162	-0.0233	0.0038	0.0082	0.0075
	Z	-0.0037	0.0152	0.0199	-0.0062	-0.0131	-0.0028
AT. 34	O X	0.0001	0.0099	0.0169	-0.0066	-0.0100	-0.0088
	Y	-0.0072	-0.0162	0.0233	-0.0038	-0.0082	-0.0075
	Z	-0.0037	-0.0152	0.0199	-0.0062	-0.0131	-0.0028
AT. 35	O X	0.0001	-0.0099	-0.0169	-0.0066	0.0100	-0.0088
	Y	0.0072	-0.0162	0.0233	0.0038	-0.0082	0.0075
	Z	-0.0037	0.0152	-0.0199	-0.0062	0.0131	-0.0028
AT. 36	O X	-0.0001	-0.0099	0.0169	0.0066	-0.0100	0.0088
	Y	-0.0072	-0.0162	-0.0233	-0.0038	0.0082	-0.0075

	Z	-0.0037	-0.0152	-0.0199	-0.0062	0.0131	-0.0028
AT. 37	O X	0.0001	0.0099	0.0169	0.0066	-0.0100	0.0088
	Y	-0.0072	-0.0162	0.0233	0.0038	-0.0082	0.0075
	Z	0.0037	0.0152	-0.0199	-0.0062	0.0131	-0.0028
AT. 38	O X	-0.0001	0.0099	-0.0169	-0.0066	0.0100	-0.0088
	Y	0.0072	-0.0162	-0.0233	-0.0038	0.0082	-0.0075
	Z	0.0037	-0.0152	-0.0199	-0.0062	0.0131	-0.0028
AT. 39	O X	0.0056	0.0029	0.0114	0.0040	0.0133	-0.0175
	Y	0.0039	0.0042	0.0118	0.0135	0.0017	-0.0182
	Z	0.0040	-0.0068	-0.0005	-0.0128	-0.0007	0.0259
AT. 40	O X	-0.0056	0.0029	-0.0114	-0.0040	-0.0133	0.0175
	Y	-0.0039	0.0042	-0.0118	-0.0135	-0.0017	0.0182
	Z	0.0040	0.0068	-0.0005	-0.0128	-0.0007	0.0259
AT. 41	O X	0.0056	-0.0029	-0.0114	-0.0040	-0.0133	0.0175
	Y	-0.0039	0.0042	0.0118	0.0135	0.0017	-0.0182
	Z	-0.0040	-0.0068	-0.0005	-0.0128	-0.0007	0.0259
AT. 42	O X	-0.0056	-0.0029	0.0114	0.0040	0.0133	-0.0175
	Y	0.0039	0.0042	-0.0118	-0.0135	-0.0017	0.0182
	Z	-0.0040	0.0068	-0.0005	-0.0128	-0.0007	0.0259
AT. 43	O X	-0.0056	0.0029	-0.0114	0.0040	-0.0133	-0.0175
	Y	-0.0039	0.0042	-0.0118	0.0135	-0.0017	-0.0182
	Z	-0.0040	-0.0068	0.0005	-0.0128	0.0007	0.0259
AT. 44	O X	0.0056	0.0029	0.0114	-0.0040	0.0133	0.0175
	Y	0.0039	0.0042	0.0118	-0.0135	0.0017	0.0182
	Z	-0.0040	0.0068	0.0005	-0.0128	0.0007	0.0259
AT. 45	O X	-0.0056	-0.0029	0.0114	-0.0040	0.0133	0.0175
	Y	0.0039	0.0042	-0.0118	0.0135	-0.0017	-0.0182
	Z	0.0040	-0.0068	0.0005	-0.0128	0.0007	0.0259
AT. 46	O X	0.0056	-0.0029	-0.0114	0.0040	-0.0133	-0.0175
	Y	-0.0039	0.0042	0.0118	-0.0135	0.0017	0.0182
	Z	0.0040	0.0068	0.0005	-0.0128	0.0007	0.0259
AT. 47	O X	-0.0036	0.0043	0.0162	0.0000	0.0108	0.0000
	Y	0.0352	-0.0013	-0.0201	0.0000	-0.0347	0.0000
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0221
AT. 48	O X	0.0036	0.0043	-0.0162	0.0000	-0.0108	0.0000
	Y	-0.0352	-0.0013	0.0201	0.0000	0.0347	0.0000
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0221
AT. 49	O X	-0.0036	-0.0043	-0.0162	0.0000	-0.0108	0.0000
	Y	-0.0352	-0.0013	-0.0201	0.0000	-0.0347	0.0000
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0221
AT. 50	O X	0.0036	-0.0043	0.0162	0.0000	0.0108	0.0000
	Y	0.0352	-0.0013	0.0201	0.0000	0.0347	0.0000
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0221
AT. 51	O X	-0.0247	0.0127	0.0216	0.0000	0.0269	0.0000
	Y	0.0107	0.0193	0.0266	0.0000	0.0072	0.0000
	Z	0.0000	0.0000	0.0000	-0.0029	0.0000	-0.0105
AT. 52	O X	0.0247	0.0127	-0.0216	0.0000	-0.0269	0.0000
	Y	-0.0107	0.0193	-0.0266	0.0000	-0.0072	0.0000
	Z	0.0000	0.0000	0.0000	-0.0029	0.0000	-0.0105
AT. 53	O X	-0.0247	-0.0127	-0.0216	0.0000	-0.0269	0.0000
	Y	-0.0107	0.0193	0.0266	0.0000	0.0072	0.0000
	Z	0.0000	0.0000	0.0000	-0.0029	0.0000	-0.0105
AT. 54	O X	0.0247	-0.0127	0.0216	0.0000	0.0269	0.0000
	Y	0.0107	0.0193	-0.0266	0.0000	-0.0072	0.0000

	Z	0.0000	0.0000	0.0000	-0.0029	0.0000	-0.0105
AT. 55 O	X	-0.0031	-0.0216	-0.0125	0.0000	0.0015	0.0000
	Y	0.0135	0.0086	0.0045	0.0000	0.0046	0.0000
	Z	0.0000	0.0000	0.0000	0.0049	0.0000	-0.0192
AT. 56 O	X	0.0031	-0.0216	0.0125	0.0000	-0.0015	0.0000
	Y	-0.0135	0.0086	-0.0045	0.0000	-0.0046	0.0000
	Z	0.0000	0.0000	0.0000	0.0049	0.0000	-0.0192
AT. 57 O	X	-0.0031	0.0216	0.0125	0.0000	-0.0015	0.0000
	Y	-0.0135	0.0086	0.0045	0.0000	0.0046	0.0000
	Z	0.0000	0.0000	0.0000	0.0049	0.0000	-0.0192
AT. 58 O	X	0.0031	0.0216	-0.0125	0.0000	0.0015	0.0000
	Y	0.0135	0.0086	-0.0045	0.0000	-0.0046	0.0000
	Z	0.0000	0.0000	0.0000	0.0049	0.0000	-0.0192

FREQ(CM\*\*-1) 255.07 260.06 265.69 266.11 267.11 267.53

AT. 1 MG	X	-0.0068	0.0092	0.0000	-0.0057	-0.0016	-0.0040
	Y	0.0000	0.0000	-0.0166	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0088	0.0000	0.0000	0.0000
AT. 2 MG	X	-0.0068	0.0092	0.0000	0.0057	0.0016	-0.0040
	Y	0.0000	0.0000	-0.0166	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0088	0.0000	0.0000	0.0000
AT. 3 MG	X	-0.0068	-0.0092	0.0000	0.0057	-0.0016	-0.0040
	Y	0.0000	0.0000	0.0166	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0088	0.0000	0.0000	0.0000
AT. 4 MG	X	-0.0068	-0.0092	0.0000	-0.0057	0.0016	-0.0040
	Y	0.0000	0.0000	0.0166	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0088	0.0000	0.0000	0.0000
AT. 5 AL	X	-0.0165	0.0129	0.0042	0.0000	0.0000	-0.0039
	Y	-0.0014	0.0089	-0.0069	0.0000	0.0000	-0.0078
	Z	0.0000	0.0000	0.0000	0.0173	-0.0058	0.0000
AT. 6 AL	X	-0.0165	0.0129	-0.0042	0.0000	0.0000	-0.0039
	Y	0.0014	-0.0089	-0.0069	0.0000	0.0000	0.0078
	Z	0.0000	0.0000	0.0000	-0.0173	0.0058	0.0000
AT. 7 AL	X	-0.0165	-0.0129	-0.0042	0.0000	0.0000	-0.0039
	Y	-0.0014	-0.0089	0.0069	0.0000	0.0000	-0.0078
	Z	0.0000	0.0000	0.0000	-0.0173	-0.0058	0.0000
AT. 8 AL	X	-0.0165	-0.0129	0.0042	0.0000	0.0000	-0.0039
	Y	0.0014	0.0089	0.0069	0.0000	0.0000	0.0078
	Z	0.0000	0.0000	0.0000	0.0173	0.0058	0.0000
AT. 9 AL	X	0.0018	0.0000	0.0000	0.0293	0.0000	0.0059
	Y	-0.0141	0.0000	0.0000	0.0111	0.0000	0.0115
	Z	0.0000	0.0080	-0.0237	0.0000	0.0047	0.0000
AT. 10 AL	X	0.0018	0.0000	0.0000	-0.0293	0.0000	0.0059
	Y	-0.0141	0.0000	0.0000	-0.0111	0.0000	0.0115
	Z	0.0000	-0.0080	0.0237	0.0000	0.0047	0.0000
AT. 11 AL	X	0.0018	0.0000	0.0000	0.0293	0.0000	0.0059
	Y	0.0141	0.0000	0.0000	-0.0111	0.0000	-0.0115
	Z	0.0000	-0.0080	-0.0237	0.0000	-0.0047	0.0000
AT. 12 AL	X	0.0018	0.0000	0.0000	-0.0293	0.0000	0.0059
	Y	0.0141	0.0000	0.0000	0.0111	0.0000	-0.0115
	Z	0.0000	0.0080	0.0237	0.0000	-0.0047	0.0000
AT. 13 SI	X	-0.0113	0.0106	0.0000	0.0000	0.0000	-0.0101
	Y	0.0000	0.0000	0.0060	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14 SI	X	-0.0113	-0.0106	0.0000	0.0000	0.0000	-0.0101
	Y	0.0000	0.0000	-0.0060	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15 SI	X	0.0241	0.0000	0.0000	-0.0003	0.0000	-0.0026
	Y	-0.0099	0.0000	0.0000	-0.0096	0.0000	-0.0090
	Z	0.0000	0.0248	-0.0059	0.0000	-0.0167	0.0000
AT. 16 SI	X	0.0241	0.0000	0.0000	0.0003	0.0000	-0.0026
	Y	-0.0099	0.0000	0.0000	0.0096	0.0000	-0.0090
	Z	0.0000	-0.0248	0.0059	0.0000	-0.0167	0.0000
AT. 17 SI	X	0.0241	0.0000	0.0000	-0.0003	0.0000	-0.0026
	Y	0.0099	0.0000	0.0000	0.0096	0.0000	0.0090
	Z	0.0000	-0.0248	-0.0059	0.0000	0.0167	0.0000
AT. 18 SI	X	0.0241	0.0000	0.0000	0.0003	0.0000	-0.0026
	Y	0.0099	0.0000	0.0000	-0.0096	0.0000	0.0090
	Z	0.0000	0.0248	0.0059	0.0000	0.0167	0.0000
AT. 19 SI	X	-0.0090	0.0000	0.0000	-0.0298	0.0000	0.0061
	Y	-0.0041	0.0000	0.0000	-0.0044	0.0000	-0.0142
	Z	0.0000	0.0120	0.0139	0.0000	-0.0135	0.0000
AT. 20 SI	X	-0.0090	0.0000	0.0000	0.0298	0.0000	0.0061
	Y	-0.0041	0.0000	0.0000	0.0044	0.0000	-0.0142
	Z	0.0000	-0.0120	-0.0139	0.0000	-0.0135	0.0000
AT. 21 SI	X	-0.0090	0.0000	0.0000	-0.0298	0.0000	0.0061
	Y	0.0041	0.0000	0.0000	0.0044	0.0000	0.0142
	Z	0.0000	-0.0120	0.0139	0.0000	0.0135	0.0000
AT. 22 SI	X	-0.0090	0.0000	0.0000	0.0298	0.0000	0.0061
	Y	0.0041	0.0000	0.0000	-0.0044	0.0000	0.0142
	Z	0.0000	0.0120	-0.0139	0.0000	0.0135	0.0000
AT. 23 O	X	0.0164	-0.0186	-0.0057	-0.0035	0.0199	-0.0051
	Y	0.0068	0.0117	0.0020	-0.0027	-0.0079	0.0123
	Z	-0.0015	-0.0345	-0.0109	-0.0035	0.0265	-0.0038
AT. 24 O	X	0.0164	-0.0186	-0.0057	0.0035	-0.0199	-0.0051
	Y	0.0068	0.0117	0.0020	0.0027	0.0079	0.0123
	Z	0.0015	0.0345	0.0109	-0.0035	0.0265	0.0038
AT. 25 O	X	0.0164	-0.0186	0.0057	-0.0035	0.0199	-0.0051
	Y	-0.0068	-0.0117	0.0020	0.0027	0.0079	-0.0123
	Z	0.0015	0.0345	-0.0109	0.0035	-0.0265	0.0038
AT. 26 O	X	0.0164	-0.0186	0.0057	0.0035	-0.0199	-0.0051
	Y	-0.0068	-0.0117	0.0020	-0.0027	-0.0079	-0.0123
	Z	-0.0015	-0.0345	0.0109	0.0035	-0.0265	-0.0038
AT. 27 O	X	0.0164	0.0186	0.0057	0.0035	0.0199	-0.0051
	Y	0.0068	-0.0117	-0.0020	0.0027	-0.0079	0.0123
	Z	-0.0015	0.0345	0.0109	0.0035	0.0265	-0.0038
AT. 28 O	X	0.0164	0.0186	0.0057	-0.0035	-0.0199	-0.0051
	Y	0.0068	-0.0117	-0.0020	-0.0027	0.0079	0.0123
	Z	0.0015	-0.0345	-0.0109	0.0035	0.0265	0.0038
AT. 29 O	X	0.0164	0.0186	-0.0057	0.0035	0.0199	-0.0051
	Y	-0.0068	0.0117	-0.0020	-0.0027	0.0079	-0.0123
	Z	0.0015	-0.0345	0.0109	-0.0035	-0.0265	0.0038
AT. 30 O	X	0.0164	0.0186	-0.0057	-0.0035	-0.0199	-0.0051
	Y	-0.0068	0.0117	-0.0020	0.0027	-0.0079	-0.0123
	Z	-0.0015	0.0345	-0.0109	-0.0035	-0.0265	-0.0038
AT. 31 O	X	-0.0130	0.0104	0.0135	0.0098	-0.0032	-0.0049
	Y	0.0112	0.0048	0.0158	-0.0137	0.0230	-0.0405

	Z	-0.0059	-0.0064	-0.0276	0.0038	-0.0199	0.0271
AT. 32	O X	-0.0130	0.0104	0.0135	-0.0098	0.0032	-0.0049
	Y	0.0112	0.0048	0.0158	0.0137	-0.0230	-0.0405
	Z	0.0059	0.0064	0.0276	0.0038	-0.0199	-0.0271
AT. 33	O X	-0.0130	0.0104	-0.0135	0.0098	-0.0032	-0.0049
	Y	-0.0112	-0.0048	0.0158	0.0137	-0.0230	0.0405
	Z	0.0059	0.0064	-0.0276	-0.0038	0.0199	-0.0271
AT. 34	O X	-0.0130	0.0104	-0.0135	-0.0098	0.0032	-0.0049
	Y	-0.0112	-0.0048	0.0158	-0.0137	0.0230	0.0405
	Z	-0.0059	-0.0064	0.0276	-0.0038	0.0199	0.0271
AT. 35	O X	-0.0130	-0.0104	-0.0135	-0.0098	-0.0032	-0.0049
	Y	0.0112	-0.0048	-0.0158	0.0137	0.0230	-0.0405
	Z	-0.0059	0.0064	0.0276	-0.0038	-0.0199	0.0271
AT. 36	O X	-0.0130	-0.0104	-0.0135	0.0098	0.0032	-0.0049
	Y	0.0112	-0.0048	-0.0158	-0.0137	-0.0230	-0.0405
	Z	0.0059	-0.0064	-0.0276	-0.0038	-0.0199	-0.0271
AT. 37	O X	-0.0130	-0.0104	0.0135	-0.0098	-0.0032	-0.0049
	Y	-0.0112	0.0048	-0.0158	-0.0137	-0.0230	0.0405
	Z	0.0059	-0.0064	0.0276	0.0038	0.0199	-0.0271
AT. 38	O X	-0.0130	-0.0104	0.0135	0.0098	0.0032	-0.0049
	Y	-0.0112	0.0048	-0.0158	0.0137	0.0230	0.0405
	Z	-0.0059	0.0064	-0.0276	0.0038	0.0199	0.0271
AT. 39	O X	-0.0215	-0.0091	0.0232	0.0199	-0.0172	-0.0005
	Y	0.0064	-0.0083	0.0058	0.0031	-0.0063	0.0090
	Z	0.0065	0.0192	-0.0246	-0.0025	0.0218	0.0038
AT. 40	O X	-0.0215	-0.0091	0.0232	-0.0199	0.0172	-0.0005
	Y	0.0064	-0.0083	0.0058	-0.0031	0.0063	0.0090
	Z	-0.0065	-0.0192	0.0246	-0.0025	0.0218	-0.0038
AT. 41	O X	-0.0215	-0.0091	-0.0232	0.0199	-0.0172	-0.0005
	Y	-0.0064	0.0083	0.0058	-0.0031	0.0063	-0.0090
	Z	-0.0065	-0.0192	-0.0246	0.0025	-0.0218	-0.0038
AT. 42	O X	-0.0215	-0.0091	-0.0232	-0.0199	0.0172	-0.0005
	Y	-0.0064	0.0083	0.0058	0.0031	-0.0063	-0.0090
	Z	0.0065	0.0192	0.0246	0.0025	-0.0218	0.0038
AT. 43	O X	-0.0215	0.0091	-0.0232	-0.0199	-0.0172	-0.0005
	Y	0.0064	0.0083	-0.0058	-0.0031	-0.0063	0.0090
	Z	0.0065	-0.0192	0.0246	0.0025	0.0218	0.0038
AT. 44	O X	-0.0215	0.0091	-0.0232	0.0199	0.0172	-0.0005
	Y	0.0064	0.0083	-0.0058	0.0031	0.0063	0.0090
	Z	-0.0065	0.0192	-0.0246	0.0025	0.0218	-0.0038
AT. 45	O X	-0.0215	0.0091	0.0232	-0.0199	-0.0172	-0.0005
	Y	-0.0064	-0.0083	-0.0058	0.0031	0.0063	-0.0090
	Z	-0.0065	0.0192	0.0246	-0.0025	-0.0218	-0.0038
AT. 46	O X	-0.0215	0.0091	0.0232	0.0199	0.0172	-0.0005
	Y	-0.0064	-0.0083	-0.0058	-0.0031	-0.0063	-0.0090
	Z	0.0065	-0.0192	-0.0246	-0.0025	-0.0218	0.0038
AT. 47	O X	-0.0082	0.0000	0.0000	-0.0276	0.0000	0.0077
	Y	0.0129	0.0000	0.0000	-0.0073	0.0000	-0.0035
	Z	0.0000	-0.0131	-0.0035	0.0000	-0.0154	0.0000
AT. 48	O X	-0.0082	0.0000	0.0000	0.0276	0.0000	0.0077
	Y	0.0129	0.0000	0.0000	0.0073	0.0000	-0.0035
	Z	0.0000	0.0131	0.0035	0.0000	-0.0154	0.0000
AT. 49	O X	-0.0082	0.0000	0.0000	-0.0276	0.0000	0.0077
	Y	-0.0129	0.0000	0.0000	0.0073	0.0000	0.0035

	Z	0.0000	0.0131	-0.0035	0.0000	0.0154	0.0000
AT. 50	O X	-0.0082	0.0000	0.0000	0.0276	0.0000	0.0077
	Y	-0.0129	0.0000	0.0000	-0.0073	0.0000	0.0035
	Z	0.0000	-0.0131	0.0035	0.0000	0.0154	0.0000
AT. 51	O X	0.0387	0.0000	0.0000	-0.0107	0.0000	0.0131
	Y	0.0140	0.0000	0.0000	-0.0238	0.0000	0.0132
	Z	0.0000	0.0021	0.0007	0.0000	-0.0011	0.0000
AT. 52	O X	0.0387	0.0000	0.0000	0.0107	0.0000	0.0131
	Y	0.0140	0.0000	0.0000	0.0238	0.0000	0.0132
	Z	0.0000	-0.0021	-0.0007	0.0000	-0.0011	0.0000
AT. 53	O X	0.0387	0.0000	0.0000	-0.0107	0.0000	0.0131
	Y	-0.0140	0.0000	0.0000	0.0238	0.0000	-0.0132
	Z	0.0000	-0.0021	0.0007	0.0000	0.0011	0.0000
AT. 54	O X	0.0387	0.0000	0.0000	0.0107	0.0000	0.0131
	Y	-0.0140	0.0000	0.0000	-0.0238	0.0000	-0.0132
	Z	0.0000	0.0021	-0.0007	0.0000	0.0011	0.0000
AT. 55	O X	0.0244	0.0000	0.0000	0.0017	0.0000	0.0047
	Y	-0.0117	0.0000	0.0000	-0.0119	0.0000	-0.0114
	Z	0.0000	-0.0155	-0.0034	0.0000	-0.0095	0.0000
AT. 56	O X	0.0244	0.0000	0.0000	-0.0017	0.0000	0.0047
	Y	-0.0117	0.0000	0.0000	0.0119	0.0000	-0.0114
	Z	0.0000	0.0155	0.0034	0.0000	-0.0095	0.0000
AT. 57	O X	0.0244	0.0000	0.0000	0.0017	0.0000	0.0047
	Y	0.0117	0.0000	0.0000	0.0119	0.0000	0.0114
	Z	0.0000	0.0155	-0.0034	0.0000	0.0095	0.0000
AT. 58	O X	0.0244	0.0000	0.0000	-0.0017	0.0000	0.0047
	Y	0.0117	0.0000	0.0000	-0.0119	0.0000	0.0114
	Z	0.0000	-0.0155	0.0034	0.0000	0.0095	0.0000

FREQ(CM\*\*-1) 271.57 271.59 288.15 292.56 297.27 297.73

AT. 1	MG X	0.0000	0.0000	-0.0135	0.0000	0.0000	0.0171
	Y	-0.0204	-0.0062	0.0000	0.0459	0.0019	0.0000
	Z	0.0379	-0.0186	0.0000	0.0008	0.0205	0.0000
AT. 2	MG X	0.0000	0.0000	-0.0135	0.0000	0.0000	-0.0171
	Y	0.0204	-0.0062	0.0000	-0.0459	-0.0019	0.0000
	Z	0.0379	0.0186	0.0000	0.0008	0.0205	0.0000
AT. 3	MG X	0.0000	0.0000	0.0135	0.0000	0.0000	-0.0171
	Y	0.0204	-0.0062	0.0000	0.0459	-0.0019	0.0000
	Z	-0.0379	-0.0186	0.0000	0.0008	-0.0205	0.0000
AT. 4	MG X	0.0000	0.0000	0.0135	0.0000	0.0000	0.0171
	Y	-0.0204	-0.0062	0.0000	-0.0459	0.0019	0.0000
	Z	-0.0379	0.0186	0.0000	0.0008	-0.0205	0.0000
AT. 5	AL X	0.0000	0.0196	0.0302	0.0000	0.0000	0.0000
	Y	0.0000	0.0130	0.0243	0.0000	0.0000	0.0000
	Z	0.0131	0.0000	0.0000	0.0032	0.0046	-0.0015
AT. 6	AL X	0.0000	-0.0196	0.0302	0.0000	0.0000	0.0000
	Y	0.0000	0.0130	-0.0243	0.0000	0.0000	0.0000
	Z	0.0131	0.0000	0.0000	0.0032	0.0046	0.0015
AT. 7	AL X	0.0000	0.0196	-0.0302	0.0000	0.0000	0.0000
	Y	0.0000	0.0130	-0.0243	0.0000	0.0000	0.0000
	Z	-0.0131	0.0000	0.0000	0.0032	-0.0046	0.0015
AT. 8	AL X	0.0000	-0.0196	-0.0302	0.0000	0.0000	0.0000
	Y	0.0000	0.0130	0.0243	0.0000	0.0000	0.0000

	Z	-0.0131	0.0000	0.0000	0.0032	-0.0046	-0.0015
AT. 9	AL X	0.0013	-0.0113	0.0000	0.0000	-0.0041	-0.0058
	Y	0.0088	-0.0046	0.0000	0.0000	-0.0265	-0.0010
	Z	0.0000	0.0000	0.0065	-0.0159	0.0000	0.0000
AT. 10	AL X	-0.0013	-0.0113	0.0000	0.0000	0.0041	0.0058
	Y	-0.0088	-0.0046	0.0000	0.0000	0.0265	0.0010
	Z	0.0000	0.0000	-0.0065	-0.0159	0.0000	0.0000
AT. 11	AL X	-0.0013	0.0113	0.0000	0.0000	0.0041	-0.0058
	Y	0.0088	-0.0046	0.0000	0.0000	-0.0265	0.0010
	Z	0.0000	0.0000	-0.0065	-0.0159	0.0000	0.0000
AT. 12	AL X	0.0013	0.0113	0.0000	0.0000	-0.0041	0.0058
	Y	-0.0088	-0.0046	0.0000	0.0000	0.0265	-0.0010
	Z	0.0000	0.0000	0.0065	-0.0159	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	-0.0060	0.0000	0.0000	0.0000
	Y	0.0000	0.0184	0.0000	0.0000	0.0000	0.0000
	Z	0.0017	0.0000	0.0000	-0.0091	-0.0365	0.0000
AT. 14	SI X	0.0000	0.0000	0.0060	0.0000	0.0000	0.0000
	Y	0.0000	0.0184	0.0000	0.0000	0.0000	0.0000
	Z	-0.0017	0.0000	0.0000	-0.0091	0.0365	0.0000
AT. 15	SI X	0.0099	0.0039	0.0000	0.0000	-0.0011	0.0009
	Y	0.0131	0.0043	0.0000	0.0000	-0.0011	0.0127
	Z	0.0000	0.0000	0.0026	-0.0015	0.0000	0.0000
AT. 16	SI X	-0.0099	0.0039	0.0000	0.0000	0.0011	-0.0009
	Y	-0.0131	0.0043	0.0000	0.0000	0.0011	-0.0127
	Z	0.0000	0.0000	-0.0026	-0.0015	0.0000	0.0000
AT. 17	SI X	-0.0099	-0.0039	0.0000	0.0000	0.0011	0.0009
	Y	0.0131	0.0043	0.0000	0.0000	-0.0011	-0.0127
	Z	0.0000	0.0000	-0.0026	-0.0015	0.0000	0.0000
AT. 18	SI X	0.0099	-0.0039	0.0000	0.0000	-0.0011	-0.0009
	Y	-0.0131	0.0043	0.0000	0.0000	0.0011	0.0127
	Z	0.0000	0.0000	0.0026	-0.0015	0.0000	0.0000
AT. 19	SI X	0.0073	0.0003	0.0000	0.0000	0.0029	0.0030
	Y	0.0119	-0.0112	0.0000	0.0000	0.0072	0.0188
	Z	0.0000	0.0000	-0.0066	0.0077	0.0000	0.0000
AT. 20	SI X	-0.0073	0.0003	0.0000	0.0000	-0.0029	-0.0030
	Y	-0.0119	-0.0112	0.0000	0.0000	-0.0072	-0.0188
	Z	0.0000	0.0000	0.0066	0.0077	0.0000	0.0000
AT. 21	SI X	-0.0073	-0.0003	0.0000	0.0000	-0.0029	0.0030
	Y	0.0119	-0.0112	0.0000	0.0000	0.0072	-0.0188
	Z	0.0000	0.0000	0.0066	0.0077	0.0000	0.0000
AT. 22	SI X	0.0073	-0.0003	0.0000	0.0000	0.0029	-0.0030
	Y	-0.0119	-0.0112	0.0000	0.0000	-0.0072	0.0188
	Z	0.0000	0.0000	-0.0066	0.0077	0.0000	0.0000
AT. 23	O X	-0.0037	-0.0164	0.0077	-0.0015	0.0090	0.0168
	Y	0.0078	0.0195	-0.0204	0.0018	-0.0028	-0.0088
	Z	0.0056	-0.0117	0.0063	-0.0009	0.0060	0.0109
AT. 24	O X	0.0037	-0.0164	0.0077	0.0015	-0.0090	-0.0168
	Y	-0.0078	0.0195	-0.0204	-0.0018	0.0028	0.0088
	Z	0.0056	0.0117	-0.0063	-0.0009	0.0060	0.0109
AT. 25	O X	0.0037	0.0164	0.0077	0.0015	-0.0090	0.0168
	Y	0.0078	0.0195	0.0204	0.0018	-0.0028	0.0088
	Z	0.0056	-0.0117	-0.0063	-0.0009	0.0060	-0.0109
AT. 26	O X	-0.0037	0.0164	0.0077	-0.0015	0.0090	-0.0168
	Y	-0.0078	0.0195	0.0204	-0.0018	0.0028	-0.0088



	Z	0.0056	0.0117	0.0063	-0.0009	0.0060	-0.0109
AT. 27	O X	0.0037	-0.0164	-0.0077	-0.0015	-0.0090	-0.0168
	Y	-0.0078	0.0195	0.0204	0.0018	0.0028	0.0088
	Z	-0.0056	-0.0117	-0.0063	-0.0009	-0.0060	-0.0109
AT. 28	O X	-0.0037	-0.0164	-0.0077	0.0015	0.0090	0.0168
	Y	0.0078	0.0195	0.0204	-0.0018	-0.0028	-0.0088
	Z	-0.0056	0.0117	0.0063	-0.0009	-0.0060	-0.0109
AT. 29	O X	-0.0037	0.0164	-0.0077	0.0015	0.0090	-0.0168
	Y	-0.0078	0.0195	-0.0204	0.0018	0.0028	-0.0088
	Z	-0.0056	-0.0117	0.0063	-0.0009	-0.0060	0.0109
AT. 30	O X	0.0037	0.0164	-0.0077	-0.0015	-0.0090	0.0168
	Y	0.0078	0.0195	-0.0204	-0.0018	-0.0028	0.0088
	Z	-0.0056	0.0117	-0.0063	-0.0009	-0.0060	0.0109
AT. 31	O X	-0.0054	0.0141	0.0011	0.0098	-0.0033	-0.0002
	Y	0.0023	0.0101	-0.0056	-0.0202	-0.0084	-0.0004
	Z	0.0080	-0.0076	-0.0006	0.0014	-0.0166	0.0005
AT. 32	O X	0.0054	0.0141	0.0011	-0.0098	0.0033	0.0002
	Y	-0.0023	0.0101	-0.0056	0.0202	0.0084	0.0004
	Z	0.0080	0.0076	0.0006	0.0014	-0.0166	0.0005
AT. 33	O X	0.0054	-0.0141	0.0011	-0.0098	0.0033	-0.0002
	Y	0.0023	0.0101	0.0056	-0.0202	-0.0084	0.0004
	Z	0.0080	-0.0076	0.0006	0.0014	-0.0166	-0.0005
AT. 34	O X	-0.0054	-0.0141	0.0011	0.0098	-0.0033	0.0002
	Y	-0.0023	0.0101	0.0056	0.0202	0.0084	-0.0004
	Z	0.0080	0.0076	-0.0006	0.0014	-0.0166	-0.0005
AT. 35	O X	0.0054	0.0141	-0.0011	0.0098	0.0033	0.0002
	Y	-0.0023	0.0101	0.0056	-0.0202	0.0084	0.0004
	Z	-0.0080	-0.0076	0.0006	0.0014	0.0166	-0.0005
AT. 36	O X	-0.0054	0.0141	-0.0011	-0.0098	-0.0033	-0.0002
	Y	0.0023	0.0101	0.0056	0.0202	-0.0084	-0.0004
	Z	-0.0080	0.0076	-0.0006	0.0014	0.0166	-0.0005
AT. 37	O X	-0.0054	-0.0141	-0.0011	-0.0098	-0.0033	0.0002
	Y	-0.0023	0.0101	-0.0056	-0.0202	0.0084	-0.0004
	Z	-0.0080	-0.0076	-0.0006	0.0014	0.0166	0.0005
AT. 38	O X	0.0054	-0.0141	-0.0011	0.0098	0.0033	-0.0002
	Y	0.0023	0.0101	-0.0056	0.0202	-0.0084	0.0004
	Z	-0.0080	0.0076	0.0006	0.0014	0.0166	0.0005
AT. 39	O X	-0.0063	0.0036	0.0151	0.0041	0.0036	0.0061
	Y	-0.0199	-0.0081	-0.0096	0.0050	-0.0096	0.0227
	Z	0.0143	-0.0001	-0.0083	0.0005	-0.0001	-0.0059
AT. 40	O X	0.0063	0.0036	0.0151	-0.0041	-0.0036	-0.0061
	Y	0.0199	-0.0081	-0.0096	-0.0050	0.0096	-0.0227
	Z	0.0143	0.0001	0.0083	0.0005	-0.0001	-0.0059
AT. 41	O X	0.0063	-0.0036	0.0151	-0.0041	-0.0036	0.0061
	Y	-0.0199	-0.0081	0.0096	0.0050	-0.0096	-0.0227
	Z	0.0143	-0.0001	0.0083	0.0005	-0.0001	0.0059
AT. 42	O X	-0.0063	-0.0036	0.0151	0.0041	0.0036	-0.0061
	Y	0.0199	-0.0081	0.0096	-0.0050	0.0096	0.0227
	Z	0.0143	0.0001	-0.0083	0.0005	-0.0001	0.0059
AT. 43	O X	0.0063	0.0036	-0.0151	0.0041	-0.0036	-0.0061
	Y	0.0199	-0.0081	0.0096	0.0050	0.0096	-0.0227
	Z	-0.0143	-0.0001	0.0083	0.0005	0.0001	0.0059
AT. 44	O X	-0.0063	0.0036	-0.0151	-0.0041	0.0036	0.0061
	Y	-0.0199	-0.0081	0.0096	-0.0050	-0.0096	0.0227

	Z	-0.0143	0.0001	-0.0083	0.0005	0.0001	0.0059
AT. 45 O	X	-0.0063	-0.0036	-0.0151	-0.0041	0.0036	-0.0061
	Y	0.0199	-0.0081	-0.0096	0.0050	0.0096	0.0227
	Z	-0.0143	-0.0001	-0.0083	0.0005	0.0001	-0.0059
AT. 46 O	X	0.0063	-0.0036	-0.0151	0.0041	-0.0036	0.0061
	Y	-0.0199	-0.0081	-0.0096	-0.0050	-0.0096	-0.0227
	Z	-0.0143	0.0001	0.0083	0.0005	0.0001	-0.0059
AT. 47 O	X	0.0067	0.0029	0.0000	0.0000	0.0045	0.0081
	Y	-0.0166	-0.0432	0.0000	0.0000	0.0047	-0.0210
	Z	0.0000	0.0000	-0.0309	0.0213	0.0000	0.0000
AT. 48 O	X	-0.0067	0.0029	0.0000	0.0000	-0.0045	-0.0081
	Y	0.0166	-0.0432	0.0000	0.0000	-0.0047	0.0210
	Z	0.0000	0.0000	0.0309	0.0213	0.0000	0.0000
AT. 49 O	X	-0.0067	-0.0029	0.0000	0.0000	-0.0045	0.0081
	Y	-0.0166	-0.0432	0.0000	0.0000	0.0047	0.0210
	Z	0.0000	0.0000	0.0309	0.0213	0.0000	0.0000
AT. 50 O	X	0.0067	-0.0029	0.0000	0.0000	0.0045	-0.0081
	Y	0.0166	-0.0432	0.0000	0.0000	-0.0047	-0.0210
	Z	0.0000	0.0000	-0.0309	0.0213	0.0000	0.0000
AT. 51 O	X	-0.0100	-0.0038	0.0000	0.0000	-0.0042	-0.0330
	Y	-0.0072	-0.0028	0.0000	0.0000	-0.0105	-0.0283
	Z	0.0000	0.0000	0.0036	0.0199	0.0000	0.0000
AT. 52 O	X	0.0100	-0.0038	0.0000	0.0000	0.0042	0.0330
	Y	0.0072	-0.0028	0.0000	0.0000	0.0105	0.0283
	Z	0.0000	0.0000	-0.0036	0.0199	0.0000	0.0000
AT. 53 O	X	0.0100	0.0038	0.0000	0.0000	0.0042	-0.0330
	Y	-0.0072	-0.0028	0.0000	0.0000	-0.0105	0.0283
	Z	0.0000	0.0000	-0.0036	0.0199	0.0000	0.0000
AT. 54 O	X	-0.0100	0.0038	0.0000	0.0000	-0.0042	0.0330
	Y	0.0072	-0.0028	0.0000	0.0000	0.0105	-0.0283
	Z	0.0000	0.0000	0.0036	0.0199	0.0000	0.0000
AT. 55 O	X	0.0268	0.0142	0.0000	0.0000	-0.0399	-0.0081
	Y	0.0052	-0.0070	0.0000	0.0000	0.0158	0.0175
	Z	0.0000	0.0000	-0.0261	-0.0261	0.0000	0.0000
AT. 56 O	X	-0.0268	0.0142	0.0000	0.0000	0.0399	0.0081
	Y	-0.0052	-0.0070	0.0000	0.0000	-0.0158	-0.0175
	Z	0.0000	0.0000	0.0261	-0.0261	0.0000	0.0000
AT. 57 O	X	-0.0268	-0.0142	0.0000	0.0000	0.0399	-0.0081
	Y	0.0052	-0.0070	0.0000	0.0000	0.0158	-0.0175
	Z	0.0000	0.0000	0.0261	-0.0261	0.0000	0.0000
AT. 58 O	X	0.0268	-0.0142	0.0000	0.0000	-0.0399	0.0081
	Y	-0.0052	-0.0070	0.0000	0.0000	-0.0158	0.0175
	Z	0.0000	0.0000	-0.0261	-0.0261	0.0000	0.0000

FREQ(CM\*\*-1) 297.93 298.15 298.32 302.65 306.24 314.56

AT. 1 MG	X	0.0000	0.0002	0.0068	0.0000	0.0000	-0.0093
	Y	-0.0037	0.0000	0.0000	-0.0041	0.0091	0.0000
	Z	-0.0384	0.0000	0.0000	-0.0119	-0.0199	0.0000
AT. 2 MG	X	0.0000	0.0002	-0.0068	0.0000	0.0000	0.0093
	Y	-0.0037	0.0000	0.0000	0.0041	0.0091	0.0000
	Z	0.0384	0.0000	0.0000	-0.0119	0.0199	0.0000
AT. 3 MG	X	0.0000	0.0002	0.0068	0.0000	0.0000	0.0093
	Y	0.0037	0.0000	0.0000	0.0041	-0.0091	0.0000

	Z	0.0384	0.0000	0.0000	0.0119	0.0199	0.0000
AT. 4	MG X	0.0000	0.0002	-0.0068	0.0000	0.0000	-0.0093
	Y	0.0037	0.0000	0.0000	-0.0041	-0.0091	0.0000
	Z	-0.0384	0.0000	0.0000	0.0119	-0.0199	0.0000
AT. 5	AL X	0.0249	-0.0077	0.0000	0.0000	-0.0208	0.0000
	Y	0.0180	-0.0046	0.0000	0.0000	-0.0081	0.0000
	Z	0.0000	0.0000	0.0021	-0.0031	0.0000	0.0156
AT. 6	AL X	-0.0249	-0.0077	0.0000	0.0000	0.0208	0.0000
	Y	0.0180	0.0046	0.0000	0.0000	-0.0081	0.0000
	Z	0.0000	0.0000	-0.0021	-0.0031	0.0000	-0.0156
AT. 7	AL X	-0.0249	-0.0077	0.0000	0.0000	0.0208	0.0000
	Y	-0.0180	-0.0046	0.0000	0.0000	0.0081	0.0000
	Z	0.0000	0.0000	0.0021	0.0031	0.0000	-0.0156
AT. 8	AL X	0.0249	-0.0077	0.0000	0.0000	-0.0208	0.0000
	Y	-0.0180	0.0046	0.0000	0.0000	0.0081	0.0000
	Z	0.0000	0.0000	-0.0021	0.0031	0.0000	0.0156
AT. 9	AL X	0.0000	0.0060	0.0000	0.0084	0.0000	0.0003
	Y	0.0000	0.0202	0.0000	-0.0044	0.0000	0.0196
	Z	-0.0144	0.0000	-0.0207	0.0000	-0.0165	0.0000
AT. 10	AL X	0.0000	0.0060	0.0000	-0.0084	0.0000	-0.0003
	Y	0.0000	0.0202	0.0000	0.0044	0.0000	-0.0196
	Z	0.0144	0.0000	-0.0207	0.0000	0.0165	0.0000
AT. 11	AL X	0.0000	0.0060	0.0000	-0.0084	0.0000	0.0003
	Y	0.0000	-0.0202	0.0000	-0.0044	0.0000	-0.0196
	Z	-0.0144	0.0000	0.0207	0.0000	-0.0165	0.0000
AT. 12	AL X	0.0000	0.0060	0.0000	0.0084	0.0000	-0.0003
	Y	0.0000	-0.0202	0.0000	0.0044	0.0000	0.0196
	Z	0.0144	0.0000	0.0207	0.0000	0.0165	0.0000
AT. 13	SI X	0.0000	-0.0049	0.0000	0.0000	0.0000	0.0000
	Y	-0.0094	0.0000	0.0000	0.0000	-0.0268	0.0000
	Z	0.0000	0.0000	0.0000	0.0118	0.0000	0.0000
AT. 14	SI X	0.0000	-0.0049	0.0000	0.0000	0.0000	0.0000
	Y	0.0094	0.0000	0.0000	0.0000	0.0268	0.0000
	Z	0.0000	0.0000	0.0000	-0.0118	0.0000	0.0000
AT. 15	SI X	0.0000	-0.0116	0.0000	0.0026	0.0000	0.0110
	Y	0.0000	0.0013	0.0000	-0.0011	0.0000	0.0178
	Z	0.0099	0.0000	-0.0079	0.0000	0.0005	0.0000
AT. 16	SI X	0.0000	-0.0116	0.0000	-0.0026	0.0000	-0.0110
	Y	0.0000	0.0013	0.0000	0.0011	0.0000	-0.0178
	Z	-0.0099	0.0000	-0.0079	0.0000	-0.0005	0.0000
AT. 17	SI X	0.0000	-0.0116	0.0000	-0.0026	0.0000	0.0110
	Y	0.0000	-0.0013	0.0000	-0.0011	0.0000	-0.0178
	Z	0.0099	0.0000	0.0079	0.0000	0.0005	0.0000
AT. 18	SI X	0.0000	-0.0116	0.0000	0.0026	0.0000	-0.0110
	Y	0.0000	-0.0013	0.0000	0.0011	0.0000	0.0178
	Z	-0.0099	0.0000	0.0079	0.0000	-0.0005	0.0000
AT. 19	SI X	0.0000	0.0086	0.0000	-0.0113	0.0000	0.0098
	Y	0.0000	-0.0065	0.0000	0.0072	0.0000	0.0032
	Z	-0.0122	0.0000	-0.0112	0.0000	0.0025	0.0000
AT. 20	SI X	0.0000	0.0086	0.0000	0.0113	0.0000	-0.0098
	Y	0.0000	-0.0065	0.0000	-0.0072	0.0000	-0.0032
	Z	0.0122	0.0000	-0.0112	0.0000	-0.0025	0.0000
AT. 21	SI X	0.0000	0.0086	0.0000	0.0113	0.0000	0.0098
	Y	0.0000	0.0065	0.0000	0.0072	0.0000	-0.0032

	Z	-0.0122	0.0000	0.0112	0.0000	0.0025	0.0000
AT. 22	SI X	0.0000	0.0086	0.0000	-0.0113	0.0000	-0.0098
	Y	0.0000	0.0065	0.0000	-0.0072	0.0000	0.0032
	Z	0.0122	0.0000	0.0112	0.0000	-0.0025	0.0000
AT. 23	O X	0.0008	-0.0191	0.0107	-0.0210	0.0018	0.0053
	Y	0.0054	0.0109	-0.0070	0.0069	-0.0091	-0.0114
	Z	0.0099	-0.0092	0.0140	-0.0160	0.0040	-0.0028
AT. 24	O X	0.0008	-0.0191	-0.0107	0.0210	0.0018	-0.0053
	Y	0.0054	0.0109	0.0070	-0.0069	-0.0091	0.0114
	Z	-0.0099	0.0092	0.0140	-0.0160	-0.0040	-0.0028
AT. 25	O X	-0.0008	-0.0191	0.0107	0.0210	-0.0018	0.0053
	Y	0.0054	-0.0109	0.0070	0.0069	-0.0091	0.0114
	Z	0.0099	0.0092	-0.0140	-0.0160	0.0040	0.0028
AT. 26	O X	-0.0008	-0.0191	-0.0107	-0.0210	-0.0018	-0.0053
	Y	0.0054	-0.0109	-0.0070	-0.0069	-0.0091	-0.0114
	Z	-0.0099	-0.0092	-0.0140	-0.0160	-0.0040	0.0028
AT. 27	O X	-0.0008	-0.0191	0.0107	0.0210	-0.0018	-0.0053
	Y	-0.0054	0.0109	-0.0070	-0.0069	0.0091	0.0114
	Z	-0.0099	-0.0092	0.0140	0.0160	-0.0040	0.0028
AT. 28	O X	-0.0008	-0.0191	-0.0107	-0.0210	-0.0018	0.0053
	Y	-0.0054	0.0109	0.0070	0.0069	0.0091	-0.0114
	Z	0.0099	0.0092	0.0140	0.0160	0.0040	0.0028
AT. 29	O X	0.0008	-0.0191	0.0107	-0.0210	0.0018	-0.0053
	Y	-0.0054	-0.0109	0.0070	-0.0069	0.0091	-0.0114
	Z	-0.0099	0.0092	-0.0140	0.0160	-0.0040	-0.0028
AT. 30	O X	0.0008	-0.0191	-0.0107	0.0210	0.0018	0.0053
	Y	-0.0054	-0.0109	-0.0070	0.0069	0.0091	0.0114
	Z	0.0099	-0.0092	-0.0140	0.0160	0.0040	-0.0028
AT. 31	O X	0.0086	0.0013	0.0002	0.0104	-0.0033	0.0067
	Y	-0.0003	0.0142	-0.0294	-0.0211	0.0015	-0.0129
	Z	-0.0126	-0.0194	0.0322	0.0158	-0.0156	0.0023
AT. 32	O X	0.0086	0.0013	-0.0002	-0.0104	-0.0033	-0.0067
	Y	-0.0003	0.0142	0.0294	0.0211	0.0015	0.0129
	Z	0.0126	0.0194	0.0322	0.0158	0.0156	0.0023
AT. 33	O X	-0.0086	0.0013	0.0002	-0.0104	0.0033	0.0067
	Y	-0.0003	-0.0142	0.0294	-0.0211	0.0015	0.0129
	Z	-0.0126	0.0194	-0.0322	0.0158	-0.0156	-0.0023
AT. 34	O X	-0.0086	0.0013	-0.0002	0.0104	0.0033	-0.0067
	Y	-0.0003	-0.0142	-0.0294	0.0211	0.0015	-0.0129
	Z	0.0126	-0.0194	-0.0322	0.0158	0.0156	-0.0023
AT. 35	O X	-0.0086	0.0013	0.0002	-0.0104	0.0033	-0.0067
	Y	0.0003	0.0142	-0.0294	0.0211	-0.0015	0.0129
	Z	0.0126	-0.0194	0.0322	-0.0158	0.0156	-0.0023
AT. 36	O X	-0.0086	0.0013	-0.0002	0.0104	0.0033	0.0067
	Y	0.0003	0.0142	0.0294	-0.0211	-0.0015	-0.0129
	Z	-0.0126	0.0194	0.0322	-0.0158	-0.0156	-0.0023
AT. 37	O X	0.0086	0.0013	0.0002	0.0104	-0.0033	-0.0067
	Y	0.0003	-0.0142	0.0294	0.0211	-0.0015	-0.0129
	Z	0.0126	0.0194	-0.0322	-0.0158	0.0156	0.0023
AT. 38	O X	0.0086	0.0013	-0.0002	-0.0104	-0.0033	0.0067
	Y	0.0003	-0.0142	-0.0294	-0.0211	-0.0015	0.0129
	Z	-0.0126	-0.0194	-0.0322	-0.0158	-0.0156	0.0023
AT. 39	O X	0.0017	0.0128	-0.0076	-0.0074	-0.0127	-0.0025
	Y	0.0033	0.0174	-0.0046	-0.0094	-0.0011	-0.0047

	Z	0.0106	-0.0118	0.0143	0.0002	0.0039	0.0037
AT. 40	O X	0.0017	0.0128	0.0076	0.0074	-0.0127	0.0025
	Y	0.0033	0.0174	0.0046	0.0094	-0.0011	0.0047
	Z	-0.0106	0.0118	0.0143	0.0002	-0.0039	0.0037
AT. 41	O X	-0.0017	0.0128	-0.0076	0.0074	0.0127	-0.0025
	Y	0.0033	-0.0174	0.0046	-0.0094	-0.0011	0.0047
	Z	0.0106	0.0118	-0.0143	0.0002	0.0039	-0.0037
AT. 42	O X	-0.0017	0.0128	0.0076	-0.0074	0.0127	0.0025
	Y	0.0033	-0.0174	-0.0046	0.0094	-0.0011	-0.0047
	Z	-0.0106	-0.0118	-0.0143	0.0002	-0.0039	-0.0037
AT. 43	O X	-0.0017	0.0128	-0.0076	0.0074	0.0127	0.0025
	Y	-0.0033	0.0174	-0.0046	0.0094	0.0011	0.0047
	Z	-0.0106	-0.0118	0.0143	-0.0002	-0.0039	-0.0037
AT. 44	O X	-0.0017	0.0128	0.0076	-0.0074	0.0127	-0.0025
	Y	-0.0033	0.0174	0.0046	-0.0094	0.0011	-0.0047
	Z	0.0106	0.0118	0.0143	-0.0002	0.0039	-0.0037
AT. 45	O X	0.0017	0.0128	-0.0076	-0.0074	-0.0127	0.0025
	Y	-0.0033	-0.0174	0.0046	0.0094	0.0011	-0.0047
	Z	-0.0106	0.0118	-0.0143	-0.0002	-0.0039	0.0037
AT. 46	O X	0.0017	0.0128	0.0076	0.0074	-0.0127	-0.0025
	Y	-0.0033	-0.0174	-0.0046	-0.0094	0.0011	0.0047
	Z	0.0106	-0.0118	-0.0143	-0.0002	0.0039	0.0037
AT. 47	O X	0.0000	0.0063	0.0000	-0.0052	0.0000	0.0102
	Y	0.0000	0.0192	0.0000	-0.0168	0.0000	-0.0321
	Z	0.0158	0.0000	-0.0046	0.0000	-0.0422	0.0000
AT. 48	O X	0.0000	0.0063	0.0000	0.0052	0.0000	-0.0102
	Y	0.0000	0.0192	0.0000	0.0168	0.0000	0.0321
	Z	-0.0158	0.0000	-0.0046	0.0000	0.0422	0.0000
AT. 49	O X	0.0000	0.0063	0.0000	0.0052	0.0000	0.0102
	Y	0.0000	-0.0192	0.0000	-0.0168	0.0000	0.0321
	Z	0.0158	0.0000	0.0046	0.0000	-0.0422	0.0000
AT. 50	O X	0.0000	0.0063	0.0000	-0.0052	0.0000	-0.0102
	Y	0.0000	-0.0192	0.0000	0.0168	0.0000	-0.0321
	Z	-0.0158	0.0000	0.0046	0.0000	0.0422	0.0000
AT. 51	O X	0.0000	0.0142	0.0000	-0.0174	0.0000	0.0074
	Y	0.0000	0.0286	0.0000	-0.0271	0.0000	0.0176
	Z	0.0092	0.0000	-0.0065	0.0000	0.0142	0.0000
AT. 52	O X	0.0000	0.0142	0.0000	0.0174	0.0000	-0.0074
	Y	0.0000	0.0286	0.0000	0.0271	0.0000	-0.0176
	Z	-0.0092	0.0000	-0.0065	0.0000	-0.0142	0.0000
AT. 53	O X	0.0000	0.0142	0.0000	0.0174	0.0000	0.0074
	Y	0.0000	-0.0286	0.0000	-0.0271	0.0000	-0.0176
	Z	0.0092	0.0000	0.0065	0.0000	0.0142	0.0000
AT. 54	O X	0.0000	0.0142	0.0000	-0.0174	0.0000	-0.0074
	Y	0.0000	-0.0286	0.0000	0.0271	0.0000	0.0176
	Z	-0.0092	0.0000	0.0065	0.0000	-0.0142	0.0000
AT. 55	O X	0.0000	0.0011	0.0000	-0.0235	0.0000	0.0387
	Y	0.0000	-0.0034	0.0000	0.0088	0.0000	0.0001
	Z	-0.0178	0.0000	-0.0052	0.0000	0.0208	0.0000
AT. 56	O X	0.0000	0.0011	0.0000	0.0235	0.0000	-0.0387
	Y	0.0000	-0.0034	0.0000	-0.0088	0.0000	-0.0001
	Z	0.0178	0.0000	-0.0052	0.0000	-0.0208	0.0000
AT. 57	O X	0.0000	0.0011	0.0000	0.0235	0.0000	0.0387
	Y	0.0000	0.0034	0.0000	0.0088	0.0000	-0.0001

	Z	-0.0178	0.0000	0.0052	0.0000	0.0208	0.0000
AT. 58 O	X	0.0000	0.0011	0.0000	-0.0235	0.0000	-0.0387
	Y	0.0000	0.0034	0.0000	-0.0088	0.0000	0.0001
	Z	0.0178	0.0000	0.0052	0.0000	-0.0208	0.0000

FREQ(CM\*\*-1) 322.13 326.98 330.03 330.12 331.55 340.48

AT. 1 MG	X	0.0535	0.0033	0.0039	0.0094	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0352	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	0.0119	0.0052
AT. 2 MG	X	-0.0535	0.0033	-0.0039	0.0094	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0352	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	-0.0119	-0.0052
AT. 3 MG	X	0.0535	0.0033	-0.0039	-0.0094	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0352	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	0.0119	0.0052
AT. 4 MG	X	-0.0535	0.0033	0.0039	-0.0094	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0352	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	-0.0119	-0.0052
AT. 5 AL	X	0.0000	-0.0112	0.0000	0.0155	0.0033	-0.0015
	Y	0.0000	0.0256	0.0000	-0.0217	0.0042	-0.0052
	Z	0.0042	0.0000	0.0274	0.0000	0.0000	0.0000
AT. 6 AL	X	0.0000	-0.0112	0.0000	0.0155	-0.0033	0.0015
	Y	0.0000	-0.0256	0.0000	0.0217	0.0042	-0.0052
	Z	-0.0042	0.0000	-0.0274	0.0000	0.0000	0.0000
AT. 7 AL	X	0.0000	-0.0112	0.0000	-0.0155	0.0033	-0.0015
	Y	0.0000	0.0256	0.0000	0.0217	0.0042	-0.0052
	Z	0.0042	0.0000	-0.0274	0.0000	0.0000	0.0000
AT. 8 AL	X	0.0000	-0.0112	0.0000	-0.0155	-0.0033	0.0015
	Y	0.0000	-0.0256	0.0000	-0.0217	0.0042	-0.0052
	Z	-0.0042	0.0000	0.0274	0.0000	0.0000	0.0000
AT. 9 AL	X	0.0000	-0.0066	0.0058	0.0000	-0.0042	-0.0014
	Y	0.0000	-0.0028	-0.0073	0.0000	0.0106	0.0037
	Z	-0.0114	0.0000	0.0000	0.0092	0.0000	0.0000
AT. 10 AL	X	0.0000	-0.0066	-0.0058	0.0000	-0.0042	-0.0014
	Y	0.0000	-0.0028	0.0073	0.0000	0.0106	0.0037
	Z	-0.0114	0.0000	0.0000	-0.0092	0.0000	0.0000
AT. 11 AL	X	0.0000	-0.0066	0.0058	0.0000	0.0042	0.0014
	Y	0.0000	0.0028	0.0073	0.0000	0.0106	0.0037
	Z	0.0114	0.0000	0.0000	-0.0092	0.0000	0.0000
AT. 12 AL	X	0.0000	-0.0066	-0.0058	0.0000	0.0042	0.0014
	Y	0.0000	0.0028	-0.0073	0.0000	0.0106	0.0037
	Z	0.0114	0.0000	0.0000	0.0092	0.0000	0.0000
AT. 13 SI	X	0.0000	0.0248	0.0000	-0.0233	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0038	-0.0062
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14 SI	X	0.0000	0.0248	0.0000	0.0233	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0038	-0.0062
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15 SI	X	0.0000	-0.0013	0.0071	0.0000	-0.0066	-0.0036
	Y	0.0000	0.0040	0.0082	0.0000	0.0184	0.0065
	Z	0.0088	0.0000	0.0000	-0.0001	0.0000	0.0000
AT. 16 SI	X	0.0000	-0.0013	-0.0071	0.0000	-0.0066	-0.0036
	Y	0.0000	0.0040	-0.0082	0.0000	0.0184	0.0065

	Z	0.0088	0.0000	0.0000	0.0001	0.0000	0.0000
AT. 17	SI X	0.0000	-0.0013	0.0071	0.0000	0.0066	0.0036
	Y	0.0000	-0.0040	-0.0082	0.0000	0.0184	0.0065
	Z	-0.0088	0.0000	0.0000	0.0001	0.0000	0.0000
AT. 18	SI X	0.0000	-0.0013	-0.0071	0.0000	0.0066	0.0036
	Y	0.0000	-0.0040	0.0082	0.0000	0.0184	0.0065
	Z	-0.0088	0.0000	0.0000	-0.0001	0.0000	0.0000
AT. 19	SI X	0.0000	-0.0065	-0.0060	0.0000	0.0113	0.0018
	Y	0.0000	-0.0110	0.0042	0.0000	0.0072	0.0024
	Z	0.0001	0.0000	0.0000	0.0027	0.0000	0.0000
AT. 20	SI X	0.0000	-0.0065	0.0060	0.0000	0.0113	0.0018
	Y	0.0000	-0.0110	-0.0042	0.0000	0.0072	0.0024
	Z	0.0001	0.0000	0.0000	-0.0027	0.0000	0.0000
AT. 21	SI X	0.0000	-0.0065	-0.0060	0.0000	-0.0113	-0.0018
	Y	0.0000	0.0110	-0.0042	0.0000	0.0072	0.0024
	Z	-0.0001	0.0000	0.0000	-0.0027	0.0000	0.0000
AT. 22	SI X	0.0000	-0.0065	0.0060	0.0000	-0.0113	-0.0018
	Y	0.0000	0.0110	0.0042	0.0000	0.0072	0.0024
	Z	-0.0001	0.0000	0.0000	0.0027	0.0000	0.0000
AT. 23	O X	0.0075	-0.0004	-0.0002	-0.0006	0.0150	-0.0184
	Y	0.0009	-0.0198	-0.0105	0.0182	0.0065	0.0115
	Z	-0.0019	0.0007	-0.0056	-0.0032	0.0066	-0.0184
AT. 24	O X	-0.0075	-0.0004	0.0002	-0.0006	0.0150	-0.0184
	Y	-0.0009	-0.0198	0.0105	0.0182	0.0065	0.0115
	Z	-0.0019	-0.0007	-0.0056	0.0032	-0.0066	0.0184
AT. 25	O X	0.0075	-0.0004	-0.0002	-0.0006	-0.0150	0.0184
	Y	-0.0009	0.0198	0.0105	-0.0182	0.0065	0.0115
	Z	0.0019	-0.0007	0.0056	0.0032	0.0066	-0.0184
AT. 26	O X	-0.0075	-0.0004	0.0002	-0.0006	-0.0150	0.0184
	Y	0.0009	0.0198	-0.0105	-0.0182	0.0065	0.0115
	Z	0.0019	0.0007	0.0056	-0.0032	-0.0066	0.0184
AT. 27	O X	0.0075	-0.0004	0.0002	0.0006	0.0150	-0.0184
	Y	0.0009	-0.0198	0.0105	-0.0182	0.0065	0.0115
	Z	-0.0019	0.0007	0.0056	0.0032	0.0066	-0.0184
AT. 28	O X	-0.0075	-0.0004	-0.0002	0.0006	0.0150	-0.0184
	Y	-0.0009	-0.0198	-0.0105	-0.0182	0.0065	0.0115
	Z	-0.0019	-0.0007	0.0056	-0.0032	-0.0066	0.0184
AT. 29	O X	0.0075	-0.0004	0.0002	0.0006	-0.0150	0.0184
	Y	-0.0009	0.0198	-0.0105	0.0182	0.0065	0.0115
	Z	0.0019	-0.0007	-0.0056	-0.0032	0.0066	-0.0184
AT. 30	O X	-0.0075	-0.0004	-0.0002	0.0006	-0.0150	0.0184
	Y	0.0009	0.0198	0.0105	0.0182	0.0065	0.0115
	Z	0.0019	0.0007	-0.0056	0.0032	-0.0066	0.0184
AT. 31	O X	-0.0082	0.0185	-0.0033	-0.0166	-0.0012	-0.0045
	Y	0.0111	-0.0013	0.0223	-0.0083	-0.0147	-0.0031
	Z	-0.0035	0.0058	-0.0147	-0.0001	0.0111	0.0015
AT. 32	O X	0.0082	0.0185	0.0033	-0.0166	-0.0012	-0.0045
	Y	-0.0111	-0.0013	-0.0223	-0.0083	-0.0147	-0.0031
	Z	-0.0035	-0.0058	-0.0147	0.0001	-0.0111	-0.0015
AT. 33	O X	-0.0082	0.0185	-0.0033	-0.0166	0.0012	0.0045
	Y	-0.0111	0.0013	-0.0223	0.0083	-0.0147	-0.0031
	Z	0.0035	-0.0058	0.0147	0.0001	0.0111	0.0015
AT. 34	O X	0.0082	0.0185	0.0033	-0.0166	0.0012	0.0045
	Y	0.0111	0.0013	0.0223	0.0083	-0.0147	-0.0031

	Z	0.0035	0.0058	0.0147	-0.0001	-0.0111	-0.0015
AT. 35	O X	-0.0082	0.0185	0.0033	0.0166	-0.0012	-0.0045
	Y	0.0111	-0.0013	-0.0223	0.0083	-0.0147	-0.0031
	Z	-0.0035	0.0058	0.0147	0.0001	0.0111	0.0015
AT. 36	O X	0.0082	0.0185	-0.0033	0.0166	-0.0012	-0.0045
	Y	-0.0111	-0.0013	0.0223	0.0083	-0.0147	-0.0031
	Z	-0.0035	-0.0058	0.0147	-0.0001	-0.0111	-0.0015
AT. 37	O X	-0.0082	0.0185	0.0033	0.0166	0.0012	0.0045
	Y	-0.0111	0.0013	0.0223	-0.0083	-0.0147	-0.0031
	Z	0.0035	-0.0058	-0.0147	-0.0001	0.0111	0.0015
AT. 38	O X	0.0082	0.0185	-0.0033	0.0166	0.0012	0.0045
	Y	0.0111	0.0013	-0.0223	-0.0083	-0.0147	-0.0031
	Z	0.0035	0.0058	-0.0147	0.0001	-0.0111	-0.0015
AT. 39	O X	0.0033	-0.0082	-0.0087	0.0173	-0.0062	-0.0212
	Y	0.0004	0.0206	-0.0177	-0.0058	-0.0017	-0.0129
	Z	-0.0006	-0.0043	0.0201	-0.0021	0.0020	0.0180
AT. 40	O X	-0.0033	-0.0082	0.0087	0.0173	-0.0062	-0.0212
	Y	-0.0004	0.0206	0.0177	-0.0058	-0.0017	-0.0129
	Z	-0.0006	0.0043	0.0201	0.0021	-0.0020	-0.0180
AT. 41	O X	0.0033	-0.0082	-0.0087	0.0173	0.0062	0.0212
	Y	-0.0004	-0.0206	0.0177	0.0058	-0.0017	-0.0129
	Z	0.0006	0.0043	-0.0201	0.0021	0.0020	0.0180
AT. 42	O X	-0.0033	-0.0082	0.0087	0.0173	0.0062	0.0212
	Y	0.0004	-0.0206	-0.0177	0.0058	-0.0017	-0.0129
	Z	0.0006	-0.0043	-0.0201	-0.0021	-0.0020	-0.0180
AT. 43	O X	0.0033	-0.0082	0.0087	-0.0173	-0.0062	-0.0212
	Y	0.0004	0.0206	0.0177	0.0058	-0.0017	-0.0129
	Z	-0.0006	-0.0043	-0.0201	0.0021	0.0020	0.0180
AT. 44	O X	-0.0033	-0.0082	-0.0087	-0.0173	-0.0062	-0.0212
	Y	-0.0004	0.0206	-0.0177	0.0058	-0.0017	-0.0129
	Z	-0.0006	0.0043	-0.0201	-0.0021	-0.0020	-0.0180
AT. 45	O X	0.0033	-0.0082	0.0087	-0.0173	0.0062	0.0212
	Y	-0.0004	-0.0206	-0.0177	-0.0058	-0.0017	-0.0129
	Z	0.0006	0.0043	0.0201	-0.0021	0.0020	0.0180
AT. 46	O X	-0.0033	-0.0082	-0.0087	-0.0173	0.0062	0.0212
	Y	0.0004	-0.0206	0.0177	-0.0058	-0.0017	-0.0129
	Z	0.0006	-0.0043	0.0201	0.0021	-0.0020	-0.0180
AT. 47	O X	0.0000	-0.0030	-0.0022	0.0000	0.0098	-0.0012
	Y	0.0000	-0.0181	-0.0084	0.0000	-0.0129	0.0143
	Z	0.0202	0.0000	0.0000	-0.0278	0.0000	0.0000
AT. 48	O X	0.0000	-0.0030	0.0022	0.0000	0.0098	-0.0012
	Y	0.0000	-0.0181	0.0084	0.0000	-0.0129	0.0143
	Z	0.0202	0.0000	0.0000	0.0278	0.0000	0.0000
AT. 49	O X	0.0000	-0.0030	-0.0022	0.0000	-0.0098	0.0012
	Y	0.0000	0.0181	0.0084	0.0000	-0.0129	0.0143
	Z	-0.0202	0.0000	0.0000	0.0278	0.0000	0.0000
AT. 50	O X	0.0000	-0.0030	0.0022	0.0000	-0.0098	0.0012
	Y	0.0000	0.0181	-0.0084	0.0000	-0.0129	0.0143
	Z	-0.0202	0.0000	0.0000	-0.0278	0.0000	0.0000
AT. 51	O X	0.0000	0.0113	-0.0036	0.0000	-0.0059	-0.0195
	Y	0.0000	0.0180	-0.0076	0.0000	0.0143	-0.0131
	Z	-0.0122	0.0000	0.0000	-0.0187	0.0000	0.0000
AT. 52	O X	0.0000	0.0113	0.0036	0.0000	-0.0059	-0.0195
	Y	0.0000	0.0180	0.0076	0.0000	0.0143	-0.0131



	Z	-0.0122	0.0000	0.0000	0.0187	0.0000	0.0000
AT. 53	O X	0.0000	0.0113	-0.0036	0.0000	0.0059	0.0195
	Y	0.0000	-0.0180	0.0076	0.0000	0.0143	-0.0131
	Z	0.0122	0.0000	0.0000	0.0187	0.0000	0.0000
AT. 54	O X	0.0000	0.0113	0.0036	0.0000	0.0059	0.0195
	Y	0.0000	-0.0180	-0.0076	0.0000	0.0143	-0.0131
	Z	0.0122	0.0000	0.0000	-0.0187	0.0000	0.0000
AT. 55	O X	0.0000	-0.0110	-0.0198	0.0000	0.0206	-0.0263
	Y	0.0000	-0.0008	0.0104	0.0000	0.0049	0.0123
	Z	-0.0077	0.0000	0.0000	0.0239	0.0000	0.0000
AT. 56	O X	0.0000	-0.0110	0.0198	0.0000	0.0206	-0.0263
	Y	0.0000	-0.0008	-0.0104	0.0000	0.0049	0.0123
	Z	-0.0077	0.0000	0.0000	-0.0239	0.0000	0.0000
AT. 57	O X	0.0000	-0.0110	-0.0198	0.0000	-0.0206	0.0263
	Y	0.0000	0.0008	-0.0104	0.0000	0.0049	0.0123
	Z	0.0077	0.0000	0.0000	-0.0239	0.0000	0.0000
AT. 58	O X	0.0000	-0.0110	0.0198	0.0000	-0.0206	0.0263
	Y	0.0000	0.0008	0.0104	0.0000	0.0049	0.0123
	Z	0.0077	0.0000	0.0000	0.0239	0.0000	0.0000

FREQ(CM\*\*-1) 342.18 342.38 358.61 358.86 359.68 363.03

AT. 1	MG X	0.0000	0.0000	0.0000	0.0000	-0.0259	0.0451
	Y	0.0358	0.0426	0.0199	-0.0235	0.0000	0.0000
	Z	-0.0029	0.0115	0.0047	0.0149	0.0000	0.0000
AT. 2	MG X	0.0000	0.0000	0.0000	0.0000	-0.0259	-0.0451
	Y	-0.0358	-0.0426	0.0199	0.0235	0.0000	0.0000
	Z	-0.0029	0.0115	-0.0047	0.0149	0.0000	0.0000
AT. 3	MG X	0.0000	0.0000	0.0000	0.0000	-0.0259	-0.0451
	Y	0.0358	-0.0426	0.0199	0.0235	0.0000	0.0000
	Z	-0.0029	-0.0115	0.0047	-0.0149	0.0000	0.0000
AT. 4	MG X	0.0000	0.0000	0.0000	0.0000	-0.0259	0.0451
	Y	-0.0358	0.0426	0.0199	-0.0235	0.0000	0.0000
	Z	-0.0029	-0.0115	-0.0047	-0.0149	0.0000	0.0000
AT. 5	AL X	0.0000	0.0000	-0.0044	0.0000	0.0091	0.0000
	Y	0.0000	0.0000	0.0008	0.0000	0.0093	0.0000
	Z	0.0007	-0.0038	0.0000	-0.0140	0.0000	0.0086
AT. 6	AL X	0.0000	0.0000	0.0044	0.0000	0.0091	0.0000
	Y	0.0000	0.0000	0.0008	0.0000	-0.0093	0.0000
	Z	0.0007	-0.0038	0.0000	-0.0140	0.0000	-0.0086
AT. 7	AL X	0.0000	0.0000	-0.0044	0.0000	0.0091	0.0000
	Y	0.0000	0.0000	0.0008	0.0000	0.0093	0.0000
	Z	0.0007	0.0038	0.0000	0.0140	0.0000	-0.0086
AT. 8	AL X	0.0000	0.0000	0.0044	0.0000	0.0091	0.0000
	Y	0.0000	0.0000	0.0008	0.0000	-0.0093	0.0000
	Z	0.0007	0.0038	0.0000	0.0140	0.0000	0.0086
AT. 9	AL X	0.0000	-0.0032	-0.0199	-0.0098	0.0154	-0.0049
	Y	0.0000	0.0079	0.0036	0.0068	-0.0125	-0.0032
	Z	0.0186	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0000	0.0032	-0.0199	0.0098	0.0154	0.0049
	Y	0.0000	-0.0079	0.0036	-0.0068	-0.0125	0.0032
	Z	0.0186	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0000	0.0032	0.0199	0.0098	0.0154	-0.0049
	Y	0.0000	0.0079	0.0036	0.0068	0.0125	0.0032

	Z	0.0186	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0000	-0.0032	0.0199	-0.0098	0.0154	0.0049
	Y	0.0000	-0.0079	0.0036	-0.0068	0.0125	-0.0032
	Z	0.0186	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	-0.0114	0.0000	0.0000	0.0000
	Z	0.0157	-0.0048	0.0000	0.0028	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	-0.0114	0.0000	0.0000	0.0000
	Z	0.0157	0.0048	0.0000	-0.0028	0.0000	0.0000
AT. 15	SI X	0.0000	-0.0011	-0.0128	0.0011	0.0055	0.0001
	Y	0.0000	0.0076	0.0014	0.0079	-0.0142	0.0019
	Z	-0.0073	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0000	0.0011	-0.0128	-0.0011	0.0055	-0.0001
	Y	0.0000	-0.0076	0.0014	-0.0079	-0.0142	-0.0019
	Z	-0.0073	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	0.0000	0.0011	0.0128	-0.0011	0.0055	0.0001
	Y	0.0000	0.0076	0.0014	0.0079	0.0142	-0.0019
	Z	-0.0073	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0000	-0.0011	0.0128	0.0011	0.0055	-0.0001
	Y	0.0000	-0.0076	0.0014	-0.0079	0.0142	0.0019
	Z	-0.0073	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	0.0000	0.0008	-0.0102	0.0070	-0.0007	0.0021
	Y	0.0000	0.0002	-0.0128	0.0034	-0.0071	-0.0031
	Z	0.0048	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0000	-0.0008	-0.0102	-0.0070	-0.0007	-0.0021
	Y	0.0000	-0.0002	-0.0128	-0.0034	-0.0071	0.0031
	Z	0.0048	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0000	-0.0008	0.0102	-0.0070	-0.0007	0.0021
	Y	0.0000	0.0002	-0.0128	0.0034	0.0071	0.0031
	Z	0.0048	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	0.0000	0.0008	0.0102	0.0070	-0.0007	-0.0021
	Y	0.0000	-0.0002	-0.0128	-0.0034	0.0071	-0.0031
	Z	0.0048	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0091	-0.0156	0.0026	-0.0162	0.0023	-0.0114
	Y	0.0046	0.0161	0.0065	0.0002	0.0031	0.0014
	Z	-0.0006	-0.0136	-0.0057	-0.0099	-0.0019	-0.0091
AT. 24	O X	-0.0091	0.0156	0.0026	0.0162	0.0023	0.0114
	Y	-0.0046	-0.0161	0.0065	-0.0002	0.0031	-0.0014
	Z	-0.0006	-0.0136	0.0057	-0.0099	0.0019	-0.0091
AT. 25	O X	-0.0091	0.0156	-0.0026	0.0162	0.0023	-0.0114
	Y	0.0046	0.0161	0.0065	0.0002	-0.0031	-0.0014
	Z	-0.0006	-0.0136	-0.0057	-0.0099	0.0019	0.0091
AT. 26	O X	0.0091	-0.0156	-0.0026	-0.0162	0.0023	0.0114
	Y	-0.0046	-0.0161	0.0065	-0.0002	-0.0031	0.0014
	Z	-0.0006	-0.0136	0.0057	-0.0099	-0.0019	0.0091
AT. 27	O X	0.0091	0.0156	0.0026	0.0162	0.0023	0.0114
	Y	0.0046	-0.0161	0.0065	-0.0002	0.0031	-0.0014
	Z	-0.0006	0.0136	-0.0057	0.0099	-0.0019	0.0091
AT. 28	O X	-0.0091	-0.0156	0.0026	-0.0162	0.0023	-0.0114
	Y	-0.0046	0.0161	0.0065	0.0002	0.0031	0.0014
	Z	-0.0006	0.0136	0.0057	0.0099	0.0019	0.0091
AT. 29	O X	-0.0091	-0.0156	-0.0026	-0.0162	0.0023	0.0114
	Y	0.0046	-0.0161	0.0065	-0.0002	-0.0031	0.0014

	Z	-0.0006	0.0136	-0.0057	0.0099	0.0019	-0.0091
AT. 30	O X	0.0091	0.0156	-0.0026	0.0162	0.0023	-0.0114
	Y	-0.0046	0.0161	0.0065	0.0002	-0.0031	-0.0014
	Z	-0.0006	0.0136	0.0057	0.0099	-0.0019	-0.0091
AT. 31	O X	-0.0116	-0.0096	0.0013	0.0015	0.0043	-0.0045
	Y	0.0278	0.0141	-0.0075	0.0088	-0.0003	-0.0173
	Z	-0.0043	-0.0071	0.0020	-0.0017	0.0016	0.0157
AT. 32	O X	0.0116	0.0096	0.0013	-0.0015	0.0043	0.0045
	Y	-0.0278	-0.0141	-0.0075	-0.0088	-0.0003	0.0173
	Z	-0.0043	-0.0071	-0.0020	-0.0017	-0.0016	0.0157
AT. 33	O X	0.0116	0.0096	-0.0013	-0.0015	0.0043	-0.0045
	Y	0.0278	0.0141	-0.0075	0.0088	0.0003	0.0173
	Z	-0.0043	-0.0071	0.0020	-0.0017	-0.0016	-0.0157
AT. 34	O X	-0.0116	-0.0096	-0.0013	0.0015	0.0043	0.0045
	Y	-0.0278	-0.0141	-0.0075	-0.0088	0.0003	-0.0173
	Z	-0.0043	-0.0071	-0.0020	-0.0017	0.0016	-0.0157
AT. 35	O X	-0.0116	0.0096	0.0013	-0.0015	0.0043	0.0045
	Y	0.0278	-0.0141	-0.0075	-0.0088	-0.0003	0.0173
	Z	-0.0043	0.0071	0.0020	0.0017	0.0016	-0.0157
AT. 36	O X	0.0116	-0.0096	0.0013	0.0015	0.0043	-0.0045
	Y	-0.0278	0.0141	-0.0075	0.0088	-0.0003	-0.0173
	Z	-0.0043	0.0071	-0.0020	0.0017	-0.0016	-0.0157
AT. 37	O X	0.0116	-0.0096	-0.0013	0.0015	0.0043	0.0045
	Y	0.0278	-0.0141	-0.0075	-0.0088	0.0003	-0.0173
	Z	-0.0043	0.0071	0.0020	0.0017	-0.0016	0.0157
AT. 38	O X	-0.0116	0.0096	-0.0013	-0.0015	0.0043	-0.0045
	Y	-0.0278	0.0141	-0.0075	0.0088	0.0003	0.0173
	Z	-0.0043	0.0071	-0.0020	0.0017	0.0016	0.0157
AT. 39	O X	-0.0014	-0.0058	-0.0056	0.0179	0.0063	0.0035
	Y	0.0029	-0.0001	-0.0171	0.0177	0.0061	-0.0116
	Z	0.0010	0.0040	0.0065	-0.0169	-0.0039	0.0023
AT. 40	O X	0.0014	0.0058	-0.0056	-0.0179	0.0063	-0.0035
	Y	-0.0029	0.0001	-0.0171	-0.0177	0.0061	0.0116
	Z	0.0010	0.0040	-0.0065	-0.0169	0.0039	0.0023
AT. 41	O X	0.0014	0.0058	0.0056	-0.0179	0.0063	0.0035
	Y	0.0029	-0.0001	-0.0171	0.0177	-0.0061	0.0116
	Z	0.0010	0.0040	0.0065	-0.0169	0.0039	-0.0023
AT. 42	O X	-0.0014	-0.0058	0.0056	0.0179	0.0063	-0.0035
	Y	-0.0029	0.0001	-0.0171	-0.0177	-0.0061	-0.0116
	Z	0.0010	0.0040	-0.0065	-0.0169	-0.0039	-0.0023
AT. 43	O X	-0.0014	0.0058	-0.0056	-0.0179	0.0063	-0.0035
	Y	0.0029	0.0001	-0.0171	-0.0177	0.0061	0.0116
	Z	0.0010	-0.0040	0.0065	0.0169	-0.0039	-0.0023
AT. 44	O X	0.0014	-0.0058	-0.0056	0.0179	0.0063	0.0035
	Y	-0.0029	-0.0001	-0.0171	0.0177	0.0061	-0.0116
	Z	0.0010	-0.0040	-0.0065	0.0169	0.0039	-0.0023
AT. 45	O X	0.0014	-0.0058	0.0056	0.0179	0.0063	-0.0035
	Y	0.0029	0.0001	-0.0171	-0.0177	-0.0061	-0.0116
	Z	0.0010	-0.0040	0.0065	0.0169	0.0039	0.0023
AT. 46	O X	-0.0014	0.0058	0.0056	-0.0179	0.0063	0.0035
	Y	-0.0029	-0.0001	-0.0171	0.0177	-0.0061	0.0116
	Z	0.0010	-0.0040	-0.0065	0.0169	-0.0039	0.0023
AT. 47	O X	0.0000	-0.0021	-0.0130	0.0055	-0.0028	0.0020
	Y	0.0000	0.0036	0.0103	0.0155	0.0274	-0.0013

	Z	-0.0225	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	0.0000	0.0021	-0.0130	-0.0055	-0.0028	-0.0020
	Y	0.0000	-0.0036	0.0103	-0.0155	0.0274	0.0013
	Z	-0.0225	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	0.0000	0.0021	0.0130	-0.0055	-0.0028	0.0020
	Y	0.0000	0.0036	0.0103	0.0155	-0.0274	0.0013
	Z	-0.0225	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	0.0000	-0.0021	0.0130	0.0055	-0.0028	-0.0020
	Y	0.0000	-0.0036	0.0103	-0.0155	-0.0274	-0.0013
	Z	-0.0225	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	0.0000	-0.0092	0.0139	-0.0114	0.0054	-0.0010
	Y	0.0000	-0.0011	0.0323	-0.0039	-0.0142	0.0050
	Z	-0.0060	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	0.0000	0.0092	0.0139	0.0114	0.0054	0.0010
	Y	0.0000	0.0011	0.0323	0.0039	-0.0142	-0.0050
	Z	-0.0060	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	0.0000	0.0092	-0.0139	0.0114	0.0054	-0.0010
	Y	0.0000	-0.0011	0.0323	-0.0039	0.0142	-0.0050
	Z	-0.0060	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	0.0000	-0.0092	-0.0139	-0.0114	0.0054	0.0010
	Y	0.0000	0.0011	0.0323	0.0039	0.0142	0.0050
	Z	-0.0060	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	0.0000	-0.0021	0.0175	-0.0100	-0.0390	-0.0047
	Y	0.0000	0.0068	-0.0137	0.0075	0.0042	-0.0012
	Z	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56	O X	0.0000	0.0021	0.0175	0.0100	-0.0390	0.0047
	Y	0.0000	-0.0068	-0.0137	-0.0075	0.0042	0.0012
	Z	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57	O X	0.0000	0.0021	-0.0175	0.0100	-0.0390	-0.0047
	Y	0.0000	0.0068	-0.0137	0.0075	-0.0042	0.0012
	Z	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58	O X	0.0000	-0.0021	-0.0175	-0.0100	-0.0390	0.0047
	Y	0.0000	-0.0068	-0.0137	-0.0075	-0.0042	-0.0012
	Z	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000

FREQ(CM\*\*-1) 363.77 370.33 370.42 371.56 378.32 379.78

AT. 1	MG X	0.0249	0.0000	-0.0112	-0.0073	0.0000	0.0000
	Y	0.0000	-0.0049	0.0000	0.0000	0.0405	-0.0147
	Z	0.0000	0.0077	0.0000	0.0000	-0.0025	-0.0203
AT. 2	MG X	0.0249	0.0000	0.0112	0.0073	0.0000	0.0000
	Y	0.0000	0.0049	0.0000	0.0000	0.0405	-0.0147
	Z	0.0000	0.0077	0.0000	0.0000	0.0025	0.0203
AT. 3	MG X	0.0249	0.0000	0.0112	-0.0073	0.0000	0.0000
	Y	0.0000	-0.0049	0.0000	0.0000	-0.0405	-0.0147
	Z	0.0000	0.0077	0.0000	0.0000	0.0025	-0.0203
AT. 4	MG X	0.0249	0.0000	-0.0112	0.0073	0.0000	0.0000
	Y	0.0000	0.0049	0.0000	0.0000	-0.0405	-0.0147
	Z	0.0000	0.0077	0.0000	0.0000	-0.0025	0.0203
AT. 5	AL X	0.0097	0.0000	0.0000	0.0000	0.0120	-0.0108
	Y	0.0003	0.0000	0.0000	0.0000	-0.0165	-0.0008
	Z	0.0000	0.0275	-0.0016	0.0250	0.0000	0.0000
AT. 6	AL X	0.0097	0.0000	0.0000	0.0000	-0.0120	0.0108
	Y	-0.0003	0.0000	0.0000	0.0000	-0.0165	-0.0008

	Z	0.0000	0.0275	0.0016	-0.0250	0.0000	0.0000
AT. 7	AL X	0.0097	0.0000	0.0000	0.0000	-0.0120	-0.0108
	Y	0.0003	0.0000	0.0000	0.0000	0.0165	-0.0008
	Z	0.0000	0.0275	0.0016	0.0250	0.0000	0.0000
AT. 8	AL X	0.0097	0.0000	0.0000	0.0000	0.0120	0.0108
	Y	-0.0003	0.0000	0.0000	0.0000	0.0165	-0.0008
	Z	0.0000	0.0275	-0.0016	-0.0250	0.0000	0.0000
AT. 9	AL X	-0.0171	0.0000	0.0004	0.0000	0.0000	-0.0106
	Y	-0.0003	0.0000	0.0013	0.0000	0.0000	-0.0175
	Z	0.0000	0.0018	0.0000	0.0170	-0.0018	0.0000
AT. 10	AL X	-0.0171	0.0000	-0.0004	0.0000	0.0000	-0.0106
	Y	-0.0003	0.0000	-0.0013	0.0000	0.0000	-0.0175
	Z	0.0000	0.0018	0.0000	0.0170	0.0018	0.0000
AT. 11	AL X	-0.0171	0.0000	0.0004	0.0000	0.0000	0.0106
	Y	0.0003	0.0000	-0.0013	0.0000	0.0000	-0.0175
	Z	0.0000	0.0018	0.0000	-0.0170	-0.0018	0.0000
AT. 12	AL X	-0.0171	0.0000	-0.0004	0.0000	0.0000	0.0106
	Y	0.0003	0.0000	0.0013	0.0000	0.0000	-0.0175
	Z	0.0000	0.0018	0.0000	-0.0170	0.0018	0.0000
AT. 13	SI X	-0.0116	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0038	-0.0026
	Z	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	-0.0116	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0038	-0.0026
	Z	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	-0.0008	0.0000	0.0044	0.0000	0.0000	0.0051
	Y	-0.0008	0.0000	-0.0010	0.0000	0.0000	0.0019
	Z	0.0000	0.0120	0.0000	0.0042	-0.0062	0.0000
AT. 16	SI X	-0.0008	0.0000	-0.0044	0.0000	0.0000	0.0051
	Y	-0.0008	0.0000	0.0010	0.0000	0.0000	0.0019
	Z	0.0000	0.0120	0.0000	0.0042	0.0062	0.0000
AT. 17	SI X	-0.0008	0.0000	0.0044	0.0000	0.0000	-0.0051
	Y	0.0008	0.0000	0.0010	0.0000	0.0000	0.0019
	Z	0.0000	0.0120	0.0000	-0.0042	-0.0062	0.0000
AT. 18	SI X	-0.0008	0.0000	-0.0044	0.0000	0.0000	-0.0051
	Y	0.0008	0.0000	-0.0010	0.0000	0.0000	0.0019
	Z	0.0000	0.0120	0.0000	-0.0042	0.0062	0.0000
AT. 19	SI X	-0.0108	0.0000	0.0019	0.0000	0.0000	-0.0057
	Y	-0.0084	0.0000	-0.0035	0.0000	0.0000	0.0097
	Z	0.0000	0.0010	0.0000	-0.0144	-0.0065	0.0000
AT. 20	SI X	-0.0108	0.0000	-0.0019	0.0000	0.0000	-0.0057
	Y	-0.0084	0.0000	0.0035	0.0000	0.0000	0.0097
	Z	0.0000	0.0010	0.0000	-0.0144	0.0065	0.0000
AT. 21	SI X	-0.0108	0.0000	0.0019	0.0000	0.0000	0.0057
	Y	0.0084	0.0000	0.0035	0.0000	0.0000	0.0097
	Z	0.0000	0.0010	0.0000	0.0144	-0.0065	0.0000
AT. 22	SI X	-0.0108	0.0000	-0.0019	0.0000	0.0000	0.0057
	Y	0.0084	0.0000	-0.0035	0.0000	0.0000	0.0097
	Z	0.0000	0.0010	0.0000	0.0144	0.0065	0.0000
AT. 23	O X	0.0156	-0.0169	0.0198	0.0170	-0.0020	0.0027
	Y	-0.0054	0.0172	-0.0066	-0.0142	-0.0171	-0.0042
	Z	0.0093	-0.0059	0.0120	0.0078	-0.0005	0.0049
AT. 24	O X	0.0156	0.0169	-0.0198	-0.0170	-0.0020	0.0027
	Y	-0.0054	-0.0172	0.0066	0.0142	-0.0171	-0.0042

	Z	-0.0093	-0.0059	0.0120	0.0078	0.0005	-0.0049
AT. 25	O X	0.0156	0.0169	0.0198	0.0170	0.0020	-0.0027
	Y	0.0054	0.0172	0.0066	0.0142	-0.0171	-0.0042
	Z	-0.0093	-0.0059	-0.0120	-0.0078	-0.0005	0.0049
AT. 26	O X	0.0156	-0.0169	-0.0198	-0.0170	0.0020	-0.0027
	Y	0.0054	-0.0172	-0.0066	-0.0142	-0.0171	-0.0042
	Z	0.0093	-0.0059	-0.0120	-0.0078	0.0005	-0.0049
AT. 27	O X	0.0156	-0.0169	-0.0198	0.0170	0.0020	0.0027
	Y	-0.0054	0.0172	0.0066	-0.0142	0.0171	-0.0042
	Z	0.0093	-0.0059	-0.0120	0.0078	0.0005	0.0049
AT. 28	O X	0.0156	0.0169	0.0198	-0.0170	0.0020	0.0027
	Y	-0.0054	-0.0172	-0.0066	0.0142	0.0171	-0.0042
	Z	-0.0093	-0.0059	-0.0120	0.0078	-0.0005	-0.0049
AT. 29	O X	0.0156	0.0169	-0.0198	0.0170	-0.0020	-0.0027
	Y	0.0054	0.0172	-0.0066	0.0142	0.0171	-0.0042
	Z	-0.0093	-0.0059	0.0120	-0.0078	0.0005	0.0049
AT. 30	O X	0.0156	-0.0169	0.0198	-0.0170	-0.0020	-0.0027
	Y	0.0054	-0.0172	0.0066	-0.0142	0.0171	-0.0042
	Z	0.0093	-0.0059	0.0120	-0.0078	-0.0005	-0.0049
AT. 31	O X	-0.0151	0.0040	0.0053	0.0064	-0.0001	0.0181
	Y	-0.0037	0.0019	-0.0222	-0.0060	0.0023	0.0009
	Z	0.0030	-0.0019	0.0155	-0.0038	-0.0033	-0.0153
AT. 32	O X	-0.0151	-0.0040	-0.0053	-0.0064	-0.0001	0.0181
	Y	-0.0037	-0.0019	0.0222	0.0060	0.0023	0.0009
	Z	-0.0030	-0.0019	0.0155	-0.0038	0.0033	0.0153
AT. 33	O X	-0.0151	-0.0040	0.0053	0.0064	0.0001	-0.0181
	Y	0.0037	0.0019	0.0222	0.0060	0.0023	0.0009
	Z	-0.0030	-0.0019	-0.0155	0.0038	-0.0033	-0.0153
AT. 34	O X	-0.0151	0.0040	-0.0053	-0.0064	0.0001	-0.0181
	Y	0.0037	-0.0019	-0.0222	-0.0060	0.0023	0.0009
	Z	0.0030	-0.0019	-0.0155	0.0038	0.0033	0.0153
AT. 35	O X	-0.0151	0.0040	-0.0053	0.0064	0.0001	0.0181
	Y	-0.0037	0.0019	0.0222	-0.0060	-0.0023	0.0009
	Z	0.0030	-0.0019	-0.0155	-0.0038	0.0033	-0.0153
AT. 36	O X	-0.0151	-0.0040	0.0053	-0.0064	0.0001	0.0181
	Y	-0.0037	-0.0019	-0.0222	0.0060	-0.0023	0.0009
	Z	-0.0030	-0.0019	-0.0155	-0.0038	-0.0033	0.0153
AT. 37	O X	-0.0151	-0.0040	-0.0053	0.0064	-0.0001	-0.0181
	Y	0.0037	0.0019	-0.0222	0.0060	-0.0023	0.0009
	Z	-0.0030	-0.0019	0.0155	0.0038	0.0033	-0.0153
AT. 38	O X	-0.0151	0.0040	0.0053	-0.0064	-0.0001	-0.0181
	Y	0.0037	-0.0019	0.0222	-0.0060	-0.0023	0.0009
	Z	0.0030	-0.0019	0.0155	0.0038	-0.0033	0.0153
AT. 39	O X	0.0151	0.0225	-0.0173	0.0199	0.0165	-0.0173
	Y	0.0142	0.0011	-0.0136	0.0152	-0.0115	0.0105
	Z	-0.0114	-0.0103	0.0128	-0.0044	-0.0004	0.0091
AT. 40	O X	0.0151	-0.0225	0.0173	-0.0199	0.0165	-0.0173
	Y	0.0142	-0.0011	0.0136	-0.0152	-0.0115	0.0105
	Z	0.0114	-0.0103	0.0128	-0.0044	0.0004	-0.0091
AT. 41	O X	0.0151	-0.0225	-0.0173	0.0199	-0.0165	0.0173
	Y	-0.0142	0.0011	0.0136	-0.0152	-0.0115	0.0105
	Z	0.0114	-0.0103	-0.0128	0.0044	-0.0004	0.0091
AT. 42	O X	0.0151	0.0225	0.0173	-0.0199	-0.0165	0.0173
	Y	-0.0142	-0.0011	-0.0136	0.0152	-0.0115	0.0105

	Z	-0.0114	-0.0103	-0.0128	0.0044	0.0004	-0.0091
AT. 43 O	X	0.0151	0.0225	0.0173	0.0199	-0.0165	-0.0173
	Y	0.0142	0.0011	0.0136	0.0152	0.0115	0.0105
	Z	-0.0114	-0.0103	-0.0128	-0.0044	0.0004	0.0091
AT. 44 O	X	0.0151	-0.0225	-0.0173	-0.0199	-0.0165	-0.0173
	Y	0.0142	-0.0011	-0.0136	-0.0152	0.0115	0.0105
	Z	0.0114	-0.0103	-0.0128	-0.0044	-0.0004	-0.0091
AT. 45 O	X	0.0151	-0.0225	0.0173	0.0199	0.0165	0.0173
	Y	-0.0142	0.0011	-0.0136	-0.0152	0.0115	0.0105
	Z	0.0114	-0.0103	0.0128	0.0044	0.0004	0.0091
AT. 46 O	X	0.0151	0.0225	-0.0173	-0.0199	0.0165	0.0173
	Y	-0.0142	-0.0011	0.0136	0.0152	0.0115	0.0105
	Z	-0.0114	-0.0103	0.0128	0.0044	-0.0004	-0.0091
AT. 47 O	X	-0.0163	0.0000	-0.0023	0.0000	0.0000	-0.0114
	Y	0.0218	0.0000	0.0192	0.0000	0.0000	0.0160
	Z	0.0000	-0.0191	0.0000	0.0170	0.0138	0.0000
AT. 48 O	X	-0.0163	0.0000	0.0023	0.0000	0.0000	-0.0114
	Y	0.0218	0.0000	-0.0192	0.0000	0.0000	0.0160
	Z	0.0000	-0.0191	0.0000	0.0170	-0.0138	0.0000
AT. 49 O	X	-0.0163	0.0000	-0.0023	0.0000	0.0000	0.0114
	Y	-0.0218	0.0000	-0.0192	0.0000	0.0000	0.0160
	Z	0.0000	-0.0191	0.0000	-0.0170	0.0138	0.0000
AT. 50 O	X	-0.0163	0.0000	0.0023	0.0000	0.0000	0.0114
	Y	-0.0218	0.0000	0.0192	0.0000	0.0000	0.0160
	Z	0.0000	-0.0191	0.0000	-0.0170	-0.0138	0.0000
AT. 51 O	X	-0.0045	0.0000	-0.0062	0.0000	0.0000	0.0050
	Y	0.0016	0.0000	-0.0111	0.0000	0.0000	0.0013
	Z	0.0000	-0.0095	0.0000	-0.0126	-0.0032	0.0000
AT. 52 O	X	-0.0045	0.0000	0.0062	0.0000	0.0000	0.0050
	Y	0.0016	0.0000	0.0111	0.0000	0.0000	0.0013
	Z	0.0000	-0.0095	0.0000	-0.0126	0.0032	0.0000
AT. 53 O	X	-0.0045	0.0000	-0.0062	0.0000	0.0000	-0.0050
	Y	-0.0016	0.0000	0.0111	0.0000	0.0000	0.0013
	Z	0.0000	-0.0095	0.0000	0.0126	-0.0032	0.0000
AT. 54 O	X	-0.0045	0.0000	0.0062	0.0000	0.0000	-0.0050
	Y	-0.0016	0.0000	-0.0111	0.0000	0.0000	0.0013
	Z	0.0000	-0.0095	0.0000	0.0126	0.0032	0.0000
AT. 55 O	X	-0.0052	0.0000	-0.0170	0.0000	0.0000	0.0140
	Y	-0.0037	0.0000	0.0049	0.0000	0.0000	0.0032
	Z	0.0000	-0.0212	0.0000	-0.0049	0.0038	0.0000
AT. 56 O	X	-0.0052	0.0000	0.0170	0.0000	0.0000	0.0140
	Y	-0.0037	0.0000	-0.0049	0.0000	0.0000	0.0032
	Z	0.0000	-0.0212	0.0000	-0.0049	-0.0038	0.0000
AT. 57 O	X	-0.0052	0.0000	-0.0170	0.0000	0.0000	-0.0140
	Y	0.0037	0.0000	-0.0049	0.0000	0.0000	0.0032
	Z	0.0000	-0.0212	0.0000	0.0049	0.0038	0.0000
AT. 58 O	X	-0.0052	0.0000	0.0170	0.0000	0.0000	-0.0140
	Y	0.0037	0.0000	0.0049	0.0000	0.0000	0.0032
	Z	0.0000	-0.0212	0.0000	0.0049	-0.0038	0.0000

FREQ(CM\*\*-1) 385.74 397.72 405.11 409.88 417.16 424.33

AT. 1 MG	X	0.0354	0.0239	0.0062	0.0000	0.0240	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	-0.0065

	Z	0.0000	0.0000	0.0000	0.0023	0.0000	-0.0022
AT. 2	MG X	0.0354	0.0239	0.0062	0.0000	0.0240	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0065
	Z	0.0000	0.0000	0.0000	-0.0023	0.0000	-0.0022
AT. 3	MG X	-0.0354	-0.0239	0.0062	0.0000	0.0240	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0065
	Z	0.0000	0.0000	0.0000	0.0023	0.0000	0.0022
AT. 4	MG X	-0.0354	-0.0239	0.0062	0.0000	0.0240	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	-0.0065
	Z	0.0000	0.0000	0.0000	-0.0023	0.0000	0.0022
AT. 5	AL X	-0.0075	0.0000	-0.0035	-0.0188	-0.0139	0.0000
	Y	0.0102	0.0050	-0.0015	-0.0225	0.0098	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0261
AT. 6	AL X	-0.0075	0.0000	-0.0035	0.0188	-0.0139	0.0000
	Y	-0.0102	-0.0050	0.0015	-0.0225	-0.0098	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0261
AT. 7	AL X	0.0075	0.0000	-0.0035	-0.0188	-0.0139	0.0000
	Y	-0.0102	-0.0050	-0.0015	-0.0225	0.0098	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0261
AT. 8	AL X	0.0075	0.0000	-0.0035	0.0188	-0.0139	0.0000
	Y	0.0102	0.0050	0.0015	-0.0225	-0.0098	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0261
AT. 9	AL X	0.0000	0.0000	0.0124	-0.0135	0.0147	-0.0178
	Y	0.0000	0.0000	0.0233	0.0093	-0.0054	-0.0028
	Z	0.0262	-0.0340	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0000	0.0000	0.0124	-0.0135	0.0147	0.0178
	Y	0.0000	0.0000	0.0233	0.0093	-0.0054	0.0028
	Z	-0.0262	0.0340	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0000	0.0000	0.0124	0.0135	0.0147	0.0178
	Y	0.0000	0.0000	-0.0233	0.0093	0.0054	-0.0028
	Z	-0.0262	0.0340	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0000	0.0000	0.0124	0.0135	0.0147	-0.0178
	Y	0.0000	0.0000	-0.0233	0.0093	0.0054	0.0028
	Z	0.0262	-0.0340	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	-0.0171	0.0003	-0.0123	0.0000	-0.0104	0.0000
	Y	0.0000	0.0000	0.0000	0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0147
AT. 14	SI X	0.0171	-0.0003	-0.0123	0.0000	-0.0104	0.0000
	Y	0.0000	0.0000	0.0000	0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0147
AT. 15	SI X	0.0000	0.0000	-0.0046	-0.0016	0.0146	-0.0099
	Y	0.0000	0.0000	-0.0042	0.0001	0.0068	0.0012
	Z	0.0021	0.0093	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0000	0.0000	-0.0046	-0.0016	0.0146	0.0099
	Y	0.0000	0.0000	-0.0042	0.0001	0.0068	-0.0012
	Z	-0.0021	-0.0093	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	0.0000	0.0000	-0.0046	0.0016	0.0146	0.0099
	Y	0.0000	0.0000	0.0042	0.0001	-0.0068	0.0012
	Z	-0.0021	-0.0093	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0000	0.0000	-0.0046	0.0016	0.0146	-0.0099
	Y	0.0000	0.0000	0.0042	0.0001	-0.0068	-0.0012
	Z	0.0021	0.0093	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	0.0000	0.0000	0.0100	-0.0032	0.0068	0.0040
	Y	0.0000	0.0000	-0.0122	0.0094	0.0117	0.0014



	Z	-0.0039	-0.0052	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0000	0.0000	0.0100	-0.0032	0.0068	-0.0040
	Y	0.0000	0.0000	-0.0122	0.0094	0.0117	-0.0014
	Z	0.0039	0.0052	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0000	0.0000	0.0100	0.0032	0.0068	-0.0040
	Y	0.0000	0.0000	0.0122	0.0094	-0.0117	0.0014
	Z	0.0039	0.0052	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	0.0000	0.0000	0.0100	0.0032	0.0068	0.0040
	Y	0.0000	0.0000	0.0122	0.0094	-0.0117	-0.0014
	Z	-0.0039	-0.0052	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	-0.0008	0.0067	0.0148	-0.0172	-0.0099	-0.0045
	Y	-0.0124	-0.0030	-0.0086	-0.0039	-0.0004	-0.0087
	Z	0.0017	-0.0016	0.0141	-0.0138	-0.0135	-0.0114
AT. 24	O X	-0.0008	0.0067	0.0148	-0.0172	-0.0099	0.0045
	Y	-0.0124	-0.0030	-0.0086	-0.0039	-0.0004	0.0087
	Z	-0.0017	0.0016	-0.0141	0.0138	0.0135	-0.0114
AT. 25	O X	-0.0008	0.0067	0.0148	0.0172	-0.0099	0.0045
	Y	0.0124	0.0030	0.0086	-0.0039	0.0004	-0.0087
	Z	-0.0017	0.0016	-0.0141	-0.0138	0.0135	-0.0114
AT. 26	O X	-0.0008	0.0067	0.0148	0.0172	-0.0099	-0.0045
	Y	0.0124	0.0030	0.0086	-0.0039	0.0004	0.0087
	Z	0.0017	-0.0016	0.0141	0.0138	-0.0135	-0.0114
AT. 27	O X	0.0008	-0.0067	0.0148	-0.0172	-0.0099	0.0045
	Y	0.0124	0.0030	-0.0086	-0.0039	-0.0004	0.0087
	Z	-0.0017	0.0016	0.0141	-0.0138	-0.0135	0.0114
AT. 28	O X	0.0008	-0.0067	0.0148	-0.0172	-0.0099	-0.0045
	Y	0.0124	0.0030	-0.0086	-0.0039	-0.0004	-0.0087
	Z	0.0017	-0.0016	-0.0141	0.0138	0.0135	0.0114
AT. 29	O X	0.0008	-0.0067	0.0148	0.0172	-0.0099	-0.0045
	Y	-0.0124	-0.0030	0.0086	-0.0039	0.0004	0.0087
	Z	0.0017	-0.0016	-0.0141	-0.0138	0.0135	0.0114
AT. 30	O X	0.0008	-0.0067	0.0148	0.0172	-0.0099	0.0045
	Y	-0.0124	-0.0030	0.0086	-0.0039	0.0004	-0.0087
	Z	-0.0017	0.0016	0.0141	0.0138	-0.0135	0.0114
AT. 31	O X	-0.0097	-0.0204	-0.0024	0.0005	-0.0142	0.0040
	Y	-0.0118	0.0145	0.0019	-0.0051	-0.0028	-0.0045
	Z	-0.0018	0.0043	-0.0112	0.0086	0.0027	-0.0098
AT. 32	O X	-0.0097	-0.0204	-0.0024	0.0005	-0.0142	-0.0040
	Y	-0.0118	0.0145	0.0019	-0.0051	-0.0028	0.0045
	Z	0.0018	-0.0043	0.0112	-0.0086	-0.0027	-0.0098
AT. 33	O X	-0.0097	-0.0204	-0.0024	-0.0005	-0.0142	-0.0040
	Y	0.0118	-0.0145	-0.0019	-0.0051	0.0028	-0.0045
	Z	0.0018	-0.0043	0.0112	0.0086	-0.0027	-0.0098
AT. 34	O X	-0.0097	-0.0204	-0.0024	-0.0005	-0.0142	0.0040
	Y	0.0118	-0.0145	-0.0019	-0.0051	0.0028	0.0045
	Z	-0.0018	0.0043	-0.0112	-0.0086	0.0027	-0.0098
AT. 35	O X	0.0097	0.0204	-0.0024	0.0005	-0.0142	-0.0040
	Y	0.0118	-0.0145	0.0019	-0.0051	-0.0028	0.0045
	Z	0.0018	-0.0043	-0.0112	0.0086	0.0027	0.0098
AT. 36	O X	0.0097	0.0204	-0.0024	0.0005	-0.0142	0.0040
	Y	0.0118	-0.0145	0.0019	-0.0051	-0.0028	-0.0045
	Z	-0.0018	0.0043	0.0112	-0.0086	-0.0027	0.0098
AT. 37	O X	0.0097	0.0204	-0.0024	-0.0005	-0.0142	0.0040
	Y	-0.0118	0.0145	-0.0019	-0.0051	0.0028	0.0045

	Z	-0.0018	0.0043	0.0112	0.0086	-0.0027	0.0098
AT. 38	O X	0.0097	0.0204	-0.0024	-0.0005	-0.0142	-0.0040
	Y	-0.0118	0.0145	-0.0019	-0.0051	0.0028	-0.0045
	Z	0.0018	-0.0043	-0.0112	-0.0086	0.0027	0.0098
AT. 39	O X	-0.0073	-0.0033	-0.0160	0.0076	-0.0042	-0.0156
	Y	0.0063	0.0006	0.0045	0.0141	0.0085	-0.0066
	Z	-0.0016	-0.0014	0.0143	-0.0082	-0.0052	0.0041
AT. 40	O X	-0.0073	-0.0033	-0.0160	0.0076	-0.0042	0.0156
	Y	0.0063	0.0006	0.0045	0.0141	0.0085	0.0066
	Z	0.0016	0.0014	-0.0143	0.0082	0.0052	0.0041
AT. 41	O X	-0.0073	-0.0033	-0.0160	-0.0076	-0.0042	0.0156
	Y	-0.0063	-0.0006	-0.0045	0.0141	-0.0085	-0.0066
	Z	0.0016	0.0014	-0.0143	-0.0082	0.0052	0.0041
AT. 42	O X	-0.0073	-0.0033	-0.0160	-0.0076	-0.0042	-0.0156
	Y	-0.0063	-0.0006	-0.0045	0.0141	-0.0085	0.0066
	Z	-0.0016	-0.0014	0.0143	0.0082	-0.0052	0.0041
AT. 43	O X	0.0073	0.0033	-0.0160	0.0076	-0.0042	0.0156
	Y	-0.0063	-0.0006	0.0045	0.0141	0.0085	0.0066
	Z	0.0016	0.0014	0.0143	-0.0082	-0.0052	-0.0041
AT. 44	O X	0.0073	0.0033	-0.0160	0.0076	-0.0042	-0.0156
	Y	-0.0063	-0.0006	0.0045	0.0141	0.0085	-0.0066
	Z	-0.0016	-0.0014	-0.0143	0.0082	0.0052	-0.0041
AT. 45	O X	0.0073	0.0033	-0.0160	-0.0076	-0.0042	-0.0156
	Y	0.0063	0.0006	-0.0045	0.0141	-0.0085	0.0066
	Z	-0.0016	-0.0014	-0.0143	-0.0082	0.0052	-0.0041
AT. 46	O X	0.0073	0.0033	-0.0160	-0.0076	-0.0042	0.0156
	Y	0.0063	0.0006	-0.0045	0.0141	-0.0085	-0.0066
	Z	0.0016	0.0014	0.0143	0.0082	-0.0052	-0.0041
AT. 47	O X	0.0000	0.0000	0.0108	-0.0033	0.0076	0.0125
	Y	0.0000	0.0000	-0.0004	-0.0083	-0.0024	-0.0205
	Z	0.0105	-0.0143	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	0.0000	0.0000	0.0108	-0.0033	0.0076	-0.0125
	Y	0.0000	0.0000	-0.0004	-0.0083	-0.0024	0.0205
	Z	-0.0105	0.0143	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	0.0000	0.0000	0.0108	0.0033	0.0076	-0.0125
	Y	0.0000	0.0000	0.0004	-0.0083	0.0024	-0.0205
	Z	-0.0105	0.0143	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	0.0000	0.0000	0.0108	0.0033	0.0076	0.0125
	Y	0.0000	0.0000	0.0004	-0.0083	0.0024	0.0205
	Z	0.0105	-0.0143	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	0.0000	0.0000	-0.0097	-0.0086	-0.0031	0.0034
	Y	0.0000	0.0000	-0.0068	-0.0027	-0.0146	0.0153
	Z	-0.0083	0.0009	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	0.0000	0.0000	-0.0097	-0.0086	-0.0031	-0.0034
	Y	0.0000	0.0000	-0.0068	-0.0027	-0.0146	-0.0153
	Z	0.0083	-0.0009	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	0.0000	0.0000	-0.0097	0.0086	-0.0031	-0.0034
	Y	0.0000	0.0000	0.0068	-0.0027	0.0146	0.0153
	Z	0.0083	-0.0009	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	0.0000	0.0000	-0.0097	0.0086	-0.0031	0.0034
	Y	0.0000	0.0000	0.0068	-0.0027	0.0146	-0.0153
	Z	-0.0083	0.0009	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	0.0000	0.0000	-0.0167	0.0202	-0.0137	0.0106
	Y	0.0000	0.0000	-0.0017	-0.0018	0.0131	-0.0041

	Z	-0.0111	-0.0077	0.0000	0.0000	0.0000	0.0000
AT. 56 O	X	0.0000	0.0000	-0.0167	0.0202	-0.0137	-0.0106
	Y	0.0000	0.0000	-0.0017	-0.0018	0.0131	0.0041
	Z	0.0111	0.0077	0.0000	0.0000	0.0000	0.0000
AT. 57 O	X	0.0000	0.0000	-0.0167	-0.0202	-0.0137	-0.0106
	Y	0.0000	0.0000	0.0017	-0.0018	-0.0131	-0.0041
	Z	0.0111	0.0077	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	0.0000	0.0000	-0.0167	-0.0202	-0.0137	0.0106
	Y	0.0000	0.0000	0.0017	-0.0018	-0.0131	0.0041
	Z	-0.0111	-0.0077	0.0000	0.0000	0.0000	0.0000

FREQ(CM\*\*-1) 431.46 435.39 449.49 460.77 462.04 465.66

AT. 1 MG	X	0.0000	-0.0147	-0.0178	0.0037	0.0000	0.0000
	Y	0.0207	0.0000	0.0000	0.0000	0.0077	0.0007
	Z	-0.0081	0.0000	0.0000	0.0000	-0.0004	0.0004
AT. 2 MG	X	0.0000	0.0147	-0.0178	0.0037	0.0000	0.0000
	Y	0.0207	0.0000	0.0000	0.0000	-0.0077	0.0007
	Z	0.0081	0.0000	0.0000	0.0000	-0.0004	-0.0004
AT. 3 MG	X	0.0000	0.0147	-0.0178	-0.0037	0.0000	0.0000
	Y	0.0207	0.0000	0.0000	0.0000	-0.0077	-0.0007
	Z	-0.0081	0.0000	0.0000	0.0000	0.0004	-0.0004
AT. 4 MG	X	0.0000	-0.0147	-0.0178	-0.0037	0.0000	0.0000
	Y	0.0207	0.0000	0.0000	0.0000	0.0077	-0.0007
	Z	0.0081	0.0000	0.0000	0.0000	0.0004	0.0004
AT. 5 AL	X	0.0158	0.0000	-0.0221	0.0048	0.0000	0.0008
	Y	-0.0090	0.0000	-0.0086	-0.0024	0.0000	0.0061
	Z	0.0000	0.0049	0.0000	0.0000	-0.0128	0.0000
AT. 6 AL	X	-0.0158	0.0000	-0.0221	0.0048	0.0000	-0.0008
	Y	-0.0090	0.0000	0.0086	0.0024	0.0000	0.0061
	Z	0.0000	-0.0049	0.0000	0.0000	-0.0128	0.0000
AT. 7 AL	X	0.0158	0.0000	-0.0221	-0.0048	0.0000	-0.0008
	Y	-0.0090	0.0000	-0.0086	0.0024	0.0000	-0.0061
	Z	0.0000	-0.0049	0.0000	0.0000	0.0128	0.0000
AT. 8 AL	X	-0.0158	0.0000	-0.0221	-0.0048	0.0000	0.0008
	Y	-0.0090	0.0000	0.0086	-0.0024	0.0000	-0.0061
	Z	0.0000	0.0049	0.0000	0.0000	0.0128	0.0000
AT. 9 AL	X	-0.0044	0.0026	-0.0036	0.0000	0.0141	0.0000
	Y	0.0053	-0.0212	0.0086	0.0000	0.0005	0.0000
	Z	0.0000	0.0000	0.0000	-0.0016	0.0000	0.0003
AT. 10 AL	X	-0.0044	-0.0026	-0.0036	0.0000	-0.0141	0.0000
	Y	0.0053	0.0212	0.0086	0.0000	-0.0005	0.0000
	Z	0.0000	0.0000	0.0000	0.0016	0.0000	-0.0003
AT. 11 AL	X	0.0044	0.0026	-0.0036	0.0000	-0.0141	0.0000
	Y	0.0053	0.0212	-0.0086	0.0000	0.0005	0.0000
	Z	0.0000	0.0000	0.0000	0.0016	0.0000	0.0003
AT. 12 AL	X	0.0044	-0.0026	-0.0036	0.0000	0.0141	0.0000
	Y	0.0053	-0.0212	-0.0086	0.0000	-0.0005	0.0000
	Z	0.0000	0.0000	0.0000	-0.0016	0.0000	-0.0003
AT. 13 SI	X	0.0000	0.0000	-0.0029	0.0016	0.0000	0.0000
	Y	-0.0033	0.0000	0.0000	0.0000	0.0000	-0.0112
	Z	0.0000	0.0000	0.0000	0.0000	-0.0158	0.0000
AT. 14 SI	X	0.0000	0.0000	-0.0029	-0.0016	0.0000	0.0000
	Y	-0.0033	0.0000	0.0000	0.0000	0.0000	0.0112

	Z	0.0000	0.0000	0.0000	0.0000	0.0158	0.0000
AT. 15	SI X	0.0041	0.0138	0.0086	0.0000	0.0008	0.0000
	Y	0.0136	-0.0046	0.0080	0.0000	0.0123	0.0000
	Z	0.0000	0.0000	0.0000	-0.0173	0.0000	0.0162
AT. 16	SI X	0.0041	-0.0138	0.0086	0.0000	-0.0008	0.0000
	Y	0.0136	0.0046	0.0080	0.0000	-0.0123	0.0000
	Z	0.0000	0.0000	0.0000	0.0173	0.0000	-0.0162
AT. 17	SI X	-0.0041	0.0138	0.0086	0.0000	-0.0008	0.0000
	Y	0.0136	0.0046	-0.0080	0.0000	0.0123	0.0000
	Z	0.0000	0.0000	0.0000	0.0173	0.0000	0.0162
AT. 18	SI X	-0.0041	-0.0138	0.0086	0.0000	0.0008	0.0000
	Y	0.0136	-0.0046	-0.0080	0.0000	-0.0123	0.0000
	Z	0.0000	0.0000	0.0000	-0.0173	0.0000	-0.0162
AT. 19	SI X	-0.0011	0.0068	-0.0007	0.0000	-0.0067	0.0000
	Y	0.0167	0.0117	0.0093	0.0000	0.0181	0.0000
	Z	0.0000	0.0000	0.0000	0.0242	0.0000	0.0143
AT. 20	SI X	-0.0011	-0.0068	-0.0007	0.0000	0.0067	0.0000
	Y	0.0167	-0.0117	0.0093	0.0000	-0.0181	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	0.0000	-0.0143
AT. 21	SI X	0.0011	0.0068	-0.0007	0.0000	0.0067	0.0000
	Y	0.0167	-0.0117	-0.0093	0.0000	0.0181	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	0.0000	0.0143
AT. 22	SI X	0.0011	-0.0068	-0.0007	0.0000	-0.0067	0.0000
	Y	0.0167	0.0117	-0.0093	0.0000	-0.0181	0.0000
	Z	0.0000	0.0000	0.0000	0.0242	0.0000	-0.0143
AT. 23	O X	-0.0003	-0.0137	0.0169	-0.0088	0.0117	-0.0162
	Y	-0.0200	0.0097	0.0071	0.0010	0.0056	-0.0049
	Z	0.0096	-0.0173	0.0073	0.0047	0.0014	0.0034
AT. 24	O X	-0.0003	0.0137	0.0169	-0.0088	-0.0117	-0.0162
	Y	-0.0200	-0.0097	0.0071	0.0010	-0.0056	-0.0049
	Z	-0.0096	-0.0173	-0.0073	-0.0047	0.0014	-0.0034
AT. 25	O X	0.0003	-0.0137	0.0169	-0.0088	-0.0117	0.0162
	Y	-0.0200	-0.0097	-0.0071	-0.0010	0.0056	-0.0049
	Z	0.0096	0.0173	-0.0073	-0.0047	0.0014	0.0034
AT. 26	O X	0.0003	0.0137	0.0169	-0.0088	0.0117	0.0162
	Y	-0.0200	0.0097	-0.0071	-0.0010	-0.0056	-0.0049
	Z	-0.0096	0.0173	0.0073	0.0047	0.0014	-0.0034
AT. 27	O X	-0.0003	0.0137	0.0169	0.0088	-0.0117	0.0162
	Y	-0.0200	-0.0097	0.0071	-0.0010	-0.0056	0.0049
	Z	0.0096	0.0173	0.0073	-0.0047	-0.0014	-0.0034
AT. 28	O X	-0.0003	-0.0137	0.0169	0.0088	0.0117	0.0162
	Y	-0.0200	0.0097	0.0071	-0.0010	0.0056	0.0049
	Z	-0.0096	0.0173	-0.0073	0.0047	-0.0014	0.0034
AT. 29	O X	0.0003	0.0137	0.0169	0.0088	0.0117	-0.0162
	Y	-0.0200	0.0097	-0.0071	0.0010	-0.0056	0.0049
	Z	0.0096	-0.0173	-0.0073	0.0047	-0.0014	-0.0034
AT. 30	O X	0.0003	-0.0137	0.0169	0.0088	-0.0117	-0.0162
	Y	-0.0200	-0.0097	-0.0071	0.0010	0.0056	0.0049
	Z	-0.0096	-0.0173	0.0073	-0.0047	-0.0014	0.0034
AT. 31	O X	0.0005	0.0063	0.0061	-0.0010	-0.0072	-0.0245
	Y	-0.0017	-0.0082	-0.0034	0.0010	-0.0125	0.0135
	Z	0.0028	0.0108	-0.0008	0.0001	0.0027	-0.0045
AT. 32	O X	0.0005	-0.0063	0.0061	-0.0010	0.0072	-0.0245
	Y	-0.0017	0.0082	-0.0034	0.0010	0.0125	0.0135

	Z	-0.0028	0.0108	0.0008	-0.0001	0.0027	0.0045
AT. 33	O X	-0.0005	0.0063	0.0061	-0.0010	0.0072	0.0245
	Y	-0.0017	0.0082	0.0034	-0.0010	-0.0125	0.0135
	Z	0.0028	-0.0108	0.0008	-0.0001	0.0027	-0.0045
AT. 34	O X	-0.0005	-0.0063	0.0061	-0.0010	-0.0072	0.0245
	Y	-0.0017	-0.0082	0.0034	-0.0010	0.0125	0.0135
	Z	-0.0028	-0.0108	-0.0008	0.0001	0.0027	0.0045
AT. 35	O X	0.0005	-0.0063	0.0061	0.0010	0.0072	0.0245
	Y	-0.0017	0.0082	-0.0034	-0.0010	0.0125	-0.0135
	Z	0.0028	-0.0108	-0.0008	-0.0001	-0.0027	0.0045
AT. 36	O X	0.0005	0.0063	0.0061	0.0010	-0.0072	0.0245
	Y	-0.0017	-0.0082	-0.0034	-0.0010	-0.0125	-0.0135
	Z	-0.0028	-0.0108	0.0008	0.0001	-0.0027	-0.0045
AT. 37	O X	-0.0005	-0.0063	0.0061	0.0010	-0.0072	-0.0245
	Y	-0.0017	-0.0082	0.0034	0.0010	0.0125	-0.0135
	Z	0.0028	0.0108	0.0008	0.0001	-0.0027	0.0045
AT. 38	O X	-0.0005	0.0063	0.0061	0.0010	0.0072	-0.0245
	Y	-0.0017	0.0082	0.0034	0.0010	-0.0125	-0.0135
	Z	-0.0028	0.0108	-0.0008	-0.0001	-0.0027	-0.0045
AT. 39	O X	-0.0028	-0.0074	0.0086	0.0036	0.0065	-0.0044
	Y	-0.0096	0.0114	0.0102	0.0281	0.0065	-0.0094
	Z	0.0150	0.0038	-0.0173	0.0043	-0.0181	-0.0028
AT. 40	O X	-0.0028	0.0074	0.0086	0.0036	-0.0065	-0.0044
	Y	-0.0096	-0.0114	0.0102	0.0281	-0.0065	-0.0094
	Z	-0.0150	0.0038	0.0173	-0.0043	-0.0181	0.0028
AT. 41	O X	0.0028	-0.0074	0.0086	0.0036	-0.0065	0.0044
	Y	-0.0096	-0.0114	-0.0102	-0.0281	0.0065	-0.0094
	Z	0.0150	-0.0038	0.0173	-0.0043	-0.0181	-0.0028
AT. 42	O X	0.0028	0.0074	0.0086	0.0036	0.0065	0.0044
	Y	-0.0096	0.0114	-0.0102	-0.0281	-0.0065	-0.0094
	Z	-0.0150	-0.0038	-0.0173	0.0043	-0.0181	0.0028
AT. 43	O X	-0.0028	0.0074	0.0086	-0.0036	-0.0065	0.0044
	Y	-0.0096	-0.0114	0.0102	-0.0281	-0.0065	0.0094
	Z	0.0150	-0.0038	-0.0173	-0.0043	0.0181	0.0028
AT. 44	O X	-0.0028	-0.0074	0.0086	-0.0036	0.0065	0.0044
	Y	-0.0096	0.0114	0.0102	-0.0281	0.0065	0.0094
	Z	-0.0150	-0.0038	0.0173	0.0043	0.0181	-0.0028
AT. 45	O X	0.0028	0.0074	0.0086	-0.0036	0.0065	-0.0044
	Y	-0.0096	0.0114	-0.0102	0.0281	-0.0065	0.0094
	Z	0.0150	0.0038	0.0173	0.0043	0.0181	0.0028
AT. 46	O X	0.0028	-0.0074	0.0086	-0.0036	-0.0065	-0.0044
	Y	-0.0096	-0.0114	-0.0102	0.0281	0.0065	0.0094
	Z	-0.0150	0.0038	-0.0173	-0.0043	0.0181	-0.0028
AT. 47	O X	0.0024	0.0087	0.0037	0.0000	-0.0060	0.0000
	Y	-0.0154	-0.0094	-0.0112	0.0000	-0.0131	0.0000
	Z	0.0000	0.0000	0.0000	-0.0157	0.0000	0.0027
AT. 48	O X	0.0024	-0.0087	0.0037	0.0000	0.0060	0.0000
	Y	-0.0154	0.0094	-0.0112	0.0000	0.0131	0.0000
	Z	0.0000	0.0000	0.0000	0.0157	0.0000	-0.0027
AT. 49	O X	-0.0024	0.0087	0.0037	0.0000	0.0060	0.0000
	Y	-0.0154	0.0094	0.0112	0.0000	-0.0131	0.0000
	Z	0.0000	0.0000	0.0000	0.0157	0.0000	0.0027
AT. 50	O X	-0.0024	-0.0087	0.0037	0.0000	-0.0060	0.0000
	Y	-0.0154	-0.0094	0.0112	0.0000	0.0131	0.0000

	Z	0.0000	0.0000	0.0000	-0.0157	0.0000	-0.0027
AT. 51	O X	-0.0086	0.0061	-0.0092	0.0000	-0.0003	0.0000
	Y	-0.0052	-0.0148	-0.0107	0.0000	0.0018	0.0000
	Z	0.0000	0.0000	0.0000	0.0096	0.0000	-0.0167
AT. 52	O X	-0.0086	-0.0061	-0.0092	0.0000	0.0003	0.0000
	Y	-0.0052	0.0148	-0.0107	0.0000	-0.0018	0.0000
	Z	0.0000	0.0000	0.0000	-0.0096	0.0000	0.0167
AT. 53	O X	0.0086	0.0061	-0.0092	0.0000	0.0003	0.0000
	Y	-0.0052	0.0148	0.0107	0.0000	0.0018	0.0000
	Z	0.0000	0.0000	0.0000	-0.0096	0.0000	-0.0167
AT. 54	O X	0.0086	-0.0061	-0.0092	0.0000	-0.0003	0.0000
	Y	-0.0052	-0.0148	0.0107	0.0000	-0.0018	0.0000
	Z	0.0000	0.0000	0.0000	0.0096	0.0000	0.0167
AT. 55	O X	0.0081	-0.0039	0.0012	0.0000	0.0192	0.0000
	Y	0.0082	0.0076	0.0076	0.0000	0.0075	0.0000
	Z	0.0000	0.0000	0.0000	-0.0166	0.0000	-0.0182
AT. 56	O X	0.0081	0.0039	0.0012	0.0000	-0.0192	0.0000
	Y	0.0082	-0.0076	0.0076	0.0000	-0.0075	0.0000
	Z	0.0000	0.0000	0.0000	0.0166	0.0000	0.0182
AT. 57	O X	-0.0081	-0.0039	0.0012	0.0000	-0.0192	0.0000
	Y	0.0082	-0.0076	-0.0076	0.0000	0.0075	0.0000
	Z	0.0000	0.0000	0.0000	0.0166	0.0000	-0.0182
AT. 58	O X	-0.0081	0.0039	0.0012	0.0000	0.0192	0.0000
	Y	0.0082	0.0076	-0.0076	0.0000	-0.0075	0.0000
	Z	0.0000	0.0000	0.0000	-0.0166	0.0000	0.0182

FREQ(CM\*\*-1) 467.58 475.76 478.48 486.98 489.84 494.91

AT. 1	MG X	0.0196	-0.0098	0.0000	0.0000	0.0142	0.0000
	Y	0.0000	0.0000	0.0008	-0.0051	0.0000	-0.0090
	Z	0.0000	0.0000	-0.0055	-0.0064	0.0000	-0.0001
AT. 2	MG X	-0.0196	0.0098	0.0000	0.0000	-0.0142	0.0000
	Y	0.0000	0.0000	0.0008	0.0051	0.0000	-0.0090
	Z	0.0000	0.0000	0.0055	-0.0064	0.0000	0.0001
AT. 3	MG X	0.0196	-0.0098	0.0000	0.0000	-0.0142	0.0000
	Y	0.0000	0.0000	-0.0008	-0.0051	0.0000	0.0090
	Z	0.0000	0.0000	0.0055	-0.0064	0.0000	0.0001
AT. 4	MG X	-0.0196	0.0098	0.0000	0.0000	0.0142	0.0000
	Y	0.0000	0.0000	-0.0008	0.0051	0.0000	0.0090
	Z	0.0000	0.0000	-0.0055	-0.0064	0.0000	-0.0001
AT. 5	AL X	0.0000	0.0000	-0.0061	0.0000	0.0000	0.0032
	Y	0.0000	0.0000	-0.0043	0.0000	0.0000	-0.0062
	Z	-0.0111	-0.0100	0.0000	-0.0063	-0.0157	0.0000
AT. 6	AL X	0.0000	0.0000	0.0061	0.0000	0.0000	-0.0032
	Y	0.0000	0.0000	-0.0043	0.0000	0.0000	-0.0062
	Z	0.0111	0.0100	0.0000	-0.0063	0.0157	0.0000
AT. 7	AL X	0.0000	0.0000	0.0061	0.0000	0.0000	-0.0032
	Y	0.0000	0.0000	0.0043	0.0000	0.0000	0.0062
	Z	-0.0111	-0.0100	0.0000	-0.0063	0.0157	0.0000
AT. 8	AL X	0.0000	0.0000	-0.0061	0.0000	0.0000	0.0032
	Y	0.0000	0.0000	0.0043	0.0000	0.0000	0.0062
	Z	0.0111	0.0100	0.0000	-0.0063	-0.0157	0.0000
AT. 9	AL X	0.0000	0.0000	0.0000	0.0000	0.0154	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0134	0.0000

	Z	0.0287	-0.0105	-0.0008	-0.0010	0.0000	-0.0013
AT. 10	AL X	0.0000	0.0000	0.0000	0.0000	-0.0154	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0134	0.0000
	Z	0.0287	-0.0105	0.0008	-0.0010	0.0000	0.0013
AT. 11	AL X	0.0000	0.0000	0.0000	0.0000	0.0154	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0134	0.0000
	Z	-0.0287	0.0105	-0.0008	-0.0010	0.0000	-0.0013
AT. 12	AL X	0.0000	0.0000	0.0000	0.0000	-0.0154	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0134	0.0000
	Z	-0.0287	0.0105	0.0008	-0.0010	0.0000	0.0013
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0110	0.0000	0.0000	-0.0086
	Z	0.0000	0.0000	0.0000	0.0072	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	-0.0110	0.0000	0.0000	0.0086
	Z	0.0000	0.0000	0.0000	0.0072	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	0.0000	-0.0010	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	-0.0030	0.0146	0.0142	0.0061	0.0000	-0.0089
AT. 16	SI X	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	-0.0030	0.0146	-0.0142	0.0061	0.0000	0.0089
AT. 17	SI X	0.0000	0.0000	0.0000	0.0000	-0.0010	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	0.0030	-0.0146	0.0142	0.0061	0.0000	-0.0089
AT. 18	SI X	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	0.0030	-0.0146	-0.0142	0.0061	0.0000	0.0089
AT. 19	SI X	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0143	0.0000
	Z	-0.0071	-0.0092	-0.0064	0.0167	0.0000	-0.0147
AT. 20	SI X	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0143	0.0000
	Z	-0.0071	-0.0092	0.0064	0.0167	0.0000	0.0147
AT. 21	SI X	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0143	0.0000
	Z	0.0071	0.0092	-0.0064	0.0167	0.0000	-0.0147
AT. 22	SI X	0.0000	0.0000	0.0000	0.0000	0.0005	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0143	0.0000
	Z	0.0071	0.0092	0.0064	0.0167	0.0000	0.0147
AT. 23	O X	-0.0042	0.0123	-0.0238	-0.0129	-0.0070	0.0033
	Y	0.0082	0.0137	-0.0128	-0.0183	0.0074	-0.0031
	Z	-0.0020	-0.0086	0.0011	0.0045	-0.0022	-0.0019
AT. 24	O X	0.0042	-0.0123	-0.0238	0.0129	0.0070	0.0033
	Y	-0.0082	-0.0137	-0.0128	0.0183	-0.0074	-0.0031
	Z	-0.0020	-0.0086	-0.0011	0.0045	-0.0022	0.0019
AT. 25	O X	-0.0042	0.0123	0.0238	0.0129	-0.0070	-0.0033
	Y	-0.0082	-0.0137	-0.0128	-0.0183	-0.0074	-0.0031
	Z	0.0020	0.0086	0.0011	0.0045	0.0022	-0.0019
AT. 26	O X	0.0042	-0.0123	0.0238	-0.0129	0.0070	-0.0033
	Y	0.0082	0.0137	-0.0128	0.0183	0.0074	-0.0031
	Z	0.0020	0.0086	-0.0011	0.0045	0.0022	0.0019
AT. 27	O X	-0.0042	0.0123	0.0238	-0.0129	0.0070	-0.0033
	Y	0.0082	0.0137	0.0128	-0.0183	-0.0074	0.0031

	Z	-0.0020	-0.0086	-0.0011	0.0045	0.0022	0.0019
AT. 28	O X	0.0042	-0.0123	0.0238	0.0129	-0.0070	-0.0033
	Y	-0.0082	-0.0137	0.0128	0.0183	0.0074	0.0031
	Z	-0.0020	-0.0086	0.0011	0.0045	0.0022	-0.0019
AT. 29	O X	-0.0042	0.0123	-0.0238	0.0129	0.0070	0.0033
	Y	-0.0082	-0.0137	0.0128	-0.0183	0.0074	0.0031
	Z	0.0020	0.0086	-0.0011	0.0045	-0.0022	0.0019
AT. 30	O X	0.0042	-0.0123	-0.0238	-0.0129	-0.0070	0.0033
	Y	0.0082	0.0137	0.0128	0.0183	-0.0074	0.0031
	Z	0.0020	0.0086	0.0011	0.0045	-0.0022	-0.0019
AT. 31	O X	0.0134	0.0012	0.0125	0.0065	0.0086	-0.0232
	Y	-0.0169	0.0041	-0.0068	0.0039	0.0005	0.0116
	Z	-0.0055	0.0008	0.0032	-0.0040	-0.0097	-0.0027
AT. 32	O X	-0.0134	-0.0012	0.0125	-0.0065	-0.0086	-0.0232
	Y	0.0169	-0.0041	-0.0068	-0.0039	-0.0005	0.0116
	Z	-0.0055	0.0008	-0.0032	-0.0040	-0.0097	0.0027
AT. 33	O X	0.0134	0.0012	-0.0125	-0.0065	0.0086	0.0232
	Y	0.0169	-0.0041	-0.0068	0.0039	-0.0005	0.0116
	Z	0.0055	-0.0008	0.0032	-0.0040	0.0097	-0.0027
AT. 34	O X	-0.0134	-0.0012	-0.0125	0.0065	-0.0086	0.0232
	Y	-0.0169	0.0041	-0.0068	-0.0039	0.0005	0.0116
	Z	0.0055	-0.0008	-0.0032	-0.0040	0.0097	0.0027
AT. 35	O X	0.0134	0.0012	-0.0125	0.0065	-0.0086	0.0232
	Y	-0.0169	0.0041	0.0068	0.0039	-0.0005	-0.0116
	Z	-0.0055	0.0008	-0.0032	-0.0040	0.0097	0.0027
AT. 36	O X	-0.0134	-0.0012	-0.0125	-0.0065	0.0086	0.0232
	Y	0.0169	-0.0041	0.0068	-0.0039	0.0005	-0.0116
	Z	-0.0055	0.0008	0.0032	-0.0040	0.0097	-0.0027
AT. 37	O X	0.0134	0.0012	0.0125	-0.0065	-0.0086	-0.0232
	Y	0.0169	-0.0041	0.0068	0.0039	0.0005	-0.0116
	Z	0.0055	-0.0008	-0.0032	-0.0040	-0.0097	0.0027
AT. 38	O X	-0.0134	-0.0012	0.0125	0.0065	0.0086	-0.0232
	Y	-0.0169	0.0041	0.0068	-0.0039	-0.0005	-0.0116
	Z	0.0055	-0.0008	0.0032	-0.0040	-0.0097	-0.0027
AT. 39	O X	-0.0047	-0.0127	-0.0014	-0.0056	-0.0192	0.0011
	Y	0.0037	0.0251	0.0206	0.0231	0.0031	0.0214
	Z	0.0055	0.0071	-0.0006	0.0081	0.0124	0.0023
AT. 40	O X	0.0047	0.0127	-0.0014	0.0056	0.0192	0.0011
	Y	-0.0037	-0.0251	0.0206	-0.0231	-0.0031	0.0214
	Z	0.0055	0.0071	0.0006	0.0081	0.0124	-0.0023
AT. 41	O X	-0.0047	-0.0127	0.0014	0.0056	-0.0192	-0.0011
	Y	-0.0037	-0.0251	0.0206	0.0231	-0.0031	0.0214
	Z	-0.0055	-0.0071	-0.0006	0.0081	-0.0124	0.0023
AT. 42	O X	0.0047	0.0127	0.0014	-0.0056	0.0192	-0.0011
	Y	0.0037	0.0251	0.0206	-0.0231	0.0031	0.0214
	Z	-0.0055	-0.0071	0.0006	0.0081	-0.0124	-0.0023
AT. 43	O X	-0.0047	-0.0127	0.0014	-0.0056	0.0192	-0.0011
	Y	0.0037	0.0251	-0.0206	0.0231	-0.0031	-0.0214
	Z	0.0055	0.0071	0.0006	0.0081	-0.0124	-0.0023
AT. 44	O X	0.0047	0.0127	0.0014	0.0056	-0.0192	-0.0011
	Y	-0.0037	-0.0251	-0.0206	-0.0231	0.0031	-0.0214
	Z	0.0055	0.0071	-0.0006	0.0081	-0.0124	0.0023
AT. 45	O X	-0.0047	-0.0127	-0.0014	0.0056	0.0192	0.0011
	Y	-0.0037	-0.0251	-0.0206	0.0231	0.0031	-0.0214



	Z	-0.0055	-0.0071	0.0006	0.0081	0.0124	-0.0023
AT. 46 O	X	0.0047	0.0127	-0.0014	-0.0056	-0.0192	0.0011
	Y	0.0037	0.0251	-0.0206	-0.0231	-0.0031	-0.0214
	Z	-0.0055	-0.0071	-0.0006	0.0081	0.0124	0.0023
AT. 47 O	X	0.0000	0.0000	0.0000	0.0000	-0.0088	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0084	0.0000
	Z	-0.0154	0.0075	-0.0003	-0.0071	0.0000	0.0172
AT. 48 O	X	0.0000	0.0000	0.0000	0.0000	0.0088	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0084	0.0000
	Z	-0.0154	0.0075	0.0003	-0.0071	0.0000	-0.0172
AT. 49 O	X	0.0000	0.0000	0.0000	0.0000	-0.0088	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0084	0.0000
	Z	0.0154	-0.0075	-0.0003	-0.0071	0.0000	0.0172
AT. 50 O	X	0.0000	0.0000	0.0000	0.0000	0.0088	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0084	0.0000
	Z	0.0154	-0.0075	0.0003	-0.0071	0.0000	-0.0172
AT. 51 O	X	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0047	0.0000
	Z	-0.0101	-0.0127	-0.0214	-0.0140	0.0000	0.0025
AT. 52 O	X	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0047	0.0000
	Z	-0.0101	-0.0127	0.0214	-0.0140	0.0000	-0.0025
AT. 53 O	X	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0047	0.0000
	Z	0.0101	0.0127	-0.0214	-0.0140	0.0000	0.0025
AT. 54 O	X	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0047	0.0000
	Z	0.0101	0.0127	0.0214	-0.0140	0.0000	-0.0025
AT. 55 O	X	0.0000	0.0000	0.0000	0.0000	0.0155	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0024	0.0000
	Z	0.0101	0.0132	0.0079	-0.0201	0.0000	0.0195
AT. 56 O	X	0.0000	0.0000	0.0000	0.0000	-0.0155	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0024	0.0000
	Z	0.0101	0.0132	-0.0079	-0.0201	0.0000	-0.0195
AT. 57 O	X	0.0000	0.0000	0.0000	0.0000	0.0155	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0024	0.0000
	Z	-0.0101	-0.0132	0.0079	-0.0201	0.0000	0.0195
AT. 58 O	X	0.0000	0.0000	0.0000	0.0000	-0.0155	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0024	0.0000
	Z	-0.0101	-0.0132	-0.0079	-0.0201	0.0000	-0.0195

FREQ(CM\*\*-1) 497.32 498.11 498.32 500.17 501.39 509.24

AT. 1 MG	X	0.0000	0.0000	0.0000	-0.0093	0.0000	0.0000
	Y	-0.0139	0.0051	-0.0033	0.0000	-0.0084	0.0134
	Z	0.0022	-0.0069	-0.0010	0.0000	-0.0011	-0.0002
AT. 2 MG	X	0.0000	0.0000	0.0000	-0.0093	0.0000	0.0000
	Y	0.0139	-0.0051	-0.0033	0.0000	-0.0084	-0.0134
	Z	0.0022	-0.0069	0.0010	0.0000	0.0011	-0.0002
AT. 3 MG	X	0.0000	0.0000	0.0000	0.0093	0.0000	0.0000
	Y	0.0139	0.0051	-0.0033	0.0000	-0.0084	0.0134
	Z	-0.0022	-0.0069	-0.0010	0.0000	-0.0011	-0.0002
AT. 4 MG	X	0.0000	0.0000	0.0000	0.0093	0.0000	0.0000
	Y	-0.0139	-0.0051	-0.0033	0.0000	-0.0084	-0.0134

	Z	-0.0022	-0.0069	0.0010	0.0000	0.0011	-0.0002
AT. 5	AL X	0.0000	0.0000	-0.0035	-0.0012	0.0035	0.0000
	Y	0.0000	0.0000	0.0169	0.0024	-0.0006	0.0000
	Z	0.0106	0.0005	0.0000	0.0000	0.0000	-0.0046
AT. 6	AL X	0.0000	0.0000	0.0035	-0.0012	-0.0035	0.0000
	Y	0.0000	0.0000	0.0169	-0.0024	-0.0006	0.0000
	Z	0.0106	0.0005	0.0000	0.0000	0.0000	-0.0046
AT. 7	AL X	0.0000	0.0000	-0.0035	0.0012	0.0035	0.0000
	Y	0.0000	0.0000	0.0169	-0.0024	-0.0006	0.0000
	Z	-0.0106	0.0005	0.0000	0.0000	0.0000	-0.0046
AT. 8	AL X	0.0000	0.0000	0.0035	0.0012	-0.0035	0.0000
	Y	0.0000	0.0000	0.0169	0.0024	-0.0006	0.0000
	Z	-0.0106	0.0005	0.0000	0.0000	0.0000	-0.0046
AT. 9	AL X	0.0058	0.0000	-0.0096	0.0000	-0.0034	0.0000
	Y	-0.0002	0.0000	0.0049	0.0000	0.0001	0.0000
	Z	0.0000	0.0044	0.0000	0.0032	0.0000	-0.0010
AT. 10	AL X	-0.0058	0.0000	-0.0096	0.0000	-0.0034	0.0000
	Y	0.0002	0.0000	0.0049	0.0000	0.0001	0.0000
	Z	0.0000	0.0044	0.0000	-0.0032	0.0000	-0.0010
AT. 11	AL X	-0.0058	0.0000	0.0096	0.0000	0.0034	0.0000
	Y	-0.0002	0.0000	0.0049	0.0000	0.0001	0.0000
	Z	0.0000	0.0044	0.0000	-0.0032	0.0000	-0.0010
AT. 12	AL X	0.0058	0.0000	0.0096	0.0000	0.0034	0.0000
	Y	0.0002	0.0000	0.0049	0.0000	0.0001	0.0000
	Z	0.0000	0.0044	0.0000	0.0032	0.0000	-0.0010
AT. 13	SI X	0.0000	0.0000	0.0000	-0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0227	0.0000	-0.0199	0.0000
	Z	-0.0183	-0.0229	0.0000	0.0000	0.0000	0.0107
AT. 14	SI X	0.0000	0.0000	0.0000	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0227	0.0000	-0.0199	0.0000
	Z	0.0183	-0.0229	0.0000	0.0000	0.0000	0.0107
AT. 15	SI X	-0.0116	0.0000	0.0117	0.0000	-0.0043	0.0000
	Y	0.0090	0.0000	-0.0082	0.0000	-0.0031	0.0000
	Z	0.0000	0.0106	0.0000	0.0139	0.0000	0.0168
AT. 16	SI X	0.0116	0.0000	0.0117	0.0000	-0.0043	0.0000
	Y	-0.0090	0.0000	-0.0082	0.0000	-0.0031	0.0000
	Z	0.0000	0.0106	0.0000	-0.0139	0.0000	0.0168
AT. 17	SI X	0.0116	0.0000	-0.0117	0.0000	0.0043	0.0000
	Y	0.0090	0.0000	-0.0082	0.0000	-0.0031	0.0000
	Z	0.0000	0.0106	0.0000	-0.0139	0.0000	0.0168
AT. 18	SI X	-0.0116	0.0000	-0.0117	0.0000	0.0043	0.0000
	Y	-0.0090	0.0000	-0.0082	0.0000	-0.0031	0.0000
	Z	0.0000	0.0106	0.0000	0.0139	0.0000	0.0168
AT. 19	SI X	-0.0052	0.0000	-0.0120	0.0000	-0.0118	0.0000
	Y	-0.0145	0.0000	-0.0065	0.0000	0.0014	0.0000
	Z	0.0000	-0.0061	0.0000	-0.0004	0.0000	-0.0143
AT. 20	SI X	0.0052	0.0000	-0.0120	0.0000	-0.0118	0.0000
	Y	0.0145	0.0000	-0.0065	0.0000	0.0014	0.0000
	Z	0.0000	-0.0061	0.0000	0.0004	0.0000	-0.0143
AT. 21	SI X	0.0052	0.0000	0.0120	0.0000	0.0118	0.0000
	Y	-0.0145	0.0000	-0.0065	0.0000	0.0014	0.0000
	Z	0.0000	-0.0061	0.0000	0.0004	0.0000	-0.0143
AT. 22	SI X	-0.0052	0.0000	0.0120	0.0000	0.0118	0.0000
	Y	0.0145	0.0000	-0.0065	0.0000	0.0014	0.0000

	Z	0.0000	-0.0061	0.0000	-0.0004	0.0000	-0.0143
AT. 23	O X	0.0008	-0.0087	-0.0039	0.0259	-0.0008	-0.0177
	Y	0.0206	-0.0019	-0.0049	0.0160	-0.0016	-0.0093
	Z	-0.0106	0.0035	0.0113	-0.0011	-0.0012	0.0077
AT. 24	O X	-0.0008	0.0087	-0.0039	0.0259	-0.0008	0.0177
	Y	-0.0206	0.0019	-0.0049	0.0160	-0.0016	0.0093
	Z	-0.0106	0.0035	-0.0113	0.0011	0.0012	0.0077
AT. 25	O X	-0.0008	0.0087	0.0039	0.0259	0.0008	0.0177
	Y	0.0206	-0.0019	-0.0049	-0.0160	-0.0016	-0.0093
	Z	-0.0106	0.0035	0.0113	0.0011	-0.0012	0.0077
AT. 26	O X	0.0008	-0.0087	0.0039	0.0259	0.0008	-0.0177
	Y	-0.0206	0.0019	-0.0049	-0.0160	-0.0016	0.0093
	Z	-0.0106	0.0035	-0.0113	-0.0011	0.0012	0.0077
AT. 27	O X	-0.0008	-0.0087	-0.0039	-0.0259	-0.0008	-0.0177
	Y	-0.0206	-0.0019	-0.0049	-0.0160	-0.0016	-0.0093
	Z	0.0106	0.0035	0.0113	0.0011	-0.0012	0.0077
AT. 28	O X	0.0008	0.0087	-0.0039	-0.0259	-0.0008	0.0177
	Y	0.0206	0.0019	-0.0049	-0.0160	-0.0016	0.0093
	Z	0.0106	0.0035	-0.0113	-0.0011	0.0012	0.0077
AT. 29	O X	0.0008	0.0087	0.0039	-0.0259	0.0008	0.0177
	Y	-0.0206	-0.0019	-0.0049	0.0160	-0.0016	-0.0093
	Z	0.0106	0.0035	0.0113	-0.0011	-0.0012	0.0077
AT. 30	O X	-0.0008	-0.0087	0.0039	-0.0259	0.0008	-0.0177
	Y	0.0206	0.0019	-0.0049	0.0160	-0.0016	0.0093
	Z	0.0106	0.0035	-0.0113	0.0011	0.0012	0.0077
AT. 31	O X	-0.0012	-0.0310	-0.0062	0.0025	-0.0292	0.0078
	Y	-0.0107	-0.0101	-0.0034	-0.0017	0.0161	0.0059
	Z	-0.0012	0.0142	0.0216	-0.0002	-0.0088	-0.0043
AT. 32	O X	0.0012	0.0310	-0.0062	0.0025	-0.0292	-0.0078
	Y	0.0107	0.0101	-0.0034	-0.0017	0.0161	-0.0059
	Z	-0.0012	0.0142	-0.0216	0.0002	0.0088	-0.0043
AT. 33	O X	0.0012	0.0310	0.0062	0.0025	0.0292	-0.0078
	Y	-0.0107	-0.0101	-0.0034	0.0017	0.0161	0.0059
	Z	-0.0012	0.0142	0.0216	0.0002	-0.0088	-0.0043
AT. 34	O X	-0.0012	-0.0310	0.0062	0.0025	0.0292	0.0078
	Y	0.0107	0.0101	-0.0034	0.0017	0.0161	-0.0059
	Z	-0.0012	0.0142	-0.0216	-0.0002	0.0088	-0.0043
AT. 35	O X	0.0012	-0.0310	-0.0062	-0.0025	-0.0292	0.0078
	Y	0.0107	-0.0101	-0.0034	0.0017	0.0161	0.0059
	Z	0.0012	0.0142	0.0216	0.0002	-0.0088	-0.0043
AT. 36	O X	-0.0012	0.0310	-0.0062	-0.0025	-0.0292	-0.0078
	Y	-0.0107	0.0101	-0.0034	0.0017	0.0161	-0.0059
	Z	0.0012	0.0142	-0.0216	-0.0002	0.0088	-0.0043
AT. 37	O X	-0.0012	0.0310	0.0062	-0.0025	0.0292	-0.0078
	Y	0.0107	-0.0101	-0.0034	-0.0017	0.0161	0.0059
	Z	0.0012	0.0142	0.0216	-0.0002	-0.0088	-0.0043
AT. 38	O X	0.0012	-0.0310	0.0062	-0.0025	0.0292	0.0078
	Y	-0.0107	0.0101	-0.0034	-0.0017	0.0161	-0.0059
	Z	0.0012	0.0142	-0.0216	0.0002	0.0088	-0.0043
AT. 39	O X	-0.0051	-0.0056	-0.0102	-0.0048	-0.0059	-0.0044
	Y	0.0115	0.0036	0.0037	0.0168	0.0091	-0.0185
	Z	0.0076	-0.0013	0.0060	-0.0013	0.0047	-0.0048
AT. 40	O X	0.0051	0.0056	-0.0102	-0.0048	-0.0059	0.0044
	Y	-0.0115	-0.0036	0.0037	0.0168	0.0091	0.0185

	Z	0.0076	-0.0013	-0.0060	0.0013	-0.0047	-0.0048
AT. 41	O X	0.0051	0.0056	0.0102	-0.0048	0.0059	0.0044
	Y	0.0115	0.0036	0.0037	-0.0168	0.0091	-0.0185
	Z	0.0076	-0.0013	0.0060	0.0013	0.0047	-0.0048
AT. 42	O X	-0.0051	-0.0056	0.0102	-0.0048	0.0059	-0.0044
	Y	-0.0115	-0.0036	0.0037	-0.0168	0.0091	0.0185
	Z	0.0076	-0.0013	-0.0060	-0.0013	-0.0047	-0.0048
AT. 43	O X	0.0051	-0.0056	-0.0102	0.0048	-0.0059	-0.0044
	Y	-0.0115	0.0036	0.0037	-0.0168	0.0091	-0.0185
	Z	-0.0076	-0.0013	0.0060	0.0013	0.0047	-0.0048
AT. 44	O X	-0.0051	0.0056	-0.0102	0.0048	-0.0059	0.0044
	Y	0.0115	-0.0036	0.0037	-0.0168	0.0091	0.0185
	Z	-0.0076	-0.0013	-0.0060	-0.0013	-0.0047	-0.0048
AT. 45	O X	-0.0051	0.0056	0.0102	0.0048	0.0059	0.0044
	Y	-0.0115	0.0036	0.0037	0.0168	0.0091	-0.0185
	Z	-0.0076	-0.0013	0.0060	-0.0013	0.0047	-0.0048
AT. 46	O X	0.0051	-0.0056	0.0102	0.0048	0.0059	-0.0044
	Y	0.0115	-0.0036	0.0037	0.0168	0.0091	0.0185
	Z	-0.0076	-0.0013	-0.0060	0.0013	-0.0047	-0.0048
AT. 47	O X	-0.0069	0.0000	-0.0107	0.0000	-0.0035	0.0000
	Y	0.0056	0.0000	-0.0019	0.0000	-0.0136	0.0000
	Z	0.0000	-0.0054	0.0000	0.0000	0.0000	0.0118
AT. 48	O X	0.0069	0.0000	-0.0107	0.0000	-0.0035	0.0000
	Y	-0.0056	0.0000	-0.0019	0.0000	-0.0136	0.0000
	Z	0.0000	-0.0054	0.0000	0.0000	0.0000	0.0118
AT. 49	O X	0.0069	0.0000	0.0107	0.0000	0.0035	0.0000
	Y	0.0056	0.0000	-0.0019	0.0000	-0.0136	0.0000
	Z	0.0000	-0.0054	0.0000	0.0000	0.0000	0.0118
AT. 50	O X	-0.0069	0.0000	0.0107	0.0000	0.0035	0.0000
	Y	-0.0056	0.0000	-0.0019	0.0000	-0.0136	0.0000
	Z	0.0000	-0.0054	0.0000	0.0000	0.0000	0.0118
AT. 51	O X	0.0022	0.0000	0.0007	0.0000	0.0013	0.0000
	Y	0.0174	0.0000	-0.0087	0.0000	0.0041	0.0000
	Z	0.0000	-0.0079	0.0000	-0.0222	0.0000	-0.0189
AT. 52	O X	-0.0022	0.0000	0.0007	0.0000	0.0013	0.0000
	Y	-0.0174	0.0000	-0.0087	0.0000	0.0041	0.0000
	Z	0.0000	-0.0079	0.0000	0.0222	0.0000	-0.0189
AT. 53	O X	-0.0022	0.0000	-0.0007	0.0000	-0.0013	0.0000
	Y	0.0174	0.0000	-0.0087	0.0000	0.0041	0.0000
	Z	0.0000	-0.0079	0.0000	0.0222	0.0000	-0.0189
AT. 54	O X	0.0022	0.0000	-0.0007	0.0000	-0.0013	0.0000
	Y	-0.0174	0.0000	-0.0087	0.0000	0.0041	0.0000
	Z	0.0000	-0.0079	0.0000	-0.0222	0.0000	-0.0189
AT. 55	O X	-0.0020	0.0000	-0.0035	0.0000	0.0076	0.0000
	Y	-0.0055	0.0000	-0.0064	0.0000	-0.0041	0.0000
	Z	0.0000	-0.0050	0.0000	-0.0166	0.0000	0.0063
AT. 56	O X	0.0020	0.0000	-0.0035	0.0000	0.0076	0.0000
	Y	0.0055	0.0000	-0.0064	0.0000	-0.0041	0.0000
	Z	0.0000	-0.0050	0.0000	0.0166	0.0000	0.0063
AT. 57	O X	0.0020	0.0000	0.0035	0.0000	-0.0076	0.0000
	Y	-0.0055	0.0000	-0.0064	0.0000	-0.0041	0.0000
	Z	0.0000	-0.0050	0.0000	0.0166	0.0000	0.0063
AT. 58	O X	-0.0020	0.0000	0.0035	0.0000	-0.0076	0.0000
	Y	0.0055	0.0000	-0.0064	0.0000	-0.0041	0.0000

Z 0.0000 -0.0050 0.0000 -0.0166 0.0000 0.0063

FREQ(CM\*\*-1) 532.77 541.20 556.13 562.22 571.19 571.72

AT. 1 MG X 0.0019 -0.0066 0.0000 -0.0027 -0.0041 0.0000

Y 0.0000 0.0000 -0.0010 0.0000 0.0000 -0.0021

Z 0.0000 0.0000 -0.0071 0.0000 0.0000 0.0008

AT. 2 MG X 0.0019 0.0066 0.0000 0.0027 -0.0041 0.0000

Y 0.0000 0.0000 0.0010 0.0000 0.0000 0.0021

Z 0.0000 0.0000 -0.0071 0.0000 0.0000 0.0008

AT. 3 MG X 0.0019 -0.0066 0.0000 0.0027 -0.0041 0.0000

Y 0.0000 0.0000 0.0010 0.0000 0.0000 -0.0021

Z 0.0000 0.0000 0.0071 0.0000 0.0000 0.0008

AT. 4 MG X 0.0019 0.0066 0.0000 -0.0027 -0.0041 0.0000

Y 0.0000 0.0000 -0.0010 0.0000 0.0000 0.0021

Z 0.0000 0.0000 0.0071 0.0000 0.0000 0.0008

AT. 5 AL X -0.0154 0.0000 0.0000 0.0000 0.0003 0.0000

Y -0.0075 0.0000 0.0000 0.0000 -0.0114 0.0000

Z 0.0000 0.0003 -0.0009 0.0050 0.0000 -0.0013

AT. 6 AL X -0.0154 0.0000 0.0000 0.0000 0.0003 0.0000

Y 0.0075 0.0000 0.0000 0.0000 0.0114 0.0000

Z 0.0000 -0.0003 -0.0009 -0.0050 0.0000 -0.0013

AT. 7 AL X -0.0154 0.0000 0.0000 0.0000 0.0003 0.0000

Y -0.0075 0.0000 0.0000 0.0000 -0.0114 0.0000

Z 0.0000 0.0003 0.0009 -0.0050 0.0000 -0.0013

AT. 8 AL X -0.0154 0.0000 0.0000 0.0000 0.0003 0.0000

Y 0.0075 0.0000 0.0000 0.0000 0.0114 0.0000

Z 0.0000 -0.0003 0.0009 0.0050 0.0000 -0.0013

AT. 9 AL X 0.0131 0.0000 -0.0065 -0.0144 -0.0052 0.0000

Y -0.0141 0.0000 -0.0003 0.0198 -0.0162 0.0000

Z 0.0000 0.0038 0.0000 0.0000 0.0000 -0.0035

AT. 10 AL X 0.0131 0.0000 0.0065 0.0144 -0.0052 0.0000

Y -0.0141 0.0000 0.0003 -0.0198 -0.0162 0.0000

Z 0.0000 0.0038 0.0000 0.0000 0.0000 -0.0035

AT. 11 AL X 0.0131 0.0000 0.0065 -0.0144 -0.0052 0.0000

Y 0.0141 0.0000 -0.0003 -0.0198 0.0162 0.0000

Z 0.0000 -0.0038 0.0000 0.0000 0.0000 -0.0035

AT. 12 AL X 0.0131 0.0000 -0.0065 0.0144 -0.0052 0.0000

Y 0.0141 0.0000 0.0003 0.0198 0.0162 0.0000

Z 0.0000 -0.0038 0.0000 0.0000 0.0000 -0.0035

AT. 13 SI X -0.0038 0.0000 0.0000 0.0000 0.0126 0.0000

Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

Z 0.0000 0.0000 -0.0048 0.0000 0.0000 0.0066

AT. 14 SI X -0.0038 0.0000 0.0000 0.0000 0.0126 0.0000

Y 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

Z 0.0000 0.0000 0.0048 0.0000 0.0000 0.0066

AT. 15 SI X -0.0116 0.0000 0.0035 0.0098 -0.0067 0.0000

Y -0.0087 0.0000 0.0054 -0.0024 0.0174 0.0000

Z 0.0000 0.0136 0.0000 0.0000 0.0000 0.0144

AT. 16 SI X -0.0116 0.0000 -0.0035 -0.0098 -0.0067 0.0000

Y -0.0087 0.0000 -0.0054 0.0024 0.0174 0.0000

Z 0.0000 0.0136 0.0000 0.0000 0.0000 0.0144

AT. 17 SI X -0.0116 0.0000 -0.0035 0.0098 -0.0067 0.0000

Y 0.0087 0.0000 0.0054 0.0024 -0.0174 0.0000

	Z	0.0000	-0.0136	0.0000	0.0000	0.0000	0.0144
AT. 18	SI X	-0.0116	0.0000	0.0035	-0.0098	-0.0067	0.0000
	Y	0.0087	0.0000	-0.0054	-0.0024	-0.0174	0.0000
	Z	0.0000	-0.0136	0.0000	0.0000	0.0000	0.0144
AT. 19	SI X	0.0042	0.0000	0.0089	0.0014	0.0174	0.0000
	Y	0.0020	0.0000	0.0009	0.0017	-0.0025	0.0000
	Z	0.0000	0.0107	0.0000	0.0000	0.0000	-0.0137
AT. 20	SI X	0.0042	0.0000	-0.0089	-0.0014	0.0174	0.0000
	Y	0.0020	0.0000	-0.0009	-0.0017	-0.0025	0.0000
	Z	0.0000	0.0107	0.0000	0.0000	0.0000	-0.0137
AT. 21	SI X	0.0042	0.0000	-0.0089	0.0014	0.0174	0.0000
	Y	-0.0020	0.0000	0.0009	-0.0017	0.0025	0.0000
	Z	0.0000	-0.0107	0.0000	0.0000	0.0000	-0.0137
AT. 22	SI X	0.0042	0.0000	0.0089	-0.0014	0.0174	0.0000
	Y	-0.0020	0.0000	-0.0009	0.0017	0.0025	0.0000
	Z	0.0000	-0.0107	0.0000	0.0000	0.0000	-0.0137
AT. 23	O X	-0.0048	0.0205	-0.0020	0.0094	0.0022	0.0056
	Y	-0.0178	0.0122	-0.0097	0.0242	0.0033	0.0224
	Z	0.0176	-0.0055	0.0031	-0.0125	0.0048	0.0019
AT. 24	O X	-0.0048	-0.0205	0.0020	-0.0094	0.0022	-0.0056
	Y	-0.0178	-0.0122	0.0097	-0.0242	0.0033	-0.0224
	Z	-0.0176	-0.0055	0.0031	-0.0125	-0.0048	0.0019
AT. 25	O X	-0.0048	0.0205	0.0020	0.0094	0.0022	-0.0056
	Y	0.0178	-0.0122	-0.0097	-0.0242	-0.0033	0.0224
	Z	-0.0176	0.0055	0.0031	0.0125	-0.0048	0.0019
AT. 26	O X	-0.0048	-0.0205	-0.0020	-0.0094	0.0022	0.0056
	Y	0.0178	0.0122	0.0097	0.0242	-0.0033	-0.0224
	Z	0.0176	0.0055	0.0031	0.0125	0.0048	0.0019
AT. 27	O X	-0.0048	0.0205	0.0020	-0.0094	0.0022	0.0056
	Y	-0.0178	0.0122	0.0097	-0.0242	0.0033	0.0224
	Z	0.0176	-0.0055	-0.0031	0.0125	0.0048	0.0019
AT. 28	O X	-0.0048	-0.0205	-0.0020	0.0094	0.0022	-0.0056
	Y	-0.0178	-0.0122	-0.0097	0.0242	0.0033	-0.0224
	Z	-0.0176	-0.0055	-0.0031	0.0125	-0.0048	0.0019
AT. 29	O X	-0.0048	0.0205	-0.0020	-0.0094	0.0022	-0.0056
	Y	0.0178	-0.0122	0.0097	0.0242	-0.0033	0.0224
	Z	-0.0176	0.0055	-0.0031	-0.0125	-0.0048	0.0019
AT. 30	O X	-0.0048	-0.0205	0.0020	0.0094	0.0022	0.0056
	Y	0.0178	0.0122	-0.0097	-0.0242	-0.0033	-0.0224
	Z	0.0176	0.0055	-0.0031	-0.0125	0.0048	0.0019
AT. 31	O X	-0.0040	0.0036	-0.0276	-0.0016	-0.0049	0.0040
	Y	-0.0003	-0.0032	-0.0065	0.0002	0.0057	0.0040
	Z	0.0029	-0.0005	0.0157	-0.0051	0.0092	-0.0020
AT. 32	O X	-0.0040	-0.0036	0.0276	0.0016	-0.0049	-0.0040
	Y	-0.0003	0.0032	0.0065	-0.0002	0.0057	-0.0040
	Z	-0.0029	-0.0005	0.0157	-0.0051	-0.0092	-0.0020
AT. 33	O X	-0.0040	0.0036	0.0276	-0.0016	-0.0049	-0.0040
	Y	0.0003	0.0032	-0.0065	-0.0002	-0.0057	0.0040
	Z	-0.0029	0.0005	0.0157	0.0051	-0.0092	-0.0020
AT. 34	O X	-0.0040	-0.0036	-0.0276	0.0016	-0.0049	0.0040
	Y	0.0003	-0.0032	0.0065	0.0002	-0.0057	-0.0040
	Z	0.0029	0.0005	0.0157	0.0051	0.0092	-0.0020
AT. 35	O X	-0.0040	0.0036	0.0276	0.0016	-0.0049	0.0040
	Y	-0.0003	-0.0032	0.0065	-0.0002	0.0057	0.0040

	Z	0.0029	-0.0005	-0.0157	0.0051	0.0092	-0.0020
AT. 36	O X	-0.0040	-0.0036	-0.0276	-0.0016	-0.0049	-0.0040
	Y	-0.0003	0.0032	-0.0065	0.0002	0.0057	-0.0040
	Z	-0.0029	-0.0005	-0.0157	0.0051	-0.0092	-0.0020
AT. 37	O X	-0.0040	0.0036	-0.0276	0.0016	-0.0049	-0.0040
	Y	0.0003	0.0032	0.0065	0.0002	-0.0057	0.0040
	Z	-0.0029	0.0005	-0.0157	-0.0051	-0.0092	-0.0020
AT. 38	O X	-0.0040	-0.0036	0.0276	-0.0016	-0.0049	0.0040
	Y	0.0003	-0.0032	-0.0065	-0.0002	-0.0057	-0.0040
	Z	0.0029	0.0005	-0.0157	-0.0051	0.0092	-0.0020
AT. 39	O X	0.0074	0.0001	-0.0109	0.0060	-0.0047	-0.0201
	Y	-0.0089	-0.0188	0.0102	-0.0064	0.0127	0.0152
	Z	-0.0095	-0.0042	0.0059	-0.0003	0.0095	0.0000
AT. 40	O X	0.0074	-0.0001	0.0109	-0.0060	-0.0047	0.0201
	Y	-0.0089	0.0188	-0.0102	0.0064	0.0127	-0.0152
	Z	0.0095	-0.0042	0.0059	-0.0003	-0.0095	0.0000
AT. 41	O X	0.0074	0.0001	0.0109	0.0060	-0.0047	0.0201
	Y	0.0089	0.0188	0.0102	0.0064	-0.0127	0.0152
	Z	0.0095	0.0042	0.0059	0.0003	-0.0095	0.0000
AT. 42	O X	0.0074	-0.0001	-0.0109	-0.0060	-0.0047	-0.0201
	Y	0.0089	-0.0188	-0.0102	-0.0064	-0.0127	-0.0152
	Z	-0.0095	0.0042	0.0059	0.0003	0.0095	0.0000
AT. 43	O X	0.0074	0.0001	0.0109	-0.0060	-0.0047	-0.0201
	Y	-0.0089	-0.0188	-0.0102	0.0064	0.0127	0.0152
	Z	-0.0095	-0.0042	-0.0059	0.0003	0.0095	0.0000
AT. 44	O X	0.0074	-0.0001	-0.0109	0.0060	-0.0047	0.0201
	Y	-0.0089	0.0188	0.0102	-0.0064	0.0127	-0.0152
	Z	0.0095	-0.0042	-0.0059	0.0003	-0.0095	0.0000
AT. 45	O X	0.0074	0.0001	-0.0109	-0.0060	-0.0047	0.0201
	Y	0.0089	0.0188	-0.0102	-0.0064	-0.0127	0.0152
	Z	0.0095	0.0042	-0.0059	-0.0003	-0.0095	0.0000
AT. 46	O X	0.0074	-0.0001	0.0109	0.0060	-0.0047	-0.0201
	Y	0.0089	-0.0188	0.0102	0.0064	-0.0127	-0.0152
	Z	-0.0095	0.0042	-0.0059	-0.0003	0.0095	0.0000
AT. 47	O X	0.0072	0.0000	0.0046	0.0024	0.0066	0.0000
	Y	0.0025	0.0000	0.0083	0.0040	0.0115	0.0000
	Z	0.0000	-0.0106	0.0000	0.0000	0.0000	0.0078
AT. 48	O X	0.0072	0.0000	-0.0046	-0.0024	0.0066	0.0000
	Y	0.0025	0.0000	-0.0083	-0.0040	0.0115	0.0000
	Z	0.0000	-0.0106	0.0000	0.0000	0.0000	0.0078
AT. 49	O X	0.0072	0.0000	-0.0046	0.0024	0.0066	0.0000
	Y	-0.0025	0.0000	0.0083	-0.0040	-0.0115	0.0000
	Z	0.0000	0.0106	0.0000	0.0000	0.0000	0.0078
AT. 50	O X	0.0072	0.0000	0.0046	-0.0024	0.0066	0.0000
	Y	-0.0025	0.0000	-0.0083	0.0040	-0.0115	0.0000
	Z	0.0000	0.0106	0.0000	0.0000	0.0000	0.0078
AT. 51	O X	0.0095	0.0000	-0.0032	-0.0089	-0.0059	0.0000
	Y	0.0047	0.0000	-0.0019	-0.0095	0.0062	0.0000
	Z	0.0000	-0.0188	0.0000	0.0000	0.0000	0.0002
AT. 52	O X	0.0095	0.0000	0.0032	0.0089	-0.0059	0.0000
	Y	0.0047	0.0000	0.0019	0.0095	0.0062	0.0000
	Z	0.0000	-0.0188	0.0000	0.0000	0.0000	0.0002
AT. 53	O X	0.0095	0.0000	0.0032	-0.0089	-0.0059	0.0000
	Y	-0.0047	0.0000	-0.0019	0.0095	-0.0062	0.0000

	Z	0.0000	0.0188	0.0000	0.0000	0.0000	0.0002
AT. 54	O X	0.0095	0.0000	-0.0032	0.0089	-0.0059	0.0000
	Y	-0.0047	0.0000	0.0019	-0.0095	-0.0062	0.0000
	Z	0.0000	0.0188	0.0000	0.0000	0.0000	0.0002
AT. 55	O X	0.0035	0.0000	-0.0067	-0.0057	-0.0013	0.0000
	Y	-0.0026	0.0000	0.0042	0.0002	0.0105	0.0000
	Z	0.0000	-0.0204	0.0000	0.0000	0.0000	-0.0077
AT. 56	O X	0.0035	0.0000	0.0067	0.0057	-0.0013	0.0000
	Y	-0.0026	0.0000	-0.0042	-0.0002	0.0105	0.0000
	Z	0.0000	-0.0204	0.0000	0.0000	0.0000	-0.0077
AT. 57	O X	0.0035	0.0000	0.0067	-0.0057	-0.0013	0.0000
	Y	0.0026	0.0000	0.0042	-0.0002	-0.0105	0.0000
	Z	0.0000	0.0204	0.0000	0.0000	0.0000	-0.0077
AT. 58	O X	0.0035	0.0000	-0.0067	0.0057	-0.0013	0.0000
	Y	0.0026	0.0000	-0.0042	0.0002	-0.0105	0.0000
	Z	0.0000	0.0204	0.0000	0.0000	0.0000	-0.0077

FREQ(CM\*\*-1) 573.61 576.37 581.02 585.92 601.12 602.67

AT. 1	MG X	0.0000	0.0037	0.0000	0.0045	0.0000	0.0000
	Y	-0.0006	0.0000	-0.0029	0.0000	-0.0003	0.0042
	Z	-0.0012	0.0000	-0.0008	0.0000	0.0036	-0.0016
AT. 2	MG X	0.0000	-0.0037	0.0000	-0.0045	0.0000	0.0000
	Y	0.0006	0.0000	-0.0029	0.0000	-0.0003	-0.0042
	Z	-0.0012	0.0000	0.0008	0.0000	-0.0036	-0.0016
AT. 3	MG X	0.0000	0.0037	0.0000	-0.0045	0.0000	0.0000
	Y	0.0006	0.0000	-0.0029	0.0000	-0.0003	-0.0042
	Z	0.0012	0.0000	-0.0008	0.0000	0.0036	0.0016
AT. 4	MG X	0.0000	-0.0037	0.0000	0.0045	0.0000	0.0000
	Y	-0.0006	0.0000	-0.0029	0.0000	-0.0003	0.0042
	Z	0.0012	0.0000	0.0008	0.0000	-0.0036	0.0016
AT. 5	AL X	0.0000	0.0000	-0.0100	0.0000	0.0126	0.0000
	Y	0.0000	0.0000	0.0077	0.0000	0.0082	0.0000
	Z	0.0005	0.0032	0.0000	0.0005	0.0000	0.0095
AT. 6	AL X	0.0000	0.0000	0.0100	0.0000	-0.0126	0.0000
	Y	0.0000	0.0000	0.0077	0.0000	0.0082	0.0000
	Z	0.0005	-0.0032	0.0000	-0.0005	0.0000	0.0095
AT. 7	AL X	0.0000	0.0000	-0.0100	0.0000	0.0126	0.0000
	Y	0.0000	0.0000	0.0077	0.0000	0.0082	0.0000
	Z	-0.0005	0.0032	0.0000	-0.0005	0.0000	-0.0095
AT. 8	AL X	0.0000	0.0000	0.0100	0.0000	-0.0126	0.0000
	Y	0.0000	0.0000	0.0077	0.0000	0.0082	0.0000
	Z	-0.0005	-0.0032	0.0000	0.0005	0.0000	-0.0095
AT. 9	AL X	-0.0041	0.0000	-0.0141	0.0013	0.0008	-0.0022
	Y	-0.0002	0.0000	0.0113	-0.0038	0.0209	0.0250
	Z	0.0000	-0.0123	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0041	0.0000	-0.0141	-0.0013	0.0008	0.0022
	Y	0.0002	0.0000	0.0113	0.0038	0.0209	-0.0250
	Z	0.0000	-0.0123	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0041	0.0000	0.0141	0.0013	-0.0008	0.0022
	Y	-0.0002	0.0000	0.0113	0.0038	0.0209	0.0250
	Z	0.0000	0.0123	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	-0.0041	0.0000	0.0141	-0.0013	-0.0008	-0.0022
	Y	0.0002	0.0000	0.0113	-0.0038	0.0209	-0.0250



	Z	0.0000	0.0123	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	-0.0162	0.0000	-0.0149	0.0000
	Z	0.0042	0.0000	0.0000	0.0000	0.0000	-0.0228
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	-0.0162	0.0000	-0.0149	0.0000
	Z	-0.0042	0.0000	0.0000	0.0000	0.0000	0.0228
AT. 15	SI X	0.0141	0.0000	0.0128	0.0041	-0.0080	-0.0020
	Y	0.0138	0.0000	0.0125	0.0046	-0.0141	0.0009
	Z	0.0000	0.0075	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	-0.0141	0.0000	0.0128	-0.0041	-0.0080	0.0020
	Y	-0.0138	0.0000	0.0125	-0.0046	-0.0141	-0.0009
	Z	0.0000	0.0075	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	-0.0141	0.0000	-0.0128	0.0041	0.0080	0.0020
	Y	0.0138	0.0000	0.0125	-0.0046	-0.0141	0.0009
	Z	0.0000	-0.0075	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0141	0.0000	-0.0128	-0.0041	0.0080	-0.0020
	Y	-0.0138	0.0000	0.0125	0.0046	-0.0141	-0.0009
	Z	0.0000	-0.0075	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0071	0.0000	0.0055	0.0120	0.0034	-0.0038
	Y	0.0017	0.0000	-0.0114	-0.0061	-0.0023	-0.0014
	Z	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0071	0.0000	0.0055	-0.0120	0.0034	0.0038
	Y	-0.0017	0.0000	-0.0114	0.0061	-0.0023	0.0014
	Z	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0071	0.0000	-0.0055	0.0120	-0.0034	0.0038
	Y	0.0017	0.0000	-0.0114	0.0061	-0.0023	-0.0014
	Z	0.0000	-0.0125	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	-0.0071	0.0000	-0.0055	-0.0120	-0.0034	-0.0038
	Y	-0.0017	0.0000	-0.0114	-0.0061	-0.0023	0.0014
	Z	0.0000	-0.0125	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0036	-0.0016	-0.0080	-0.0015	-0.0077	-0.0104
	Y	-0.0003	-0.0168	-0.0073	-0.0039	-0.0075	-0.0147
	Z	0.0112	0.0003	0.0098	-0.0012	-0.0006	0.0073
AT. 24	O X	-0.0036	0.0016	-0.0080	0.0015	-0.0077	0.0104
	Y	0.0003	0.0168	-0.0073	0.0039	-0.0075	0.0147
	Z	0.0112	0.0003	-0.0098	-0.0012	0.0006	0.0073
AT. 25	O X	-0.0036	-0.0016	0.0080	-0.0015	0.0077	0.0104
	Y	-0.0003	0.0168	-0.0073	0.0039	-0.0075	-0.0147
	Z	0.0112	-0.0003	0.0098	0.0012	-0.0006	0.0073
AT. 26	O X	0.0036	0.0016	0.0080	0.0015	0.0077	-0.0104
	Y	0.0003	-0.0168	-0.0073	-0.0039	-0.0075	0.0147
	Z	0.0112	-0.0003	-0.0098	0.0012	0.0006	0.0073
AT. 27	O X	-0.0036	-0.0016	-0.0080	0.0015	-0.0077	0.0104
	Y	0.0003	-0.0168	-0.0073	0.0039	-0.0075	0.0147
	Z	-0.0112	0.0003	0.0098	0.0012	-0.0006	-0.0073
AT. 28	O X	0.0036	0.0016	-0.0080	-0.0015	-0.0077	-0.0104
	Y	-0.0003	0.0168	-0.0073	-0.0039	-0.0075	-0.0147
	Z	-0.0112	0.0003	-0.0098	0.0012	0.0006	-0.0073
AT. 29	O X	0.0036	-0.0016	0.0080	0.0015	0.0077	-0.0104
	Y	0.0003	0.0168	-0.0073	-0.0039	-0.0075	0.0147
	Z	-0.0112	-0.0003	0.0098	-0.0012	-0.0006	-0.0073
AT. 30	O X	-0.0036	0.0016	0.0080	-0.0015	0.0077	0.0104
	Y	-0.0003	-0.0168	-0.0073	0.0039	-0.0075	-0.0147

	Z	-0.0112	-0.0003	-0.0098	-0.0012	0.0006	-0.0073
AT. 31	O X	0.0128	0.0272	-0.0019	0.0305	0.0119	0.0047
	Y	0.0049	-0.0010	0.0022	-0.0020	-0.0063	-0.0124
	Z	-0.0087	-0.0077	-0.0112	-0.0126	-0.0069	-0.0071
AT. 32	O X	-0.0128	-0.0272	-0.0019	-0.0305	0.0119	-0.0047
	Y	-0.0049	0.0010	0.0022	0.0020	-0.0063	0.0124
	Z	-0.0087	-0.0077	0.0112	-0.0126	0.0069	-0.0071
AT. 33	O X	-0.0128	0.0272	0.0019	0.0305	-0.0119	-0.0047
	Y	0.0049	0.0010	0.0022	0.0020	-0.0063	-0.0124
	Z	-0.0087	0.0077	-0.0112	0.0126	-0.0069	-0.0071
AT. 34	O X	0.0128	-0.0272	0.0019	-0.0305	-0.0119	0.0047
	Y	-0.0049	-0.0010	0.0022	-0.0020	-0.0063	0.0124
	Z	-0.0087	0.0077	0.0112	0.0126	0.0069	-0.0071
AT. 35	O X	-0.0128	0.0272	-0.0019	-0.0305	0.0119	-0.0047
	Y	-0.0049	-0.0010	0.0022	0.0020	-0.0063	0.0124
	Z	0.0087	-0.0077	-0.0112	0.0126	-0.0069	0.0071
AT. 36	O X	0.0128	-0.0272	-0.0019	0.0305	0.0119	0.0047
	Y	0.0049	0.0010	0.0022	-0.0020	-0.0063	-0.0124
	Z	0.0087	-0.0077	0.0112	0.0126	0.0069	0.0071
AT. 37	O X	0.0128	0.0272	0.0019	-0.0305	-0.0119	0.0047
	Y	-0.0049	0.0010	0.0022	-0.0020	-0.0063	0.0124
	Z	0.0087	0.0077	-0.0112	-0.0126	-0.0069	0.0071
AT. 38	O X	-0.0128	-0.0272	0.0019	0.0305	-0.0119	-0.0047
	Y	0.0049	-0.0010	0.0022	0.0020	-0.0063	-0.0124
	Z	0.0087	0.0077	0.0112	-0.0126	0.0069	0.0071
AT. 39	O X	-0.0172	-0.0102	0.0035	0.0074	-0.0054	0.0038
	Y	0.0196	0.0063	-0.0069	-0.0047	0.0142	-0.0012
	Z	0.0041	-0.0027	-0.0129	-0.0094	0.0040	0.0004
AT. 40	O X	0.0172	0.0102	0.0035	-0.0074	-0.0054	-0.0038
	Y	-0.0196	-0.0063	-0.0069	0.0047	0.0142	0.0012
	Z	0.0041	-0.0027	0.0129	-0.0094	-0.0040	0.0004
AT. 41	O X	0.0172	-0.0102	-0.0035	0.0074	0.0054	-0.0038
	Y	0.0196	-0.0063	-0.0069	0.0047	0.0142	-0.0012
	Z	0.0041	0.0027	-0.0129	0.0094	0.0040	0.0004
AT. 42	O X	-0.0172	0.0102	-0.0035	-0.0074	0.0054	0.0038
	Y	-0.0196	0.0063	-0.0069	-0.0047	0.0142	0.0012
	Z	0.0041	0.0027	0.0129	0.0094	-0.0040	0.0004
AT. 43	O X	0.0172	-0.0102	0.0035	-0.0074	-0.0054	-0.0038
	Y	-0.0196	0.0063	-0.0069	0.0047	0.0142	0.0012
	Z	-0.0041	-0.0027	-0.0129	0.0094	0.0040	-0.0004
AT. 44	O X	-0.0172	0.0102	0.0035	0.0074	-0.0054	0.0038
	Y	0.0196	-0.0063	-0.0069	-0.0047	0.0142	-0.0012
	Z	-0.0041	-0.0027	0.0129	0.0094	-0.0040	-0.0004
AT. 45	O X	-0.0172	-0.0102	-0.0035	-0.0074	0.0054	0.0038
	Y	-0.0196	-0.0063	-0.0069	-0.0047	0.0142	0.0012
	Z	-0.0041	0.0027	-0.0129	-0.0094	0.0040	-0.0004
AT. 46	O X	0.0172	0.0102	-0.0035	0.0074	0.0054	-0.0038
	Y	0.0196	0.0063	-0.0069	0.0047	0.0142	-0.0012
	Z	-0.0041	0.0027	0.0129	-0.0094	-0.0040	-0.0004
AT. 47	O X	-0.0025	0.0000	-0.0022	0.0040	0.0048	-0.0059
	Y	-0.0091	0.0000	0.0044	0.0111	0.0016	0.0038
	Z	0.0000	-0.0086	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	0.0025	0.0000	-0.0022	-0.0040	0.0048	0.0059
	Y	0.0091	0.0000	0.0044	-0.0111	0.0016	-0.0038

	Z	0.0000	-0.0086	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	0.0025	0.0000	0.0022	0.0040	-0.0048	0.0059
	Y	-0.0091	0.0000	0.0044	-0.0111	0.0016	0.0038
	Z	0.0000	0.0086	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	-0.0025	0.0000	0.0022	-0.0040	-0.0048	-0.0059
	Y	0.0091	0.0000	0.0044	0.0111	0.0016	-0.0038
	Z	0.0000	0.0086	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	-0.0055	0.0000	-0.0103	0.0002	-0.0019	-0.0092
	Y	-0.0068	0.0000	-0.0019	-0.0014	0.0006	-0.0009
	Z	0.0000	0.0020	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	0.0055	0.0000	-0.0103	-0.0002	-0.0019	0.0092
	Y	0.0068	0.0000	-0.0019	0.0014	0.0006	0.0009
	Z	0.0000	0.0020	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	0.0055	0.0000	0.0103	0.0002	0.0019	0.0092
	Y	-0.0068	0.0000	-0.0019	0.0014	0.0006	-0.0009
	Z	0.0000	-0.0020	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	-0.0055	0.0000	0.0103	-0.0002	0.0019	-0.0092
	Y	0.0068	0.0000	-0.0019	-0.0014	0.0006	0.0009
	Z	0.0000	-0.0020	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	-0.0051	0.0000	-0.0052	-0.0078	0.0000	0.0023
	Y	0.0081	0.0000	0.0053	0.0039	-0.0098	-0.0015
	Z	0.0000	-0.0066	0.0000	0.0000	0.0000	0.0000
AT. 56	O X	0.0051	0.0000	-0.0052	0.0078	0.0000	-0.0023
	Y	-0.0081	0.0000	0.0053	-0.0039	-0.0098	0.0015
	Z	0.0000	-0.0066	0.0000	0.0000	0.0000	0.0000
AT. 57	O X	0.0051	0.0000	0.0052	-0.0078	0.0000	-0.0023
	Y	0.0081	0.0000	0.0053	-0.0039	-0.0098	-0.0015
	Z	0.0000	0.0066	0.0000	0.0000	0.0000	0.0000
AT. 58	O X	-0.0051	0.0000	0.0052	0.0078	0.0000	0.0023
	Y	-0.0081	0.0000	0.0053	0.0039	-0.0098	0.0015
	Z	0.0000	0.0066	0.0000	0.0000	0.0000	0.0000

FREQ(CM\*\*-1) 621.99 625.86 631.00 636.25 663.94 671.88

AT. 1	MG X	-0.0001	0.0000	0.0000	0.0057	0.0000	-0.0023
	Y	0.0000	-0.0014	-0.0013	0.0000	0.0019	0.0000
	Z	0.0000	0.0018	0.0024	0.0000	0.0028	0.0000
AT. 2	MG X	0.0001	0.0000	0.0000	-0.0057	0.0000	-0.0023
	Y	0.0000	0.0014	-0.0013	0.0000	0.0019	0.0000
	Z	0.0000	0.0018	-0.0024	0.0000	-0.0028	0.0000
AT. 3	MG X	-0.0001	0.0000	0.0000	-0.0057	0.0000	0.0023
	Y	0.0000	-0.0014	0.0013	0.0000	-0.0019	0.0000
	Z	0.0000	0.0018	-0.0024	0.0000	-0.0028	0.0000
AT. 4	MG X	0.0001	0.0000	0.0000	0.0057	0.0000	0.0023
	Y	0.0000	0.0014	0.0013	0.0000	-0.0019	0.0000
	Z	0.0000	0.0018	0.0024	0.0000	0.0028	0.0000
AT. 5	AL X	0.0000	0.0000	0.0081	0.0000	0.0150	-0.0220
	Y	0.0000	0.0000	0.0011	0.0000	0.0168	-0.0078
	Z	0.0011	-0.0004	0.0000	0.0176	0.0000	0.0000
AT. 6	AL X	0.0000	0.0000	-0.0081	0.0000	-0.0150	-0.0220
	Y	0.0000	0.0000	0.0011	0.0000	0.0168	0.0078
	Z	-0.0011	-0.0004	0.0000	-0.0176	0.0000	0.0000
AT. 7	AL X	0.0000	0.0000	-0.0081	0.0000	-0.0150	0.0220
	Y	0.0000	0.0000	-0.0011	0.0000	-0.0168	0.0078

	Z	0.0011	-0.0004	0.0000	-0.0176	0.0000	0.0000
AT. 8	AL X	0.0000	0.0000	0.0081	0.0000	0.0150	0.0220
	Y	0.0000	0.0000	-0.0011	0.0000	-0.0168	-0.0078
	Z	-0.0011	-0.0004	0.0000	0.0176	0.0000	0.0000
AT. 9	AL X	0.0000	0.0000	0.0000	-0.0130	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	-0.0135	-0.0307	0.0286	0.0000	-0.0084	-0.0035
AT. 10	AL X	0.0000	0.0000	0.0000	0.0130	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000
	Z	-0.0135	-0.0307	-0.0286	0.0000	0.0084	0.0035
AT. 11	AL X	0.0000	0.0000	0.0000	-0.0130	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000
	Z	0.0135	-0.0307	0.0286	0.0000	-0.0084	0.0035
AT. 12	AL X	0.0000	0.0000	0.0000	0.0130	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	0.0135	-0.0307	-0.0286	0.0000	0.0084	-0.0035
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0083
	Y	0.0000	0.0000	-0.0255	0.0000	0.0077	0.0000
	Z	0.0000	0.0250	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0083
	Y	0.0000	0.0000	0.0255	0.0000	-0.0077	0.0000
	Z	0.0000	0.0250	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	-0.0088	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0157	0.0000	0.0000
	Z	-0.0100	-0.0005	-0.0037	0.0000	-0.0166	0.0117
AT. 16	SI X	0.0000	0.0000	0.0000	0.0088	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0157	0.0000	0.0000
	Z	-0.0100	-0.0005	0.0037	0.0000	0.0166	-0.0117
AT. 17	SI X	0.0000	0.0000	0.0000	-0.0088	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0157	0.0000	0.0000
	Z	0.0100	-0.0005	-0.0037	0.0000	-0.0166	-0.0117
AT. 18	SI X	0.0000	0.0000	0.0000	0.0088	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0157	0.0000	0.0000
	Z	0.0100	-0.0005	0.0037	0.0000	0.0166	0.0117
AT. 19	SI X	0.0000	0.0000	0.0000	-0.0013	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0049	0.0000	0.0000
	Z	-0.0092	0.0013	0.0064	0.0000	0.0105	0.0165
AT. 20	SI X	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0049	0.0000	0.0000
	Z	-0.0092	0.0013	-0.0064	0.0000	-0.0105	-0.0165
AT. 21	SI X	0.0000	0.0000	0.0000	-0.0013	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0049	0.0000	0.0000
	Z	0.0092	0.0013	0.0064	0.0000	0.0105	-0.0165
AT. 22	SI X	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0049	0.0000	0.0000
	Z	0.0092	0.0013	-0.0064	0.0000	-0.0105	0.0165
AT. 23	O X	0.0008	-0.0002	-0.0005	0.0054	-0.0023	0.0035
	Y	0.0183	-0.0011	-0.0043	0.0001	-0.0177	-0.0126
	Z	0.0034	-0.0011	-0.0016	0.0021	-0.0027	-0.0023
AT. 24	O X	-0.0008	0.0002	-0.0005	-0.0054	-0.0023	0.0035
	Y	-0.0183	0.0011	-0.0043	-0.0001	-0.0177	-0.0126
	Z	0.0034	-0.0011	0.0016	0.0021	0.0027	0.0023
AT. 25	O X	0.0008	0.0002	0.0005	0.0054	0.0023	0.0035
	Y	-0.0183	-0.0011	-0.0043	-0.0001	-0.0177	0.0126

	Z	-0.0034	-0.0011	-0.0016	-0.0021	-0.0027	0.0023
AT. 26	O X	-0.0008	-0.0002	0.0005	-0.0054	0.0023	0.0035
	Y	0.0183	0.0011	-0.0043	0.0001	-0.0177	0.0126
	Z	-0.0034	-0.0011	0.0016	-0.0021	0.0027	-0.0023
AT. 27	O X	0.0008	-0.0002	0.0005	-0.0054	0.0023	-0.0035
	Y	0.0183	-0.0011	0.0043	-0.0001	0.0177	0.0126
	Z	0.0034	-0.0011	0.0016	-0.0021	0.0027	0.0023
AT. 28	O X	-0.0008	0.0002	0.0005	0.0054	0.0023	-0.0035
	Y	-0.0183	0.0011	0.0043	0.0001	0.0177	0.0126
	Z	0.0034	-0.0011	-0.0016	-0.0021	-0.0027	-0.0023
AT. 29	O X	0.0008	0.0002	-0.0005	-0.0054	-0.0023	-0.0035
	Y	-0.0183	-0.0011	0.0043	0.0001	0.0177	-0.0126
	Z	-0.0034	-0.0011	0.0016	0.0021	0.0027	-0.0023
AT. 30	O X	-0.0008	-0.0002	-0.0005	0.0054	-0.0023	-0.0035
	Y	0.0183	0.0011	0.0043	-0.0001	0.0177	-0.0126
	Z	-0.0034	-0.0011	-0.0016	0.0021	-0.0027	0.0023
AT. 31	O X	0.0209	-0.0107	0.0085	0.0092	-0.0005	0.0034
	Y	0.0033	0.0104	-0.0023	-0.0019	-0.0009	-0.0030
	Z	-0.0042	0.0137	-0.0160	-0.0048	0.0062	-0.0030
AT. 32	O X	-0.0209	0.0107	0.0085	-0.0092	-0.0005	0.0034
	Y	-0.0033	-0.0104	-0.0023	0.0019	-0.0009	-0.0030
	Z	-0.0042	0.0137	0.0160	-0.0048	-0.0062	0.0030
AT. 33	O X	0.0209	0.0107	-0.0085	0.0092	0.0005	0.0034
	Y	-0.0033	0.0104	-0.0023	0.0019	-0.0009	0.0030
	Z	0.0042	0.0137	-0.0160	0.0048	0.0062	0.0030
AT. 34	O X	-0.0209	-0.0107	-0.0085	-0.0092	0.0005	0.0034
	Y	0.0033	-0.0104	-0.0023	-0.0019	-0.0009	0.0030
	Z	0.0042	0.0137	0.0160	0.0048	-0.0062	-0.0030
AT. 35	O X	0.0209	-0.0107	-0.0085	-0.0092	0.0005	-0.0034
	Y	0.0033	0.0104	0.0023	0.0019	0.0009	0.0030
	Z	-0.0042	0.0137	0.0160	0.0048	-0.0062	0.0030
AT. 36	O X	-0.0209	0.0107	-0.0085	0.0092	0.0005	-0.0034
	Y	-0.0033	-0.0104	0.0023	-0.0019	0.0009	0.0030
	Z	-0.0042	0.0137	-0.0160	0.0048	0.0062	-0.0030
AT. 37	O X	0.0209	0.0107	0.0085	-0.0092	-0.0005	-0.0034
	Y	-0.0033	0.0104	0.0023	-0.0019	0.0009	-0.0030
	Z	0.0042	0.0137	0.0160	-0.0048	-0.0062	-0.0030
AT. 38	O X	-0.0209	-0.0107	0.0085	0.0092	-0.0005	-0.0034
	Y	0.0033	-0.0104	0.0023	0.0019	0.0009	-0.0030
	Z	0.0042	0.0137	-0.0160	-0.0048	0.0062	0.0030
AT. 39	O X	0.0154	0.0037	-0.0044	-0.0074	-0.0117	0.0151
	Y	-0.0077	-0.0007	0.0056	0.0181	0.0043	-0.0066
	Z	0.0029	-0.0002	-0.0013	0.0106	-0.0031	0.0015
AT. 40	O X	-0.0154	-0.0037	-0.0044	0.0074	-0.0117	0.0151
	Y	0.0077	0.0007	0.0056	-0.0181	0.0043	-0.0066
	Z	0.0029	-0.0002	0.0013	0.0106	0.0031	-0.0015
AT. 41	O X	0.0154	-0.0037	0.0044	-0.0074	0.0117	0.0151
	Y	0.0077	-0.0007	0.0056	-0.0181	0.0043	0.0066
	Z	-0.0029	-0.0002	-0.0013	-0.0106	-0.0031	-0.0015
AT. 42	O X	-0.0154	0.0037	0.0044	0.0074	0.0117	0.0151
	Y	-0.0077	0.0007	0.0056	0.0181	0.0043	0.0066
	Z	-0.0029	-0.0002	0.0013	-0.0106	0.0031	0.0015
AT. 43	O X	0.0154	0.0037	0.0044	0.0074	0.0117	-0.0151
	Y	-0.0077	-0.0007	-0.0056	-0.0181	-0.0043	0.0066

	Z	0.0029	-0.0002	0.0013	-0.0106	0.0031	-0.0015
AT. 44	O X	-0.0154	-0.0037	0.0044	-0.0074	0.0117	-0.0151
	Y	0.0077	0.0007	-0.0056	0.0181	-0.0043	0.0066
	Z	0.0029	-0.0002	-0.0013	-0.0106	-0.0031	0.0015
AT. 45	O X	0.0154	-0.0037	-0.0044	0.0074	-0.0117	-0.0151
	Y	0.0077	-0.0007	-0.0056	0.0181	-0.0043	-0.0066
	Z	-0.0029	-0.0002	0.0013	0.0106	0.0031	0.0015
AT. 46	O X	-0.0154	0.0037	-0.0044	-0.0074	-0.0117	-0.0151
	Y	-0.0077	0.0007	-0.0056	-0.0181	-0.0043	-0.0066
	Z	-0.0029	-0.0002	-0.0013	0.0106	-0.0031	-0.0015
AT. 47	O X	0.0000	0.0000	0.0000	0.0021	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0015	0.0000	0.0000
	Z	0.0073	-0.0007	0.0009	0.0000	-0.0061	-0.0059
AT. 48	O X	0.0000	0.0000	0.0000	-0.0021	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0015	0.0000	0.0000
	Z	0.0073	-0.0007	-0.0009	0.0000	0.0061	0.0059
AT. 49	O X	0.0000	0.0000	0.0000	0.0021	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0015	0.0000	0.0000
	Z	-0.0073	-0.0007	0.0009	0.0000	-0.0061	0.0059
AT. 50	O X	0.0000	0.0000	0.0000	-0.0021	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0015	0.0000	0.0000
	Z	-0.0073	-0.0007	-0.0009	0.0000	0.0061	-0.0059
AT. 51	O X	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0068	0.0000	0.0000
	Z	0.0059	0.0025	-0.0014	0.0000	0.0040	-0.0047
AT. 52	O X	0.0000	0.0000	0.0000	-0.0025	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0000
	Z	0.0059	0.0025	0.0014	0.0000	-0.0040	0.0047
AT. 53	O X	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0000
	Z	-0.0059	0.0025	-0.0014	0.0000	0.0040	0.0047
AT. 54	O X	0.0000	0.0000	0.0000	-0.0025	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0068	0.0000	0.0000
	Z	-0.0059	0.0025	0.0014	0.0000	-0.0040	-0.0047
AT. 55	O X	0.0000	0.0000	0.0000	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0123	0.0000	0.0000
	Z	0.0079	0.0002	0.0013	0.0000	0.0024	-0.0083
AT. 56	O X	0.0000	0.0000	0.0000	-0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0123	0.0000	0.0000
	Z	0.0079	0.0002	-0.0013	0.0000	-0.0024	0.0083
AT. 57	O X	0.0000	0.0000	0.0000	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0123	0.0000	0.0000
	Z	-0.0079	0.0002	0.0013	0.0000	0.0024	0.0083
AT. 58	O X	0.0000	0.0000	0.0000	-0.0020	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0123	0.0000	0.0000
	Z	-0.0079	0.0002	-0.0013	0.0000	-0.0024	-0.0083

FREQ(CM\*\*-1) 672.80 688.40 690.37 705.35 706.78 711.86

AT. 1 MG	X	0.0000	-0.0013	0.0010	0.0000	0.0025	0.0016
	Y	-0.0023	0.0000	0.0000	0.0003	0.0000	0.0000
	Z	-0.0016	0.0000	0.0000	-0.0020	0.0000	0.0000
AT. 2 MG	X	0.0000	0.0013	0.0010	0.0000	-0.0025	0.0016
	Y	-0.0023	0.0000	0.0000	-0.0003	0.0000	0.0000

	Z	0.0016	0.0000	0.0000	-0.0020	0.0000	0.0000
AT. 3	MG X	0.0000	0.0013	0.0010	0.0000	0.0025	0.0016
	Y	-0.0023	0.0000	0.0000	-0.0003	0.0000	0.0000
	Z	-0.0016	0.0000	0.0000	0.0020	0.0000	0.0000
AT. 4	MG X	0.0000	-0.0013	0.0010	0.0000	-0.0025	0.0016
	Y	-0.0023	0.0000	0.0000	0.0003	0.0000	0.0000
	Z	0.0016	0.0000	0.0000	0.0020	0.0000	0.0000
AT. 5	AL X	-0.0106	0.0000	0.0139	0.0000	0.0000	-0.0036
	Y	-0.0058	0.0000	0.0030	0.0000	0.0000	0.0144
	Z	0.0000	-0.0057	0.0000	-0.0065	0.0251	0.0000
AT. 6	AL X	0.0106	0.0000	0.0139	0.0000	0.0000	-0.0036
	Y	-0.0058	0.0000	-0.0030	0.0000	0.0000	-0.0144
	Z	0.0000	0.0057	0.0000	-0.0065	-0.0251	0.0000
AT. 7	AL X	-0.0106	0.0000	0.0139	0.0000	0.0000	-0.0036
	Y	-0.0058	0.0000	0.0030	0.0000	0.0000	0.0144
	Z	0.0000	0.0057	0.0000	0.0065	0.0251	0.0000
AT. 8	AL X	0.0106	0.0000	0.0139	0.0000	0.0000	-0.0036
	Y	-0.0058	0.0000	-0.0030	0.0000	0.0000	-0.0144
	Z	0.0000	-0.0057	0.0000	0.0065	-0.0251	0.0000
AT. 9	AL X	0.0139	-0.0094	0.0172	0.0248	0.0000	-0.0145
	Y	0.0173	-0.0146	-0.0019	0.0053	0.0000	0.0036
	Z	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000
AT. 10	AL X	0.0139	0.0094	0.0172	-0.0248	0.0000	-0.0145
	Y	0.0173	0.0146	-0.0019	-0.0053	0.0000	0.0036
	Z	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000
AT. 11	AL X	-0.0139	-0.0094	0.0172	-0.0248	0.0000	-0.0145
	Y	0.0173	0.0146	0.0019	0.0053	0.0000	-0.0036
	Z	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000
AT. 12	AL X	-0.0139	0.0094	0.0172	0.0248	0.0000	-0.0145
	Y	0.0173	-0.0146	0.0019	-0.0053	0.0000	-0.0036
	Z	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000
AT. 13	SI X	0.0000	0.0000	0.0010	0.0000	0.0000	0.0079
	Y	-0.0099	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0010	0.0000	0.0000	0.0079
	Y	-0.0099	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0000
AT. 15	SI X	0.0112	-0.0091	-0.0135	-0.0053	0.0000	-0.0065
	Y	-0.0008	0.0033	0.0005	0.0021	0.0000	-0.0188
	Z	0.0000	0.0000	0.0000	0.0000	-0.0142	0.0000
AT. 16	SI X	0.0112	0.0091	-0.0135	0.0053	0.0000	-0.0065
	Y	-0.0008	-0.0033	0.0005	-0.0021	0.0000	-0.0188
	Z	0.0000	0.0000	0.0000	0.0000	-0.0142	0.0000
AT. 17	SI X	-0.0112	-0.0091	-0.0135	0.0053	0.0000	-0.0065
	Y	-0.0008	-0.0033	-0.0005	0.0021	0.0000	0.0188
	Z	0.0000	0.0000	0.0000	0.0000	0.0142	0.0000
AT. 18	SI X	-0.0112	0.0091	-0.0135	-0.0053	0.0000	-0.0065
	Y	-0.0008	0.0033	-0.0005	-0.0021	0.0000	0.0188
	Z	0.0000	0.0000	0.0000	0.0000	0.0142	0.0000
AT. 19	SI X	-0.0176	-0.0125	-0.0111	0.0212	0.0000	0.0147
	Y	0.0015	0.0112	0.0144	0.0032	0.0000	0.0151
	Z	0.0000	0.0000	0.0000	0.0000	0.0148	0.0000
AT. 20	SI X	-0.0176	0.0125	-0.0111	-0.0212	0.0000	0.0147
	Y	0.0015	-0.0112	0.0144	-0.0032	0.0000	0.0151

	Z	0.0000	0.0000	0.0000	0.0000	0.0148	0.0000
AT. 21	SI X	0.0176	-0.0125	-0.0111	-0.0212	0.0000	0.0147
	Y	0.0015	-0.0112	-0.0144	0.0032	0.0000	-0.0151
	Z	0.0000	0.0000	0.0000	0.0000	-0.0148	0.0000
AT. 22	SI X	0.0176	0.0125	-0.0111	0.0212	0.0000	0.0147
	Y	0.0015	0.0112	-0.0144	-0.0032	0.0000	-0.0151
	Z	0.0000	0.0000	0.0000	0.0000	-0.0148	0.0000
AT. 23	O X	0.0064	0.0043	0.0028	0.0024	0.0023	0.0045
	Y	0.0107	0.0118	0.0095	-0.0044	0.0144	0.0073
	Z	0.0026	0.0072	0.0083	-0.0034	0.0014	0.0022
AT. 24	O X	0.0064	-0.0043	0.0028	-0.0024	-0.0023	0.0045
	Y	0.0107	-0.0118	0.0095	0.0044	-0.0144	0.0073
	Z	-0.0026	0.0072	-0.0083	-0.0034	0.0014	-0.0022
AT. 25	O X	-0.0064	0.0043	0.0028	-0.0024	0.0023	0.0045
	Y	0.0107	-0.0118	-0.0095	-0.0044	-0.0144	-0.0073
	Z	0.0026	-0.0072	-0.0083	-0.0034	-0.0014	-0.0022
AT. 26	O X	-0.0064	-0.0043	0.0028	0.0024	-0.0023	0.0045
	Y	0.0107	0.0118	-0.0095	0.0044	0.0144	-0.0073
	Z	-0.0026	-0.0072	0.0083	-0.0034	-0.0014	0.0022
AT. 27	O X	0.0064	-0.0043	0.0028	-0.0024	0.0023	0.0045
	Y	0.0107	-0.0118	0.0095	0.0044	0.0144	0.0073
	Z	0.0026	-0.0072	0.0083	0.0034	0.0014	0.0022
AT. 28	O X	0.0064	0.0043	0.0028	0.0024	-0.0023	0.0045
	Y	0.0107	0.0118	0.0095	-0.0044	-0.0144	0.0073
	Z	-0.0026	-0.0072	-0.0083	0.0034	0.0014	-0.0022
AT. 29	O X	-0.0064	-0.0043	0.0028	0.0024	0.0023	0.0045
	Y	0.0107	0.0118	-0.0095	0.0044	-0.0144	-0.0073
	Z	0.0026	0.0072	-0.0083	0.0034	-0.0014	-0.0022
AT. 30	O X	-0.0064	0.0043	0.0028	-0.0024	-0.0023	0.0045
	Y	0.0107	-0.0118	-0.0095	-0.0044	0.0144	-0.0073
	Z	-0.0026	0.0072	0.0083	0.0034	-0.0014	0.0022
AT. 31	O X	0.0071	0.0118	-0.0021	0.0075	-0.0023	-0.0039
	Y	-0.0014	0.0000	0.0012	-0.0002	-0.0016	0.0033
	Z	-0.0040	0.0020	0.0017	-0.0039	-0.0003	0.0045
AT. 32	O X	0.0071	-0.0118	-0.0021	-0.0075	0.0023	-0.0039
	Y	-0.0014	0.0000	0.0012	0.0002	0.0016	0.0033
	Z	0.0040	0.0020	-0.0017	-0.0039	-0.0003	-0.0045
AT. 33	O X	-0.0071	0.0118	-0.0021	-0.0075	-0.0023	-0.0039
	Y	-0.0014	0.0000	-0.0012	-0.0002	0.0016	-0.0033
	Z	-0.0040	-0.0020	-0.0017	-0.0039	0.0003	-0.0045
AT. 34	O X	-0.0071	-0.0118	-0.0021	0.0075	0.0023	-0.0039
	Y	-0.0014	0.0000	-0.0012	0.0002	-0.0016	-0.0033
	Z	0.0040	-0.0020	0.0017	-0.0039	0.0003	0.0045
AT. 35	O X	0.0071	-0.0118	-0.0021	-0.0075	-0.0023	-0.0039
	Y	-0.0014	0.0000	0.0012	0.0002	-0.0016	0.0033
	Z	-0.0040	-0.0020	0.0017	0.0039	-0.0003	0.0045
AT. 36	O X	0.0071	0.0118	-0.0021	0.0075	0.0023	-0.0039
	Y	-0.0014	0.0000	0.0012	-0.0002	0.0016	0.0033
	Z	0.0040	-0.0020	-0.0017	0.0039	-0.0003	-0.0045
AT. 37	O X	-0.0071	-0.0118	-0.0021	0.0075	-0.0023	-0.0039
	Y	-0.0014	0.0000	-0.0012	0.0002	0.0016	-0.0033
	Z	-0.0040	0.0020	-0.0017	0.0039	0.0003	-0.0045
AT. 38	O X	-0.0071	0.0118	-0.0021	-0.0075	0.0023	-0.0039
	Y	-0.0014	0.0000	-0.0012	-0.0002	-0.0016	-0.0033



	Z	0.0040	0.0020	0.0017	0.0039	0.0003	0.0045
AT. 39	O X	0.0043	0.0075	-0.0089	-0.0030	-0.0105	-0.0015
	Y	-0.0050	-0.0110	0.0116	0.0030	0.0086	-0.0011
	Z	0.0071	0.0089	-0.0063	0.0096	-0.0004	-0.0008
AT. 40	O X	0.0043	-0.0075	-0.0089	0.0030	0.0105	-0.0015
	Y	-0.0050	0.0110	0.0116	-0.0030	-0.0086	-0.0011
	Z	-0.0071	0.0089	0.0063	0.0096	-0.0004	0.0008
AT. 41	O X	-0.0043	0.0075	-0.0089	0.0030	-0.0105	-0.0015
	Y	-0.0050	0.0110	-0.0116	0.0030	-0.0086	0.0011
	Z	0.0071	-0.0089	0.0063	0.0096	0.0004	0.0008
AT. 42	O X	-0.0043	-0.0075	-0.0089	-0.0030	0.0105	-0.0015
	Y	-0.0050	-0.0110	-0.0116	-0.0030	0.0086	0.0011
	Z	-0.0071	-0.0089	-0.0063	0.0096	0.0004	-0.0008
AT. 43	O X	0.0043	-0.0075	-0.0089	0.0030	-0.0105	-0.0015
	Y	-0.0050	0.0110	0.0116	-0.0030	0.0086	-0.0011
	Z	0.0071	-0.0089	-0.0063	-0.0096	-0.0004	-0.0008
AT. 44	O X	0.0043	0.0075	-0.0089	-0.0030	0.0105	-0.0015
	Y	-0.0050	-0.0110	0.0116	0.0030	-0.0086	-0.0011
	Z	-0.0071	-0.0089	0.0063	-0.0096	-0.0004	0.0008
AT. 45	O X	-0.0043	-0.0075	-0.0089	-0.0030	-0.0105	-0.0015
	Y	-0.0050	-0.0110	-0.0116	-0.0030	-0.0086	0.0011
	Z	0.0071	0.0089	0.0063	-0.0096	0.0004	0.0008
AT. 46	O X	-0.0043	0.0075	-0.0089	0.0030	0.0105	-0.0015
	Y	-0.0050	0.0110	-0.0116	0.0030	0.0086	0.0011
	Z	-0.0071	0.0089	-0.0063	-0.0096	0.0004	-0.0008
AT. 47	O X	-0.0072	-0.0042	-0.0016	0.0079	0.0000	0.0087
	Y	-0.0104	-0.0125	-0.0086	0.0079	0.0000	0.0038
	Z	0.0000	0.0000	0.0000	0.0000	-0.0046	0.0000
AT. 48	O X	-0.0072	0.0042	-0.0016	-0.0079	0.0000	0.0087
	Y	-0.0104	0.0125	-0.0086	-0.0079	0.0000	0.0038
	Z	0.0000	0.0000	0.0000	0.0000	-0.0046	0.0000
AT. 49	O X	0.0072	-0.0042	-0.0016	-0.0079	0.0000	0.0087
	Y	-0.0104	0.0125	0.0086	0.0079	0.0000	-0.0038
	Z	0.0000	0.0000	0.0000	0.0000	0.0046	0.0000
AT. 50	O X	0.0072	0.0042	-0.0016	0.0079	0.0000	0.0087
	Y	-0.0104	-0.0125	0.0086	-0.0079	0.0000	-0.0038
	Z	0.0000	0.0000	0.0000	0.0000	0.0046	0.0000
AT. 51	O X	0.0033	0.0000	0.0004	0.0008	0.0000	0.0017
	Y	-0.0058	0.0062	0.0029	-0.0034	0.0000	0.0009
	Z	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000
AT. 52	O X	0.0033	0.0000	0.0004	-0.0008	0.0000	0.0017
	Y	-0.0058	-0.0062	0.0029	0.0034	0.0000	0.0009
	Z	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000
AT. 53	O X	-0.0033	0.0000	0.0004	-0.0008	0.0000	0.0017
	Y	-0.0058	-0.0062	-0.0029	-0.0034	0.0000	-0.0009
	Z	0.0000	0.0000	0.0000	0.0000	-0.0016	0.0000
AT. 54	O X	-0.0033	0.0000	0.0004	0.0008	0.0000	0.0017
	Y	-0.0058	0.0062	-0.0029	0.0034	0.0000	-0.0009
	Z	0.0000	0.0000	0.0000	0.0000	-0.0016	0.0000
AT. 55	O X	0.0001	0.0088	0.0060	-0.0028	0.0000	-0.0018
	Y	-0.0014	-0.0011	-0.0008	0.0082	0.0000	-0.0028
	Z	0.0000	0.0000	0.0000	0.0000	0.0027	0.0000
AT. 56	O X	0.0001	-0.0088	0.0060	0.0028	0.0000	-0.0018
	Y	-0.0014	0.0011	-0.0008	-0.0082	0.0000	-0.0028

	Z	0.0000	0.0000	0.0000	0.0000	0.0027	0.0000
AT. 57	O X	-0.0001	0.0088	0.0060	0.0028	0.0000	-0.0018
	Y	-0.0014	0.0011	0.0008	0.0082	0.0000	0.0028
	Z	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0000
AT. 58	O X	-0.0001	-0.0088	0.0060	-0.0028	0.0000	-0.0018
	Y	-0.0014	-0.0011	0.0008	-0.0082	0.0000	0.0028
	Z	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0000

FREQ(CM\*\*-1) 716.97 728.39 737.01 741.90 755.68 759.71

AT. 1	MG X	0.0000	-0.0005	0.0000	-0.0005	0.0000	0.0000
	Y	-0.0015	0.0000	-0.0026	0.0000	-0.0052	-0.0003
	Z	-0.0037	0.0000	-0.0027	0.0000	-0.0005	0.0037
AT. 2	MG X	0.0000	0.0005	0.0000	0.0005	0.0000	0.0000
	Y	0.0015	0.0000	0.0026	0.0000	-0.0052	0.0003
	Z	-0.0037	0.0000	-0.0027	0.0000	0.0005	0.0037
AT. 3	MG X	0.0000	0.0005	0.0000	0.0005	0.0000	0.0000
	Y	-0.0015	0.0000	0.0026	0.0000	0.0052	0.0003
	Z	-0.0037	0.0000	0.0027	0.0000	0.0005	-0.0037
AT. 4	MG X	0.0000	-0.0005	0.0000	-0.0005	0.0000	0.0000
	Y	0.0015	0.0000	-0.0026	0.0000	0.0052	-0.0003
	Z	-0.0037	0.0000	0.0027	0.0000	-0.0005	-0.0037
AT. 5	AL X	0.0000	0.0000	0.0000	0.0000	-0.0175	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0212	0.0000
	Z	-0.0253	0.0143	-0.0084	0.0008	0.0000	0.0144
AT. 6	AL X	0.0000	0.0000	0.0000	0.0000	0.0175	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0212	0.0000
	Z	-0.0253	-0.0143	-0.0084	-0.0008	0.0000	0.0144
AT. 7	AL X	0.0000	0.0000	0.0000	0.0000	0.0175	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0212	0.0000
	Z	-0.0253	-0.0143	0.0084	-0.0008	0.0000	-0.0144
AT. 8	AL X	0.0000	0.0000	0.0000	0.0000	-0.0175	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0212	0.0000
	Z	-0.0253	0.0143	0.0084	0.0008	0.0000	-0.0144
AT. 9	AL X	0.0000	0.0194	-0.0068	-0.0004	0.0000	-0.0022
	Y	0.0000	-0.0035	0.0171	0.0078	0.0000	0.0010
	Z	0.0010	0.0000	0.0000	0.0000	0.0044	0.0000
AT. 10	AL X	0.0000	-0.0194	0.0068	0.0004	0.0000	0.0022
	Y	0.0000	0.0035	-0.0171	-0.0078	0.0000	-0.0010
	Z	0.0010	0.0000	0.0000	0.0000	-0.0044	0.0000
AT. 11	AL X	0.0000	0.0194	0.0068	-0.0004	0.0000	0.0022
	Y	0.0000	0.0035	0.0171	-0.0078	0.0000	0.0010
	Z	0.0010	0.0000	0.0000	0.0000	0.0044	0.0000
AT. 12	AL X	0.0000	-0.0194	-0.0068	0.0004	0.0000	-0.0022
	Y	0.0000	-0.0035	-0.0171	0.0078	0.0000	-0.0010
	Z	0.0010	0.0000	0.0000	0.0000	-0.0044	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0010	0.0000
	Z	-0.0004	0.0000	-0.0082	0.0000	0.0000	-0.0019
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0010	0.0000
	Z	-0.0004	0.0000	0.0082	0.0000	0.0000	0.0019
AT. 15	SI X	0.0000	-0.0164	0.0160	0.0002	0.0000	-0.0090
	Y	0.0000	0.0030	-0.0136	-0.0209	0.0000	-0.0169

	Z	0.0148	0.0000	0.0000	0.0000	-0.0084	0.0000
AT. 16	SI X	0.0000	0.0164	-0.0160	-0.0002	0.0000	0.0090
	Y	0.0000	-0.0030	0.0136	0.0209	0.0000	0.0169
	Z	0.0148	0.0000	0.0000	0.0000	0.0084	0.0000
AT. 17	SI X	0.0000	-0.0164	-0.0160	0.0002	0.0000	0.0090
	Y	0.0000	-0.0030	-0.0136	0.0209	0.0000	-0.0169
	Z	0.0148	0.0000	0.0000	0.0000	-0.0084	0.0000
AT. 18	SI X	0.0000	0.0164	0.0160	-0.0002	0.0000	-0.0090
	Y	0.0000	0.0030	0.0136	-0.0209	0.0000	0.0169
	Z	0.0148	0.0000	0.0000	0.0000	0.0084	0.0000
AT. 19	SI X	0.0000	0.0145	0.0050	0.0080	0.0000	0.0004
	Y	0.0000	0.0033	0.0016	0.0205	0.0000	0.0224
	Z	0.0143	0.0000	0.0000	0.0000	-0.0124	0.0000
AT. 20	SI X	0.0000	-0.0145	-0.0050	-0.0080	0.0000	-0.0004
	Y	0.0000	-0.0033	-0.0016	-0.0205	0.0000	-0.0224
	Z	0.0143	0.0000	0.0000	0.0000	0.0124	0.0000
AT. 21	SI X	0.0000	0.0145	-0.0050	0.0080	0.0000	-0.0004
	Y	0.0000	-0.0033	0.0016	-0.0205	0.0000	0.0224
	Z	0.0143	0.0000	0.0000	0.0000	-0.0124	0.0000
AT. 22	SI X	0.0000	-0.0145	0.0050	-0.0080	0.0000	0.0004
	Y	0.0000	0.0033	-0.0016	0.0205	0.0000	-0.0224
	Z	0.0143	0.0000	0.0000	0.0000	0.0124	0.0000
AT. 23	O X	0.0043	0.0063	0.0098	-0.0045	-0.0050	-0.0018
	Y	0.0124	0.0147	0.0156	-0.0081	-0.0093	-0.0007
	Z	0.0014	0.0053	-0.0005	0.0077	0.0003	-0.0062
AT. 24	O X	-0.0043	-0.0063	-0.0098	0.0045	-0.0050	0.0018
	Y	-0.0124	-0.0147	-0.0156	0.0081	-0.0093	0.0007
	Z	0.0014	0.0053	-0.0005	0.0077	-0.0003	-0.0062
AT. 25	O X	-0.0043	0.0063	-0.0098	-0.0045	0.0050	0.0018
	Y	0.0124	-0.0147	0.0156	0.0081	-0.0093	-0.0007
	Z	0.0014	-0.0053	-0.0005	-0.0077	0.0003	-0.0062
AT. 26	O X	0.0043	-0.0063	0.0098	0.0045	0.0050	-0.0018
	Y	-0.0124	0.0147	-0.0156	-0.0081	-0.0093	0.0007
	Z	0.0014	-0.0053	-0.0005	-0.0077	-0.0003	-0.0062
AT. 27	O X	0.0043	-0.0063	-0.0098	0.0045	0.0050	0.0018
	Y	0.0124	-0.0147	-0.0156	0.0081	0.0093	0.0007
	Z	0.0014	-0.0053	0.0005	-0.0077	-0.0003	0.0062
AT. 28	O X	-0.0043	0.0063	0.0098	-0.0045	0.0050	-0.0018
	Y	-0.0124	0.0147	0.0156	-0.0081	0.0093	-0.0007
	Z	0.0014	-0.0053	0.0005	-0.0077	0.0003	0.0062
AT. 29	O X	-0.0043	-0.0063	0.0098	0.0045	-0.0050	-0.0018
	Y	0.0124	0.0147	-0.0156	-0.0081	0.0093	0.0007
	Z	0.0014	0.0053	0.0005	0.0077	-0.0003	0.0062
AT. 30	O X	0.0043	0.0063	-0.0098	-0.0045	-0.0050	0.0018
	Y	-0.0124	-0.0147	0.0156	0.0081	0.0093	-0.0007
	Z	0.0014	0.0053	0.0005	0.0077	0.0003	0.0062
AT. 31	O X	-0.0006	-0.0033	0.0000	-0.0013	-0.0003	0.0013
	Y	-0.0020	0.0003	-0.0047	-0.0012	-0.0007	0.0027
	Z	0.0002	0.0023	-0.0006	-0.0015	-0.0049	0.0005
AT. 32	O X	0.0006	0.0033	0.0000	0.0013	-0.0003	-0.0013
	Y	0.0020	-0.0003	0.0047	0.0012	-0.0007	-0.0027
	Z	0.0002	0.0023	-0.0006	-0.0015	0.0049	0.0005
AT. 33	O X	0.0006	-0.0033	0.0000	-0.0013	0.0003	-0.0013
	Y	-0.0020	-0.0003	-0.0047	0.0012	-0.0007	0.0027

	Z	0.0002	-0.0023	-0.0006	0.0015	-0.0049	0.0005
AT. 34	O X	-0.0006	0.0033	0.0000	0.0013	0.0003	0.0013
	Y	0.0020	0.0003	0.0047	-0.0012	-0.0007	-0.0027
	Z	0.0002	-0.0023	-0.0006	0.0015	0.0049	0.0005
AT. 35	O X	-0.0006	0.0033	0.0000	0.0013	0.0003	-0.0013
	Y	-0.0020	-0.0003	0.0047	0.0012	0.0007	-0.0027
	Z	0.0002	-0.0023	0.0006	0.0015	0.0049	-0.0005
AT. 36	O X	0.0006	-0.0033	0.0000	-0.0013	0.0003	0.0013
	Y	0.0020	0.0003	-0.0047	-0.0012	0.0007	0.0027
	Z	0.0002	-0.0023	0.0006	0.0015	-0.0049	-0.0005
AT. 37	O X	0.0006	0.0033	0.0000	0.0013	-0.0003	0.0013
	Y	-0.0020	0.0003	0.0047	-0.0012	0.0007	-0.0027
	Z	0.0002	0.0023	0.0006	-0.0015	0.0049	-0.0005
AT. 38	O X	-0.0006	-0.0033	0.0000	-0.0013	-0.0003	-0.0013
	Y	0.0020	-0.0003	-0.0047	0.0012	0.0007	0.0027
	Z	0.0002	0.0023	0.0006	-0.0015	-0.0049	-0.0005
AT. 39	O X	0.0102	0.0008	-0.0022	0.0092	0.0115	-0.0070
	Y	-0.0087	-0.0010	-0.0020	-0.0080	-0.0094	0.0120
	Z	0.0021	-0.0037	0.0004	0.0010	0.0002	-0.0019
AT. 40	O X	-0.0102	-0.0008	0.0022	-0.0092	0.0115	0.0070
	Y	0.0087	0.0010	0.0020	0.0080	-0.0094	-0.0120
	Z	0.0021	-0.0037	0.0004	0.0010	-0.0002	-0.0019
AT. 41	O X	-0.0102	0.0008	0.0022	0.0092	-0.0115	0.0070
	Y	-0.0087	0.0010	-0.0020	0.0080	-0.0094	0.0120
	Z	0.0021	0.0037	0.0004	-0.0010	0.0002	-0.0019
AT. 42	O X	0.0102	-0.0008	-0.0022	-0.0092	-0.0115	-0.0070
	Y	0.0087	-0.0010	0.0020	-0.0080	-0.0094	-0.0120
	Z	0.0021	0.0037	0.0004	-0.0010	-0.0002	-0.0019
AT. 43	O X	0.0102	-0.0008	0.0022	-0.0092	-0.0115	0.0070
	Y	-0.0087	0.0010	0.0020	0.0080	0.0094	-0.0120
	Z	0.0021	0.0037	-0.0004	-0.0010	-0.0002	0.0019
AT. 44	O X	-0.0102	0.0008	-0.0022	0.0092	-0.0115	-0.0070
	Y	0.0087	-0.0010	-0.0020	-0.0080	0.0094	0.0120
	Z	0.0021	0.0037	-0.0004	-0.0010	0.0002	0.0019
AT. 45	O X	-0.0102	-0.0008	-0.0022	-0.0092	0.0115	-0.0070
	Y	-0.0087	-0.0010	0.0020	-0.0080	0.0094	-0.0120
	Z	0.0021	-0.0037	-0.0004	0.0010	-0.0002	0.0019
AT. 46	O X	0.0102	0.0008	0.0022	0.0092	0.0115	0.0070
	Y	0.0087	0.0010	-0.0020	0.0080	0.0094	0.0120
	Z	0.0021	-0.0037	-0.0004	0.0010	0.0002	0.0019
AT. 47	O X	0.0000	0.0068	0.0063	0.0091	0.0000	0.0028
	Y	0.0000	0.0042	0.0046	-0.0007	0.0000	-0.0044
	Z	-0.0045	0.0000	0.0000	0.0000	0.0045	0.0000
AT. 48	O X	0.0000	-0.0068	-0.0063	-0.0091	0.0000	-0.0028
	Y	0.0000	-0.0042	-0.0046	0.0007	0.0000	0.0044
	Z	-0.0045	0.0000	0.0000	0.0000	-0.0045	0.0000
AT. 49	O X	0.0000	0.0068	-0.0063	0.0091	0.0000	-0.0028
	Y	0.0000	-0.0042	0.0046	0.0007	0.0000	-0.0044
	Z	-0.0045	0.0000	0.0000	0.0000	0.0045	0.0000
AT. 50	O X	0.0000	-0.0068	0.0063	-0.0091	0.0000	0.0028
	Y	0.0000	0.0042	-0.0046	-0.0007	0.0000	0.0044
	Z	-0.0045	0.0000	0.0000	0.0000	-0.0045	0.0000
AT. 51	O X	0.0000	-0.0011	0.0068	0.0103	0.0000	0.0056
	Y	0.0000	0.0036	-0.0064	-0.0040	0.0000	0.0016

	Z	-0.0018	0.0000	0.0000	0.0000	-0.0008	0.0000
AT. 52	O X	0.0000	0.0011	-0.0068	-0.0103	0.0000	-0.0056
	Y	0.0000	-0.0036	0.0064	0.0040	0.0000	-0.0016
	Z	-0.0018	0.0000	0.0000	0.0000	0.0008	0.0000
AT. 53	O X	0.0000	-0.0011	-0.0068	0.0103	0.0000	-0.0056
	Y	0.0000	-0.0036	-0.0064	0.0040	0.0000	0.0016
	Z	-0.0018	0.0000	0.0000	0.0000	-0.0008	0.0000
AT. 54	O X	0.0000	0.0011	0.0068	-0.0103	0.0000	0.0056
	Y	0.0000	0.0036	0.0064	-0.0040	0.0000	-0.0016
	Z	-0.0018	0.0000	0.0000	0.0000	0.0008	0.0000
AT. 55	O X	0.0000	0.0013	-0.0081	-0.0038	0.0000	0.0008
	Y	0.0000	0.0021	-0.0029	-0.0009	0.0000	-0.0035
	Z	-0.0056	0.0000	0.0000	0.0000	0.0027	0.0000
AT. 56	O X	0.0000	-0.0013	0.0081	0.0038	0.0000	-0.0008
	Y	0.0000	-0.0021	0.0029	0.0009	0.0000	0.0035
	Z	-0.0056	0.0000	0.0000	0.0000	-0.0027	0.0000
AT. 57	O X	0.0000	0.0013	0.0081	-0.0038	0.0000	-0.0008
	Y	0.0000	-0.0021	-0.0029	0.0009	0.0000	-0.0035
	Z	-0.0056	0.0000	0.0000	0.0000	0.0027	0.0000
AT. 58	O X	0.0000	-0.0013	-0.0081	0.0038	0.0000	0.0008
	Y	0.0000	0.0021	0.0029	-0.0009	0.0000	0.0035
	Z	-0.0056	0.0000	0.0000	0.0000	-0.0027	0.0000

FREQ(CM\*\*-1) 761.93 770.22 778.43 783.83 816.86 846.28

AT. 1	MG X	0.0000	0.0054	0.0043	0.0000	-0.0007	0.0004
	Y	-0.0015	0.0000	0.0000	-0.0038	0.0000	0.0000
	Z	0.0017	0.0000	0.0000	-0.0011	0.0000	0.0000
AT. 2	MG X	0.0000	0.0054	0.0043	0.0000	-0.0007	0.0004
	Y	-0.0015	0.0000	0.0000	-0.0038	0.0000	0.0000
	Z	-0.0017	0.0000	0.0000	0.0011	0.0000	0.0000
AT. 3	MG X	0.0000	-0.0054	0.0043	0.0000	0.0007	0.0004
	Y	-0.0015	0.0000	0.0000	-0.0038	0.0000	0.0000
	Z	0.0017	0.0000	0.0000	-0.0011	0.0000	0.0000
AT. 4	MG X	0.0000	-0.0054	0.0043	0.0000	0.0007	0.0004
	Y	-0.0015	0.0000	0.0000	-0.0038	0.0000	0.0000
	Z	-0.0017	0.0000	0.0000	0.0011	0.0000	0.0000
AT. 5	AL X	-0.0062	-0.0053	-0.0043	-0.0103	-0.0106	-0.0084
	Y	0.0101	0.0194	0.0100	0.0171	0.0158	0.0131
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 6	AL X	0.0062	-0.0053	-0.0043	0.0103	-0.0106	-0.0084
	Y	0.0101	-0.0194	-0.0100	0.0171	-0.0158	-0.0131
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 7	AL X	-0.0062	0.0053	-0.0043	-0.0103	0.0106	-0.0084
	Y	0.0101	-0.0194	0.0100	0.0171	-0.0158	0.0131
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 8	AL X	0.0062	0.0053	-0.0043	0.0103	0.0106	-0.0084
	Y	0.0101	0.0194	-0.0100	0.0171	0.0158	-0.0131
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 9	AL X	0.0192	0.0000	-0.0023	-0.0024	0.0000	0.0098
	Y	-0.0052	0.0000	-0.0155	0.0013	0.0000	0.0019
	Z	0.0000	-0.0110	0.0000	0.0000	0.0114	0.0000
AT. 10	AL X	0.0192	0.0000	-0.0023	-0.0024	0.0000	0.0098
	Y	-0.0052	0.0000	-0.0155	0.0013	0.0000	0.0019

	Z	0.0000	0.0110	0.0000	0.0000	-0.0114	0.0000
AT. 11	AL X	-0.0192	0.0000	-0.0023	0.0024	0.0000	0.0098
	Y	-0.0052	0.0000	0.0155	0.0013	0.0000	-0.0019
	Z	0.0000	0.0110	0.0000	0.0000	-0.0114	0.0000
AT. 12	AL X	-0.0192	0.0000	-0.0023	0.0024	0.0000	0.0098
	Y	-0.0052	0.0000	0.0155	0.0013	0.0000	-0.0019
	Z	0.0000	-0.0110	0.0000	0.0000	0.0114	0.0000
AT. 13	SI X	0.0000	-0.0204	-0.0240	0.0000	0.0176	0.0072
	Y	0.0051	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0204	-0.0240	0.0000	-0.0176	0.0072
	Y	0.0051	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	-0.0125	0.0000	-0.0093	-0.0060	0.0000	-0.0056
	Y	0.0146	0.0000	0.0042	-0.0120	0.0000	0.0087
	Z	0.0000	-0.0091	0.0000	0.0000	-0.0047	0.0000
AT. 16	SI X	-0.0125	0.0000	-0.0093	-0.0060	0.0000	-0.0056
	Y	0.0146	0.0000	0.0042	-0.0120	0.0000	0.0087
	Z	0.0000	0.0091	0.0000	0.0000	0.0047	0.0000
AT. 17	SI X	0.0125	0.0000	-0.0093	0.0060	0.0000	-0.0056
	Y	0.0146	0.0000	-0.0042	-0.0120	0.0000	-0.0087
	Z	0.0000	0.0091	0.0000	0.0000	0.0047	0.0000
AT. 18	SI X	0.0125	0.0000	-0.0093	0.0060	0.0000	-0.0056
	Y	0.0146	0.0000	-0.0042	-0.0120	0.0000	-0.0087
	Z	0.0000	-0.0091	0.0000	0.0000	-0.0047	0.0000
AT. 19	SI X	-0.0112	0.0000	0.0036	0.0010	0.0000	-0.0035
	Y	-0.0068	0.0000	-0.0011	0.0209	0.0000	-0.0113
	Z	0.0000	0.0043	0.0000	0.0000	0.0054	0.0000
AT. 20	SI X	-0.0112	0.0000	0.0036	0.0010	0.0000	-0.0035
	Y	-0.0068	0.0000	-0.0011	0.0209	0.0000	-0.0113
	Z	0.0000	-0.0043	0.0000	0.0000	-0.0054	0.0000
AT. 21	SI X	0.0112	0.0000	0.0036	-0.0010	0.0000	-0.0035
	Y	-0.0068	0.0000	0.0011	0.0209	0.0000	0.0113
	Z	0.0000	-0.0043	0.0000	0.0000	-0.0054	0.0000
AT. 22	SI X	0.0112	0.0000	0.0036	-0.0010	0.0000	-0.0035
	Y	-0.0068	0.0000	0.0011	0.0209	0.0000	0.0113
	Z	0.0000	0.0043	0.0000	0.0000	0.0054	0.0000
AT. 23	O X	-0.0092	0.0012	0.0053	-0.0020	0.0018	0.0086
	Y	-0.0113	0.0133	0.0079	-0.0050	0.0096	0.0089
	Z	-0.0013	0.0016	-0.0009	-0.0046	0.0022	-0.0032
AT. 24	O X	-0.0092	0.0012	0.0053	-0.0020	0.0018	0.0086
	Y	-0.0113	0.0133	0.0079	-0.0050	0.0096	0.0089
	Z	0.0013	-0.0016	0.0009	0.0046	-0.0022	0.0032
AT. 25	O X	0.0092	0.0012	0.0053	0.0020	0.0018	0.0086
	Y	-0.0113	-0.0133	-0.0079	-0.0050	-0.0096	-0.0089
	Z	-0.0013	-0.0016	0.0009	-0.0046	-0.0022	0.0032
AT. 26	O X	0.0092	0.0012	0.0053	0.0020	0.0018	0.0086
	Y	-0.0113	-0.0133	-0.0079	-0.0050	-0.0096	-0.0089
	Z	0.0013	0.0016	-0.0009	0.0046	0.0022	-0.0032
AT. 27	O X	-0.0092	-0.0012	0.0053	-0.0020	-0.0018	0.0086
	Y	-0.0113	-0.0133	0.0079	-0.0050	-0.0096	0.0089
	Z	-0.0013	-0.0016	-0.0009	-0.0046	-0.0022	-0.0032
AT. 28	O X	-0.0092	-0.0012	0.0053	-0.0020	-0.0018	0.0086
	Y	-0.0113	-0.0133	0.0079	-0.0050	-0.0096	0.0089

	Z	0.0013	0.0016	0.0009	0.0046	0.0022	0.0032
AT. 29	O X	0.0092	-0.0012	0.0053	0.0020	-0.0018	0.0086
	Y	-0.0113	0.0133	-0.0079	-0.0050	0.0096	-0.0089
	Z	-0.0013	0.0016	0.0009	-0.0046	0.0022	0.0032
AT. 30	O X	0.0092	-0.0012	0.0053	0.0020	-0.0018	0.0086
	Y	-0.0113	0.0133	-0.0079	-0.0050	0.0096	-0.0089
	Z	0.0013	-0.0016	-0.0009	0.0046	-0.0022	-0.0032
AT. 31	O X	0.0020	0.0089	0.0116	-0.0014	-0.0097	-0.0064
	Y	-0.0022	-0.0077	-0.0105	0.0002	0.0086	0.0074
	Z	-0.0012	-0.0109	-0.0128	-0.0033	0.0123	0.0088
AT. 32	O X	0.0020	0.0089	0.0116	-0.0014	-0.0097	-0.0064
	Y	-0.0022	-0.0077	-0.0105	0.0002	0.0086	0.0074
	Z	0.0012	0.0109	0.0128	0.0033	-0.0123	-0.0088
AT. 33	O X	-0.0020	0.0089	0.0116	0.0014	-0.0097	-0.0064
	Y	-0.0022	0.0077	0.0105	0.0002	-0.0086	-0.0074
	Z	-0.0012	0.0109	0.0128	-0.0033	-0.0123	-0.0088
AT. 34	O X	-0.0020	0.0089	0.0116	0.0014	-0.0097	-0.0064
	Y	-0.0022	0.0077	0.0105	0.0002	-0.0086	-0.0074
	Z	0.0012	-0.0109	-0.0128	0.0033	0.0123	0.0088
AT. 35	O X	0.0020	-0.0089	0.0116	-0.0014	0.0097	-0.0064
	Y	-0.0022	0.0077	-0.0105	0.0002	-0.0086	0.0074
	Z	-0.0012	0.0109	-0.0128	-0.0033	-0.0123	0.0088
AT. 36	O X	0.0020	-0.0089	0.0116	-0.0014	0.0097	-0.0064
	Y	-0.0022	0.0077	-0.0105	0.0002	-0.0086	0.0074
	Z	0.0012	-0.0109	0.0128	0.0033	0.0123	-0.0088
AT. 37	O X	-0.0020	-0.0089	0.0116	0.0014	0.0097	-0.0064
	Y	-0.0022	-0.0077	0.0105	0.0002	0.0086	-0.0074
	Z	-0.0012	-0.0109	0.0128	-0.0033	0.0123	-0.0088
AT. 38	O X	-0.0020	-0.0089	0.0116	0.0014	0.0097	-0.0064
	Y	-0.0022	-0.0077	0.0105	0.0002	0.0086	-0.0074
	Z	0.0012	0.0109	-0.0128	0.0033	-0.0123	0.0088
AT. 39	O X	0.0003	0.0019	0.0007	0.0061	0.0091	0.0043
	Y	0.0008	-0.0056	-0.0018	-0.0139	-0.0064	-0.0117
	Z	-0.0002	-0.0004	0.0034	-0.0012	0.0024	-0.0022
AT. 40	O X	0.0003	0.0019	0.0007	0.0061	0.0091	0.0043
	Y	0.0008	-0.0056	-0.0018	-0.0139	-0.0064	-0.0117
	Z	0.0002	0.0004	-0.0034	0.0012	-0.0024	0.0022
AT. 41	O X	-0.0003	0.0019	0.0007	-0.0061	0.0091	0.0043
	Y	0.0008	0.0056	0.0018	-0.0139	0.0064	0.0117
	Z	-0.0002	0.0004	-0.0034	-0.0012	-0.0024	0.0022
AT. 42	O X	-0.0003	0.0019	0.0007	-0.0061	0.0091	0.0043
	Y	0.0008	0.0056	0.0018	-0.0139	0.0064	0.0117
	Z	0.0002	-0.0004	0.0034	0.0012	0.0024	-0.0022
AT. 43	O X	0.0003	-0.0019	0.0007	0.0061	-0.0091	0.0043
	Y	0.0008	0.0056	-0.0018	-0.0139	0.0064	-0.0117
	Z	-0.0002	0.0004	0.0034	-0.0012	-0.0024	-0.0022
AT. 44	O X	0.0003	-0.0019	0.0007	0.0061	-0.0091	0.0043
	Y	0.0008	0.0056	-0.0018	-0.0139	0.0064	-0.0117
	Z	0.0002	-0.0004	-0.0034	0.0012	0.0024	0.0022
AT. 45	O X	-0.0003	-0.0019	0.0007	-0.0061	-0.0091	0.0043
	Y	0.0008	-0.0056	0.0018	-0.0139	-0.0064	0.0117
	Z	-0.0002	-0.0004	-0.0034	-0.0012	0.0024	0.0022
AT. 46	O X	-0.0003	-0.0019	0.0007	-0.0061	-0.0091	0.0043
	Y	0.0008	-0.0056	0.0018	-0.0139	-0.0064	0.0117

	Z	0.0002	0.0004	0.0034	0.0012	-0.0024	-0.0022
AT. 47 O	X	-0.0040	0.0000	0.0015	0.0014	0.0000	0.0015
	Y	-0.0025	0.0000	0.0016	-0.0035	0.0000	0.0023
	Z	0.0000	-0.0002	0.0000	0.0000	-0.0030	0.0000
AT. 48 O	X	-0.0040	0.0000	0.0015	0.0014	0.0000	0.0015
	Y	-0.0025	0.0000	0.0016	-0.0035	0.0000	0.0023
	Z	0.0000	0.0002	0.0000	0.0000	0.0030	0.0000
AT. 49 O	X	0.0040	0.0000	0.0015	-0.0014	0.0000	0.0015
	Y	-0.0025	0.0000	-0.0016	-0.0035	0.0000	-0.0023
	Z	0.0000	0.0002	0.0000	0.0000	0.0030	0.0000
AT. 50 O	X	0.0040	0.0000	0.0015	-0.0014	0.0000	0.0015
	Y	-0.0025	0.0000	-0.0016	-0.0035	0.0000	-0.0023
	Z	0.0000	-0.0002	0.0000	0.0000	-0.0030	0.0000
AT. 51 O	X	-0.0074	0.0000	-0.0033	0.0030	0.0000	-0.0090
	Y	0.0053	0.0000	0.0041	-0.0004	0.0000	0.0060
	Z	0.0000	0.0020	0.0000	0.0000	-0.0005	0.0000
AT. 52 O	X	-0.0074	0.0000	-0.0033	0.0030	0.0000	-0.0090
	Y	0.0053	0.0000	0.0041	-0.0004	0.0000	0.0060
	Z	0.0000	-0.0020	0.0000	0.0000	0.0005	0.0000
AT. 53 O	X	0.0074	0.0000	-0.0033	-0.0030	0.0000	-0.0090
	Y	0.0053	0.0000	-0.0041	-0.0004	0.0000	-0.0060
	Z	0.0000	-0.0020	0.0000	0.0000	0.0005	0.0000
AT. 54 O	X	0.0074	0.0000	-0.0033	-0.0030	0.0000	-0.0090
	Y	0.0053	0.0000	-0.0041	-0.0004	0.0000	-0.0060
	Z	0.0000	0.0020	0.0000	0.0000	-0.0005	0.0000
AT. 55 O	X	0.0052	0.0000	0.0020	0.0002	0.0000	0.0012
	Y	-0.0016	0.0000	0.0007	0.0007	0.0000	-0.0072
	Z	0.0000	0.0042	0.0000	0.0000	0.0015	0.0000
AT. 56 O	X	0.0052	0.0000	0.0020	0.0002	0.0000	0.0012
	Y	-0.0016	0.0000	0.0007	0.0007	0.0000	-0.0072
	Z	0.0000	-0.0042	0.0000	0.0000	-0.0015	0.0000
AT. 57 O	X	-0.0052	0.0000	0.0020	-0.0002	0.0000	0.0012
	Y	-0.0016	0.0000	-0.0007	0.0007	0.0000	0.0072
	Z	0.0000	-0.0042	0.0000	0.0000	-0.0015	0.0000
AT. 58 O	X	-0.0052	0.0000	0.0020	-0.0002	0.0000	0.0012
	Y	-0.0016	0.0000	-0.0007	0.0007	0.0000	0.0072
	Z	0.0000	0.0042	0.0000	0.0000	0.0015	0.0000

FREQ(CM\*\*-1) 902.16 906.29 908.86 909.37 910.16 915.10

AT. 1 MG	X	0.0000	0.0003	0.0000	0.0000	-0.0001	0.0000
	Y	0.0000	0.0000	0.0000	0.0017	0.0000	0.0002
	Z	0.0002	0.0000	0.0001	-0.0011	0.0000	0.0018
AT. 2 MG	X	0.0000	0.0003	0.0000	0.0000	0.0001	0.0000
	Y	0.0000	0.0000	0.0000	0.0017	0.0000	0.0002
	Z	-0.0002	0.0000	0.0001	0.0011	0.0000	-0.0018
AT. 3 MG	X	0.0000	-0.0003	0.0000	0.0000	-0.0001	0.0000
	Y	0.0000	0.0000	0.0000	-0.0017	0.0000	0.0002
	Z	-0.0002	0.0000	0.0001	0.0011	0.0000	0.0018
AT. 4 MG	X	0.0000	-0.0003	0.0000	0.0000	0.0001	0.0000
	Y	0.0000	0.0000	0.0000	-0.0017	0.0000	0.0002
	Z	0.0002	0.0000	0.0001	-0.0011	0.0000	-0.0018
AT. 5 AL	X	-0.0031	-0.0033	0.0000	0.0015	0.0000	0.0067
	Y	-0.0024	-0.0009	0.0000	-0.0022	0.0000	0.0028



	Z	0.0000	0.0000	0.0068	0.0000	-0.0067	0.0000
AT. 6	AL X	0.0031	-0.0033	0.0000	-0.0015	0.0000	-0.0067
	Y	-0.0024	0.0009	0.0000	-0.0022	0.0000	0.0028
	Z	0.0000	0.0000	0.0068	0.0000	0.0067	0.0000
AT. 7	AL X	0.0031	0.0033	0.0000	-0.0015	0.0000	0.0067
	Y	0.0024	0.0009	0.0000	0.0022	0.0000	0.0028
	Z	0.0000	0.0000	0.0068	0.0000	-0.0067	0.0000
AT. 8	AL X	-0.0031	0.0033	0.0000	0.0015	0.0000	-0.0067
	Y	0.0024	-0.0009	0.0000	0.0022	0.0000	0.0028
	Z	0.0000	0.0000	0.0068	0.0000	0.0067	0.0000
AT. 9	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
	Z	-0.0007	-0.0008	-0.0001	0.0032	-0.0001	0.0000
AT. 10	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
	Z	0.0007	0.0008	-0.0001	-0.0032	-0.0001	0.0000
AT. 11	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0016
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
	Z	-0.0007	0.0008	-0.0001	0.0032	0.0001	0.0000
AT. 12	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0016
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014
	Z	0.0007	-0.0008	-0.0001	-0.0032	0.0001	0.0000
AT. 13	SI X	0.0000	-0.0007	0.0000	0.0000	0.0000	0.0000
	Y	-0.0027	0.0000	0.0000	0.0260	0.0000	-0.0071
	Z	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000
	Y	0.0027	0.0000	0.0000	-0.0260	0.0000	-0.0071
	Z	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0092
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041
	Z	-0.0142	-0.0140	0.0132	-0.0023	-0.0128	0.0000
AT. 16	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0092
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041
	Z	0.0142	0.0140	0.0132	0.0023	-0.0128	0.0000
AT. 17	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0092
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041
	Z	-0.0142	0.0140	0.0132	-0.0023	0.0128	0.0000
AT. 18	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0092
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041
	Z	0.0142	-0.0140	0.0132	0.0023	0.0128	0.0000
AT. 19	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043
	Z	0.0135	-0.0141	0.0125	0.0013	0.0130	0.0000
AT. 20	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043
	Z	-0.0135	0.0141	0.0125	-0.0013	0.0130	0.0000
AT. 21	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043
	Z	0.0135	0.0141	0.0125	0.0013	-0.0130	0.0000
AT. 22	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043
	Z	-0.0135	-0.0141	0.0125	-0.0013	-0.0130	0.0000
AT. 23	O X	-0.0091	0.0082	0.0092	-0.0013	0.0084	0.0083
	Y	0.0063	-0.0050	-0.0078	0.0020	-0.0069	-0.0068

	Z	0.0155	-0.0150	-0.0153	0.0035	-0.0148	-0.0161
AT. 24	O X	-0.0091	0.0082	-0.0092	-0.0013	-0.0084	0.0083
	Y	0.0063	-0.0050	0.0078	0.0020	0.0069	-0.0068
	Z	-0.0155	0.0150	-0.0153	-0.0035	-0.0148	0.0161
AT. 25	O X	0.0091	0.0082	-0.0092	0.0013	0.0084	-0.0083
	Y	0.0063	0.0050	-0.0078	0.0020	0.0069	-0.0068
	Z	0.0155	0.0150	-0.0153	0.0035	0.0148	-0.0161
AT. 26	O X	0.0091	0.0082	0.0092	0.0013	-0.0084	-0.0083
	Y	0.0063	0.0050	0.0078	0.0020	-0.0069	-0.0068
	Z	-0.0155	-0.0150	-0.0153	-0.0035	0.0148	0.0161
AT. 27	O X	0.0091	-0.0082	0.0092	0.0013	0.0084	0.0083
	Y	-0.0063	0.0050	-0.0078	-0.0020	-0.0069	-0.0068
	Z	-0.0155	0.0150	-0.0153	-0.0035	-0.0148	-0.0161
AT. 28	O X	0.0091	-0.0082	-0.0092	0.0013	-0.0084	0.0083
	Y	-0.0063	0.0050	0.0078	-0.0020	0.0069	-0.0068
	Z	0.0155	-0.0150	-0.0153	0.0035	-0.0148	0.0161
AT. 29	O X	-0.0091	-0.0082	-0.0092	-0.0013	0.0084	-0.0083
	Y	-0.0063	-0.0050	-0.0078	-0.0020	0.0069	-0.0068
	Z	-0.0155	-0.0150	-0.0153	-0.0035	0.0148	-0.0161
AT. 30	O X	-0.0091	-0.0082	0.0092	-0.0013	-0.0084	-0.0083
	Y	-0.0063	-0.0050	0.0078	-0.0020	-0.0069	-0.0068
	Z	0.0155	0.0150	-0.0153	0.0035	0.0148	0.0161
AT. 31	O X	0.0013	0.0004	0.0001	-0.0119	-0.0006	0.0042
	Y	0.0017	-0.0006	0.0000	-0.0166	-0.0008	0.0037
	Z	0.0024	-0.0012	0.0003	-0.0166	-0.0005	0.0055
AT. 32	O X	0.0013	0.0004	-0.0001	-0.0119	0.0006	0.0042
	Y	0.0017	-0.0006	0.0000	-0.0166	0.0008	0.0037
	Z	-0.0024	0.0012	0.0003	0.0166	-0.0005	-0.0055
AT. 33	O X	-0.0013	0.0004	-0.0001	0.0119	-0.0006	-0.0042
	Y	0.0017	0.0006	0.0000	-0.0166	0.0008	0.0037
	Z	0.0024	0.0012	0.0003	-0.0166	0.0005	0.0055
AT. 34	O X	-0.0013	0.0004	0.0001	0.0119	0.0006	-0.0042
	Y	0.0017	0.0006	0.0000	-0.0166	-0.0008	0.0037
	Z	-0.0024	-0.0012	0.0003	0.0166	0.0005	-0.0055
AT. 35	O X	-0.0013	-0.0004	0.0001	0.0119	-0.0006	0.0042
	Y	-0.0017	0.0006	0.0000	0.0166	-0.0008	0.0037
	Z	-0.0024	0.0012	0.0003	0.0166	-0.0005	0.0055
AT. 36	O X	-0.0013	-0.0004	-0.0001	0.0119	0.0006	0.0042
	Y	-0.0017	0.0006	0.0000	0.0166	0.0008	0.0037
	Z	0.0024	-0.0012	0.0003	-0.0166	-0.0005	-0.0055
AT. 37	O X	0.0013	-0.0004	-0.0001	-0.0119	-0.0006	-0.0042
	Y	-0.0017	-0.0006	0.0000	0.0166	0.0008	0.0037
	Z	-0.0024	-0.0012	0.0003	0.0166	0.0005	0.0055
AT. 38	O X	0.0013	-0.0004	0.0001	-0.0119	0.0006	-0.0042
	Y	-0.0017	-0.0006	0.0000	0.0166	-0.0008	0.0037
	Z	0.0024	0.0012	0.0003	-0.0166	0.0005	-0.0055
AT. 39	O X	0.0090	0.0096	-0.0103	-0.0012	0.0109	-0.0109
	Y	0.0047	0.0048	-0.0042	0.0003	0.0043	-0.0017
	Z	0.0146	0.0157	-0.0143	0.0003	0.0150	-0.0153
AT. 40	O X	0.0090	0.0096	0.0103	-0.0012	-0.0109	-0.0109
	Y	0.0047	0.0048	0.0042	0.0003	-0.0043	-0.0017
	Z	-0.0146	-0.0157	-0.0143	-0.0003	0.0150	0.0153
AT. 41	O X	-0.0090	0.0096	0.0103	0.0012	0.0109	0.0109
	Y	0.0047	-0.0048	-0.0042	0.0003	-0.0043	-0.0017

	Z	0.0146	-0.0157	-0.0143	0.0003	-0.0150	-0.0153
AT. 42	O X	-0.0090	0.0096	-0.0103	0.0012	-0.0109	0.0109
	Y	0.0047	-0.0048	0.0042	0.0003	0.0043	-0.0017
	Z	-0.0146	0.0157	-0.0143	-0.0003	-0.0150	0.0153
AT. 43	O X	-0.0090	-0.0096	-0.0103	0.0012	0.0109	-0.0109
	Y	-0.0047	-0.0048	-0.0042	-0.0003	0.0043	-0.0017
	Z	-0.0146	-0.0157	-0.0143	-0.0003	0.0150	-0.0153
AT. 44	O X	-0.0090	-0.0096	0.0103	0.0012	-0.0109	-0.0109
	Y	-0.0047	-0.0048	0.0042	-0.0003	-0.0043	-0.0017
	Z	0.0146	0.0157	-0.0143	0.0003	0.0150	0.0153
AT. 45	O X	0.0090	-0.0096	0.0103	-0.0012	0.0109	0.0109
	Y	-0.0047	0.0048	-0.0042	-0.0003	-0.0043	-0.0017
	Z	-0.0146	0.0157	-0.0143	-0.0003	-0.0150	-0.0153
AT. 46	O X	0.0090	-0.0096	-0.0103	-0.0012	-0.0109	0.0109
	Y	-0.0047	0.0048	0.0042	-0.0003	0.0043	-0.0017
	Z	0.0146	-0.0157	-0.0143	0.0003	-0.0150	0.0153
AT. 47	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0035
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
	Z	0.0006	-0.0005	0.0007	-0.0019	0.0007	0.0000
AT. 48	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0035
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
	Z	-0.0006	0.0005	0.0007	0.0019	0.0007	0.0000
AT. 49	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0035
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
	Z	0.0006	0.0005	0.0007	-0.0019	-0.0007	0.0000
AT. 50	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0035
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
	Z	-0.0006	-0.0005	0.0007	0.0019	-0.0007	0.0000
AT. 51	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Z	-0.0003	0.0001	0.0003	0.0017	-0.0003	0.0000
AT. 52	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Z	0.0003	-0.0001	0.0003	-0.0017	-0.0003	0.0000
AT. 53	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Z	-0.0003	-0.0001	0.0003	0.0017	0.0003	0.0000
AT. 54	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Z	0.0003	0.0001	0.0003	-0.0017	0.0003	0.0000
AT. 55	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0053
	Z	-0.0005	-0.0005	0.0011	-0.0005	-0.0004	0.0000
AT. 56	O X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0053
	Z	0.0005	0.0005	0.0011	0.0005	-0.0004	0.0000
AT. 57	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0053
	Z	-0.0005	0.0005	0.0011	-0.0005	0.0004	0.0000
AT. 58	O X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0053
	Z	0.0005	-0.0005	0.0011	0.0005	0.0004	0.0000

FREQ(CM\*\*-1) 931.13 945.14 963.55 964.77 970.38 977.60

AT. 1 MG X	0.0009	0.0000	0.0000	0.0000	-0.0011	0.0000
Y	0.0000	-0.0007	-0.0008	0.0019	0.0000	-0.0009
Z	0.0000	0.0014	0.0000	-0.0009	0.0000	0.0000
AT. 2 MG X	-0.0009	0.0000	0.0000	0.0000	-0.0011	0.0000
Y	0.0000	0.0007	0.0008	0.0019	0.0000	-0.0009
Z	0.0000	0.0014	0.0000	0.0009	0.0000	0.0000
AT. 3 MG X	-0.0009	0.0000	0.0000	0.0000	-0.0011	0.0000
Y	0.0000	-0.0007	0.0008	0.0019	0.0000	0.0009
Z	0.0000	0.0014	0.0000	-0.0009	0.0000	0.0000
AT. 4 MG X	0.0009	0.0000	0.0000	0.0000	-0.0011	0.0000
Y	0.0000	0.0007	-0.0008	0.0019	0.0000	0.0009
Z	0.0000	0.0014	0.0000	0.0009	0.0000	0.0000
AT. 5 AL X	0.0000	0.0000	0.0000	0.0034	-0.0055	0.0027
Y	0.0000	0.0000	0.0000	-0.0010	-0.0047	-0.0048
Z	0.0096	0.0006	-0.0068	0.0000	0.0000	0.0000
AT. 6 AL X	0.0000	0.0000	0.0000	-0.0034	-0.0055	-0.0027
Y	0.0000	0.0000	0.0000	-0.0010	0.0047	-0.0048
Z	-0.0096	0.0006	-0.0068	0.0000	0.0000	0.0000
AT. 7 AL X	0.0000	0.0000	0.0000	0.0034	-0.0055	-0.0027
Y	0.0000	0.0000	0.0000	-0.0010	-0.0047	0.0048
Z	-0.0096	0.0006	0.0068	0.0000	0.0000	0.0000
AT. 8 AL X	0.0000	0.0000	0.0000	-0.0034	-0.0055	0.0027
Y	0.0000	0.0000	0.0000	-0.0010	0.0047	0.0048
Z	0.0096	0.0006	0.0068	0.0000	0.0000	0.0000
AT. 9 AL X	-0.0042	0.0000	-0.0018	0.0001	0.0027	0.0000
Y	-0.0002	0.0000	0.0008	0.0057	0.0008	0.0000
Z	0.0000	0.0027	0.0000	0.0000	0.0000	0.0003
AT. 10 AL X	0.0042	0.0000	0.0018	0.0001	0.0027	0.0000
Y	0.0002	0.0000	-0.0008	0.0057	0.0008	0.0000
Z	0.0000	0.0027	0.0000	0.0000	0.0000	-0.0003
AT. 11 AL X	-0.0042	0.0000	0.0018	-0.0001	0.0027	0.0000
Y	0.0002	0.0000	0.0008	0.0057	-0.0008	0.0000
Z	0.0000	0.0027	0.0000	0.0000	0.0000	0.0003
AT. 12 AL X	0.0042	0.0000	-0.0018	-0.0001	0.0027	0.0000
Y	-0.0002	0.0000	-0.0008	0.0057	-0.0008	0.0000
Z	0.0000	0.0027	0.0000	0.0000	0.0000	-0.0003
AT. 13 SI X	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0000
Y	0.0000	0.0000	0.0000	0.0226	0.0000	-0.0029
Z	0.0000	0.0282	0.0165	0.0000	0.0000	0.0000
AT. 14 SI X	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0000
Y	0.0000	0.0000	0.0000	0.0226	0.0000	0.0029
Z	0.0000	0.0282	-0.0165	0.0000	0.0000	0.0000
AT. 15 SI X	0.0100	0.0000	-0.0047	0.0009	-0.0114	0.0000
Y	0.0030	0.0000	-0.0008	0.0035	-0.0031	0.0000
Z	0.0000	0.0010	0.0000	0.0000	0.0000	-0.0101
AT. 16 SI X	-0.0100	0.0000	0.0047	0.0009	-0.0114	0.0000
Y	-0.0030	0.0000	0.0008	0.0035	-0.0031	0.0000
Z	0.0000	0.0010	0.0000	0.0000	0.0000	0.0101
AT. 17 SI X	0.0100	0.0000	0.0047	-0.0009	-0.0114	0.0000
Y	-0.0030	0.0000	-0.0008	0.0035	0.0031	0.0000
Z	0.0000	0.0010	0.0000	0.0000	0.0000	-0.0101
AT. 18 SI X	-0.0100	0.0000	-0.0047	-0.0009	-0.0114	0.0000
Y	0.0030	0.0000	0.0008	0.0035	0.0031	0.0000

	Z	0.0000	0.0010	0.0000	0.0000	0.0000	0.0101
AT. 19	SI X	-0.0064	0.0000	-0.0072	0.0001	-0.0076	0.0000
	Y	0.0048	0.0000	0.0077	0.0014	0.0083	0.0000
	Z	0.0000	-0.0016	0.0000	0.0000	0.0000	-0.0118
AT. 20	SI X	0.0064	0.0000	0.0072	0.0001	-0.0076	0.0000
	Y	-0.0048	0.0000	-0.0077	0.0014	0.0083	0.0000
	Z	0.0000	-0.0016	0.0000	0.0000	0.0000	0.0118
AT. 21	SI X	-0.0064	0.0000	0.0072	-0.0001	-0.0076	0.0000
	Y	-0.0048	0.0000	0.0077	0.0014	-0.0083	0.0000
	Z	0.0000	-0.0016	0.0000	0.0000	0.0000	-0.0118
AT. 22	SI X	0.0064	0.0000	-0.0072	-0.0001	-0.0076	0.0000
	Y	0.0048	0.0000	-0.0077	0.0014	-0.0083	0.0000
	Z	0.0000	-0.0016	0.0000	0.0000	0.0000	0.0118
AT. 23	O X	-0.0086	0.0006	-0.0027	0.0033	0.0087	-0.0091
	Y	0.0068	-0.0010	0.0032	-0.0001	-0.0076	0.0065
	Z	0.0164	-0.0018	0.0053	-0.0029	-0.0148	0.0144
AT. 24	O X	0.0086	-0.0006	0.0027	0.0033	0.0087	-0.0091
	Y	-0.0068	0.0010	-0.0032	-0.0001	-0.0076	0.0065
	Z	0.0164	-0.0018	0.0053	0.0029	0.0148	-0.0144
AT. 25	O X	-0.0086	-0.0006	0.0027	-0.0033	0.0087	0.0091
	Y	-0.0068	-0.0010	0.0032	-0.0001	0.0076	0.0065
	Z	-0.0164	-0.0018	0.0053	-0.0029	0.0148	0.0144
AT. 26	O X	0.0086	0.0006	-0.0027	-0.0033	0.0087	0.0091
	Y	0.0068	0.0010	-0.0032	-0.0001	0.0076	0.0065
	Z	-0.0164	-0.0018	0.0053	0.0029	-0.0148	-0.0144
AT. 27	O X	0.0086	0.0006	0.0027	0.0033	0.0087	0.0091
	Y	-0.0068	-0.0010	-0.0032	-0.0001	-0.0076	-0.0065
	Z	-0.0164	-0.0018	-0.0053	-0.0029	-0.0148	-0.0144
AT. 28	O X	-0.0086	-0.0006	-0.0027	0.0033	0.0087	0.0091
	Y	0.0068	0.0010	0.0032	-0.0001	-0.0076	-0.0065
	Z	-0.0164	-0.0018	-0.0053	0.0029	0.0148	0.0144
AT. 29	O X	0.0086	-0.0006	-0.0027	-0.0033	0.0087	-0.0091
	Y	0.0068	-0.0010	-0.0032	-0.0001	0.0076	-0.0065
	Z	0.0164	-0.0018	-0.0053	-0.0029	0.0148	-0.0144
AT. 30	O X	-0.0086	0.0006	0.0027	-0.0033	0.0087	-0.0091
	Y	-0.0068	0.0010	0.0032	-0.0001	0.0076	-0.0065
	Z	0.0164	-0.0018	-0.0053	0.0029	-0.0148	0.0144
AT. 31	O X	-0.0002	-0.0121	-0.0072	-0.0098	0.0002	0.0016
	Y	-0.0015	-0.0144	-0.0079	-0.0146	0.0027	0.0017
	Z	-0.0024	-0.0165	-0.0107	-0.0163	0.0034	0.0011
AT. 32	O X	0.0002	0.0121	0.0072	-0.0098	0.0002	0.0016
	Y	0.0015	0.0144	0.0079	-0.0146	0.0027	0.0017
	Z	-0.0024	-0.0165	-0.0107	0.0163	-0.0034	-0.0011
AT. 33	O X	-0.0002	0.0121	0.0072	0.0098	0.0002	-0.0016
	Y	0.0015	-0.0144	-0.0079	-0.0146	-0.0027	0.0017
	Z	0.0024	-0.0165	-0.0107	-0.0163	-0.0034	0.0011
AT. 34	O X	0.0002	-0.0121	-0.0072	0.0098	0.0002	-0.0016
	Y	-0.0015	0.0144	0.0079	-0.0146	-0.0027	0.0017
	Z	0.0024	-0.0165	-0.0107	0.0163	0.0034	-0.0011
AT. 35	O X	0.0002	-0.0121	0.0072	-0.0098	0.0002	-0.0016
	Y	0.0015	-0.0144	0.0079	-0.0146	0.0027	-0.0017
	Z	0.0024	-0.0165	0.0107	-0.0163	0.0034	-0.0011
AT. 36	O X	-0.0002	0.0121	-0.0072	-0.0098	0.0002	-0.0016
	Y	-0.0015	0.0144	-0.0079	-0.0146	0.0027	-0.0017

	Z	0.0024	-0.0165	0.0107	0.0163	-0.0034	0.0011
AT. 37	O X	0.0002	0.0121	-0.0072	0.0098	0.0002	0.0016
	Y	-0.0015	-0.0144	0.0079	-0.0146	-0.0027	-0.0017
	Z	-0.0024	-0.0165	0.0107	-0.0163	-0.0034	-0.0011
AT. 38	O X	-0.0002	-0.0121	0.0072	0.0098	0.0002	0.0016
	Y	0.0015	0.0144	-0.0079	-0.0146	-0.0027	-0.0017
	Z	-0.0024	-0.0165	0.0107	0.0163	0.0034	0.0011
AT. 39	O X	-0.0113	0.0012	0.0110	-0.0043	0.0093	-0.0099
	Y	-0.0017	0.0007	0.0045	0.0000	0.0054	-0.0058
	Z	-0.0145	0.0013	0.0164	-0.0037	0.0134	-0.0158
AT. 40	O X	0.0113	-0.0012	-0.0110	-0.0043	0.0093	-0.0099
	Y	0.0017	-0.0007	-0.0045	0.0000	0.0054	-0.0058
	Z	-0.0145	0.0013	0.0164	0.0037	-0.0134	0.0158
AT. 41	O X	-0.0113	-0.0012	-0.0110	0.0043	0.0093	0.0099
	Y	0.0017	0.0007	0.0045	0.0000	-0.0054	-0.0058
	Z	0.0145	0.0013	0.0164	-0.0037	-0.0134	-0.0158
AT. 42	O X	0.0113	0.0012	0.0110	0.0043	0.0093	0.0099
	Y	-0.0017	-0.0007	-0.0045	0.0000	-0.0054	-0.0058
	Z	0.0145	0.0013	0.0164	0.0037	0.0134	0.0158
AT. 43	O X	0.0113	0.0012	-0.0110	-0.0043	0.0093	0.0099
	Y	0.0017	0.0007	-0.0045	0.0000	0.0054	0.0058
	Z	0.0145	0.0013	-0.0164	-0.0037	0.0134	0.0158
AT. 44	O X	-0.0113	-0.0012	0.0110	-0.0043	0.0093	0.0099
	Y	-0.0017	-0.0007	0.0045	0.0000	0.0054	0.0058
	Z	0.0145	0.0013	-0.0164	0.0037	-0.0134	-0.0158
AT. 45	O X	0.0113	-0.0012	0.0110	0.0043	0.0093	-0.0099
	Y	-0.0017	0.0007	-0.0045	0.0000	-0.0054	0.0058
	Z	-0.0145	0.0013	-0.0164	-0.0037	-0.0134	0.0158
AT. 46	O X	-0.0113	0.0012	-0.0110	0.0043	0.0093	-0.0099
	Y	0.0017	-0.0007	0.0045	0.0000	-0.0054	0.0058
	Z	-0.0145	0.0013	-0.0164	0.0037	0.0134	-0.0158
AT. 47	O X	-0.0034	0.0000	0.0002	-0.0057	0.0018	0.0000
	Y	0.0002	0.0000	-0.0012	0.0001	-0.0004	0.0000
	Z	0.0000	0.0010	0.0000	0.0000	0.0000	-0.0002
AT. 48	O X	0.0034	0.0000	-0.0002	-0.0057	0.0018	0.0000
	Y	-0.0002	0.0000	0.0012	0.0001	-0.0004	0.0000
	Z	0.0000	0.0010	0.0000	0.0000	0.0000	0.0002
AT. 49	O X	-0.0034	0.0000	-0.0002	0.0057	0.0018	0.0000
	Y	-0.0002	0.0000	-0.0012	0.0001	0.0004	0.0000
	Z	0.0000	0.0010	0.0000	0.0000	0.0000	-0.0002
AT. 50	O X	0.0034	0.0000	0.0002	0.0057	0.0018	0.0000
	Y	0.0002	0.0000	0.0012	0.0001	0.0004	0.0000
	Z	0.0000	0.0010	0.0000	0.0000	0.0000	0.0002
AT. 51	O X	0.0005	0.0000	0.0045	0.0075	0.0040	0.0000
	Y	0.0002	0.0000	-0.0025	-0.0053	-0.0028	0.0000
	Z	0.0000	0.0016	0.0000	0.0000	0.0000	-0.0008
AT. 52	O X	-0.0005	0.0000	-0.0045	0.0075	0.0040	0.0000
	Y	-0.0002	0.0000	0.0025	-0.0053	-0.0028	0.0000
	Z	0.0000	0.0016	0.0000	0.0000	0.0000	0.0008
AT. 53	O X	0.0005	0.0000	-0.0045	-0.0075	0.0040	0.0000
	Y	-0.0002	0.0000	-0.0025	-0.0053	0.0028	0.0000
	Z	0.0000	0.0016	0.0000	0.0000	0.0000	-0.0008
AT. 54	O X	-0.0005	0.0000	0.0045	-0.0075	0.0040	0.0000
	Y	0.0002	0.0000	0.0025	-0.0053	0.0028	0.0000

	Z	0.0000	0.0016	0.0000	0.0000	0.0000	0.0008
AT. 55 O	X	-0.0015	0.0000	-0.0006	-0.0015	-0.0001	0.0000
	Y	-0.0065	0.0000	-0.0009	-0.0045	0.0002	0.0000
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	-0.0010
AT. 56 O	X	0.0015	0.0000	0.0006	-0.0015	-0.0001	0.0000
	Y	0.0065	0.0000	0.0009	-0.0045	0.0002	0.0000
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	0.0010
AT. 57 O	X	-0.0015	0.0000	0.0006	0.0015	-0.0001	0.0000
	Y	0.0065	0.0000	-0.0009	-0.0045	-0.0002	0.0000
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	-0.0010
AT. 58 O	X	0.0015	0.0000	-0.0006	0.0015	-0.0001	0.0000
	Y	-0.0065	0.0000	0.0009	-0.0045	-0.0002	0.0000
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	0.0010

FREQ(CM\*\*-1) 979.11 984.43 987.85 987.87 988.63 1014.81

AT. 1 MG	X	0.0000	0.0019	0.0016	0.0009	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0014	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000
AT. 2 MG	X	0.0000	-0.0019	-0.0016	0.0009	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0014	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000
AT. 3 MG	X	0.0000	0.0019	-0.0016	-0.0009	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0014	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
AT. 4 MG	X	0.0000	-0.0019	0.0016	-0.0009	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0014	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
AT. 5 AL	X	0.0053	0.0000	0.0000	0.0020	0.0000	0.0000
	Y	-0.0073	0.0000	0.0000	-0.0023	0.0000	0.0000
	Z	0.0000	0.0004	0.0015	0.0000	-0.0029	-0.0005
AT. 6 AL	X	0.0053	0.0000	0.0000	0.0020	0.0000	0.0000
	Y	0.0073	0.0000	0.0000	0.0023	0.0000	0.0000
	Z	0.0000	-0.0004	-0.0015	0.0000	-0.0029	0.0005
AT. 7 AL	X	0.0053	0.0000	0.0000	-0.0020	0.0000	0.0000
	Y	-0.0073	0.0000	0.0000	0.0023	0.0000	0.0000
	Z	0.0000	0.0004	-0.0015	0.0000	0.0029	0.0005
AT. 8 AL	X	0.0053	0.0000	0.0000	-0.0020	0.0000	0.0000
	Y	0.0073	0.0000	0.0000	-0.0023	0.0000	0.0000
	Z	0.0000	-0.0004	0.0015	0.0000	0.0029	-0.0005
AT. 9 AL	X	-0.0013	0.0000	-0.0003	0.0000	0.0035	0.0014
	Y	-0.0018	0.0000	0.0073	0.0000	-0.0001	0.0048
	Z	0.0000	0.0104	0.0000	0.0024	0.0000	0.0000
AT. 10 AL	X	-0.0013	0.0000	0.0003	0.0000	-0.0035	-0.0014
	Y	-0.0018	0.0000	-0.0073	0.0000	0.0001	-0.0048
	Z	0.0000	0.0104	0.0000	-0.0024	0.0000	0.0000
AT. 11 AL	X	-0.0013	0.0000	-0.0003	0.0000	-0.0035	0.0014
	Y	0.0018	0.0000	-0.0073	0.0000	-0.0001	-0.0048
	Z	0.0000	-0.0104	0.0000	-0.0024	0.0000	0.0000
AT. 12 AL	X	-0.0013	0.0000	0.0003	0.0000	0.0035	-0.0014
	Y	0.0018	0.0000	0.0073	0.0000	0.0001	0.0048
	Z	0.0000	-0.0104	0.0000	0.0024	0.0000	0.0000
AT. 13 SI	X	-0.0034	0.0000	0.0000	-0.0086	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	Z	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000
AT. 14	SI X	-0.0034	0.0000	0.0000	0.0086	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	-0.0045	0.0000
AT. 15	SI X	-0.0066	0.0000	-0.0011	0.0000	-0.0104	0.0086
	Y	-0.0038	0.0000	-0.0016	0.0000	-0.0039	0.0043
	Z	0.0000	-0.0029	0.0000	-0.0118	0.0000	0.0000
AT. 16	SI X	-0.0066	0.0000	0.0011	0.0000	0.0104	-0.0086
	Y	-0.0038	0.0000	0.0016	0.0000	0.0039	-0.0043
	Z	0.0000	-0.0029	0.0000	0.0118	0.0000	0.0000
AT. 17	SI X	-0.0066	0.0000	-0.0011	0.0000	0.0104	0.0086
	Y	0.0038	0.0000	0.0016	0.0000	-0.0039	-0.0043
	Z	0.0000	0.0029	0.0000	0.0118	0.0000	0.0000
AT. 18	SI X	-0.0066	0.0000	0.0011	0.0000	-0.0104	-0.0086
	Y	0.0038	0.0000	-0.0016	0.0000	0.0039	0.0043
	Z	0.0000	0.0029	0.0000	-0.0118	0.0000	0.0000
AT. 19	SI X	0.0052	0.0000	-0.0008	0.0000	0.0032	0.0047
	Y	-0.0053	0.0000	0.0032	0.0000	-0.0021	-0.0091
	Z	0.0000	-0.0009	0.0000	0.0101	0.0000	0.0000
AT. 20	SI X	0.0052	0.0000	0.0008	0.0000	-0.0032	-0.0047
	Y	-0.0053	0.0000	-0.0032	0.0000	0.0021	0.0091
	Z	0.0000	-0.0009	0.0000	-0.0101	0.0000	0.0000
AT. 21	SI X	0.0052	0.0000	-0.0008	0.0000	-0.0032	0.0047
	Y	0.0053	0.0000	-0.0032	0.0000	-0.0021	0.0091
	Z	0.0000	0.0009	0.0000	-0.0101	0.0000	0.0000
AT. 22	SI X	0.0052	0.0000	0.0008	0.0000	0.0032	-0.0047
	Y	0.0053	0.0000	0.0032	0.0000	0.0021	-0.0091
	Z	0.0000	0.0009	0.0000	0.0101	0.0000	0.0000
AT. 23	O X	0.0082	0.0018	0.0021	0.0092	-0.0103	-0.0092
	Y	-0.0058	-0.0013	-0.0020	-0.0038	0.0098	0.0058
	Z	-0.0150	-0.0033	-0.0032	-0.0147	0.0191	0.0142
AT. 24	O X	0.0082	-0.0018	-0.0021	0.0092	0.0103	0.0092
	Y	-0.0058	0.0013	0.0020	-0.0038	-0.0098	-0.0058
	Z	0.0150	-0.0033	-0.0032	0.0147	0.0191	0.0142
AT. 25	O X	0.0082	0.0018	0.0021	0.0092	0.0103	-0.0092
	Y	0.0058	0.0013	0.0020	0.0038	0.0098	-0.0058
	Z	0.0150	0.0033	0.0032	0.0147	0.0191	-0.0142
AT. 26	O X	0.0082	-0.0018	-0.0021	0.0092	-0.0103	0.0092
	Y	0.0058	-0.0013	-0.0020	0.0038	-0.0098	0.0058
	Z	-0.0150	0.0033	0.0032	-0.0147	0.0191	-0.0142
AT. 27	O X	0.0082	0.0018	-0.0021	-0.0092	0.0103	0.0092
	Y	-0.0058	-0.0013	0.0020	0.0038	-0.0098	-0.0058
	Z	-0.0150	-0.0033	0.0032	0.0147	-0.0191	-0.0142
AT. 28	O X	0.0082	-0.0018	0.0021	-0.0092	-0.0103	-0.0092
	Y	-0.0058	0.0013	-0.0020	0.0038	0.0098	0.0058
	Z	0.0150	-0.0033	0.0032	-0.0147	-0.0191	-0.0142
AT. 29	O X	0.0082	0.0018	-0.0021	-0.0092	-0.0103	0.0092
	Y	0.0058	0.0013	-0.0020	-0.0038	-0.0098	0.0058
	Z	0.0150	0.0033	-0.0032	-0.0147	-0.0191	0.0142
AT. 30	O X	0.0082	-0.0018	0.0021	-0.0092	0.0103	-0.0092
	Y	0.0058	-0.0013	0.0020	-0.0038	0.0098	-0.0058
	Z	-0.0150	0.0033	-0.0032	0.0147	-0.0191	0.0142
AT. 31	O X	0.0013	0.0094	0.0103	0.0027	-0.0021	0.0014
	Y	0.0007	0.0173	0.0171	0.0062	-0.0019	0.0051



	Z	0.0014	0.0210	0.0204	0.0074	-0.0026	0.0061
AT. 32	O X	0.0013	-0.0094	-0.0103	0.0027	0.0021	-0.0014
	Y	0.0007	-0.0173	-0.0171	0.0062	0.0019	-0.0051
	Z	-0.0014	0.0210	0.0204	-0.0074	-0.0026	0.0061
AT. 33	O X	0.0013	0.0094	0.0103	0.0027	0.0021	0.0014
	Y	-0.0007	-0.0173	-0.0171	-0.0062	-0.0019	-0.0051
	Z	-0.0014	-0.0210	-0.0204	-0.0074	-0.0026	-0.0061
AT. 34	O X	0.0013	-0.0094	-0.0103	0.0027	-0.0021	-0.0014
	Y	-0.0007	0.0173	0.0171	-0.0062	0.0019	0.0051
	Z	0.0014	-0.0210	-0.0204	0.0074	-0.0026	-0.0061
AT. 35	O X	0.0013	0.0094	-0.0103	-0.0027	0.0021	-0.0014
	Y	0.0007	0.0173	-0.0171	-0.0062	0.0019	-0.0051
	Z	0.0014	0.0210	-0.0204	-0.0074	0.0026	-0.0061
AT. 36	O X	0.0013	-0.0094	0.0103	-0.0027	-0.0021	0.0014
	Y	0.0007	-0.0173	0.0171	-0.0062	-0.0019	0.0051
	Z	-0.0014	0.0210	-0.0204	0.0074	0.0026	-0.0061
AT. 37	O X	0.0013	0.0094	-0.0103	-0.0027	-0.0021	-0.0014
	Y	-0.0007	-0.0173	0.0171	0.0062	0.0019	0.0051
	Z	-0.0014	-0.0210	0.0204	0.0074	0.0026	0.0061
AT. 38	O X	0.0013	-0.0094	0.0103	-0.0027	0.0021	0.0014
	Y	-0.0007	0.0173	-0.0171	0.0062	-0.0019	-0.0051
	Z	0.0014	-0.0210	0.0204	-0.0074	0.0026	0.0061
AT. 39	O X	-0.0118	-0.0024	-0.0043	-0.0083	-0.0084	0.0094
	Y	-0.0034	0.0000	-0.0007	-0.0056	-0.0021	0.0054
	Z	-0.0166	-0.0022	-0.0056	-0.0135	-0.0104	0.0145
AT. 40	O X	-0.0118	0.0024	0.0043	-0.0083	0.0084	-0.0094
	Y	-0.0034	0.0000	0.0007	-0.0056	0.0021	-0.0054
	Z	0.0166	-0.0022	-0.0056	0.0135	-0.0104	0.0145
AT. 41	O X	-0.0118	-0.0024	-0.0043	-0.0083	0.0084	0.0094
	Y	0.0034	0.0000	0.0007	0.0056	-0.0021	-0.0054
	Z	0.0166	0.0022	0.0056	0.0135	-0.0104	-0.0145
AT. 42	O X	-0.0118	0.0024	0.0043	-0.0083	-0.0084	-0.0094
	Y	0.0034	0.0000	-0.0007	0.0056	0.0021	0.0054
	Z	-0.0166	0.0022	0.0056	-0.0135	-0.0104	-0.0145
AT. 43	O X	-0.0118	-0.0024	0.0043	0.0083	0.0084	-0.0094
	Y	-0.0034	0.0000	0.0007	0.0056	0.0021	-0.0054
	Z	-0.0166	-0.0022	0.0056	0.0135	0.0104	-0.0145
AT. 44	O X	-0.0118	0.0024	-0.0043	0.0083	-0.0084	0.0094
	Y	-0.0034	0.0000	-0.0007	0.0056	-0.0021	0.0054
	Z	0.0166	-0.0022	0.0056	-0.0135	0.0104	-0.0145
AT. 45	O X	-0.0118	-0.0024	0.0043	0.0083	-0.0084	-0.0094
	Y	0.0034	0.0000	-0.0007	-0.0056	0.0021	0.0054
	Z	0.0166	0.0022	-0.0056	-0.0135	0.0104	0.0145
AT. 46	O X	-0.0118	0.0024	-0.0043	0.0083	0.0084	0.0094
	Y	0.0034	0.0000	0.0007	-0.0056	-0.0021	-0.0054
	Z	-0.0166	0.0022	-0.0056	0.0135	0.0104	0.0145
AT. 47	O X	0.0043	0.0000	-0.0017	0.0000	0.0086	0.0042
	Y	0.0002	0.0000	0.0008	0.0000	0.0011	0.0022
	Z	0.0000	-0.0010	0.0000	0.0001	0.0000	0.0000
AT. 48	O X	0.0043	0.0000	0.0017	0.0000	-0.0086	-0.0042
	Y	0.0002	0.0000	-0.0008	0.0000	-0.0011	-0.0022
	Z	0.0000	-0.0010	0.0000	-0.0001	0.0000	0.0000
AT. 49	O X	0.0043	0.0000	-0.0017	0.0000	-0.0086	0.0042
	Y	-0.0002	0.0000	-0.0008	0.0000	0.0011	-0.0022

	Z	0.0000	0.0010	0.0000	-0.0001	0.0000	0.0000
AT. 50	O X	0.0043	0.0000	0.0017	0.0000	0.0086	-0.0042
	Y	-0.0002	0.0000	0.0008	0.0000	-0.0011	0.0022
	Z	0.0000	0.0010	0.0000	0.0001	0.0000	0.0000
AT. 51	O X	-0.0025	0.0000	0.0001	0.0000	-0.0001	0.0014
	Y	0.0018	0.0000	0.0013	0.0000	0.0015	-0.0036
	Z	0.0000	0.0003	0.0000	0.0001	0.0000	0.0000
AT. 52	O X	-0.0025	0.0000	-0.0001	0.0000	0.0001	-0.0014
	Y	0.0018	0.0000	-0.0013	0.0000	-0.0015	0.0036
	Z	0.0000	0.0003	0.0000	-0.0001	0.0000	0.0000
AT. 53	O X	-0.0025	0.0000	0.0001	0.0000	0.0001	0.0014
	Y	-0.0018	0.0000	-0.0013	0.0000	0.0015	0.0036
	Z	0.0000	-0.0003	0.0000	-0.0001	0.0000	0.0000
AT. 54	O X	-0.0025	0.0000	-0.0001	0.0000	-0.0001	-0.0014
	Y	-0.0018	0.0000	0.0013	0.0000	-0.0015	-0.0036
	Z	0.0000	-0.0003	0.0000	0.0001	0.0000	0.0000
AT. 55	O X	0.0013	0.0000	-0.0009	0.0000	-0.0013	-0.0002
	Y	0.0055	0.0000	-0.0029	0.0000	-0.0001	0.0028
	Z	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
AT. 56	O X	0.0013	0.0000	0.0009	0.0000	0.0013	0.0002
	Y	0.0055	0.0000	0.0029	0.0000	0.0001	-0.0028
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0000
AT. 57	O X	0.0013	0.0000	-0.0009	0.0000	0.0013	-0.0002
	Y	-0.0055	0.0000	0.0029	0.0000	-0.0001	-0.0028
	Z	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0000
AT. 58	O X	0.0013	0.0000	0.0009	0.0000	-0.0013	0.0002
	Y	-0.0055	0.0000	-0.0029	0.0000	0.0001	0.0028
	Z	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000

FREQ(CM\*\*-1) 1015.20 1015.21 1025.02 1035.94 1047.95 1071.32

AT. 1	MG X	-0.0012	0.0000	0.0000	0.0000	-0.0019	-0.0008
	Y	0.0000	0.0004	-0.0022	-0.0004	0.0000	0.0000
	Z	0.0000	0.0001	0.0001	0.0034	0.0000	0.0000
AT. 2	MG X	-0.0012	0.0000	0.0000	0.0000	-0.0019	0.0008
	Y	0.0000	0.0004	0.0022	0.0004	0.0000	0.0000
	Z	0.0000	-0.0001	0.0001	0.0034	0.0000	0.0000
AT. 3	MG X	0.0012	0.0000	0.0000	0.0000	-0.0019	-0.0008
	Y	0.0000	0.0004	-0.0022	0.0004	0.0000	0.0000
	Z	0.0000	0.0001	0.0001	-0.0034	0.0000	0.0000
AT. 4	MG X	0.0012	0.0000	0.0000	0.0000	-0.0019	0.0008
	Y	0.0000	0.0004	0.0022	-0.0004	0.0000	0.0000
	Z	0.0000	-0.0001	0.0001	-0.0034	0.0000	0.0000
AT. 5	AL X	-0.0001	0.0042	0.0000	0.0000	-0.0011	0.0000
	Y	-0.0001	-0.0065	0.0000	0.0000	-0.0009	0.0000
	Z	0.0000	0.0000	-0.0001	0.0079	0.0000	-0.0003
AT. 6	AL X	-0.0001	-0.0042	0.0000	0.0000	-0.0011	0.0000
	Y	0.0001	-0.0065	0.0000	0.0000	0.0009	0.0000
	Z	0.0000	0.0000	-0.0001	0.0079	0.0000	0.0003
AT. 7	AL X	0.0001	0.0042	0.0000	0.0000	-0.0011	0.0000
	Y	0.0001	-0.0065	0.0000	0.0000	-0.0009	0.0000
	Z	0.0000	0.0000	-0.0001	-0.0079	0.0000	-0.0003
AT. 8	AL X	0.0001	-0.0042	0.0000	0.0000	-0.0011	0.0000
	Y	-0.0001	-0.0065	0.0000	0.0000	0.0009	0.0000

	Z	0.0000	0.0000	-0.0001	-0.0079	0.0000	0.0003
AT. 9	AL X	0.0000	0.0020	0.0000	0.0007	0.0015	0.0000
	Y	0.0000	0.0000	0.0000	0.0035	-0.0041	0.0000
	Z	-0.0023	0.0000	-0.0004	0.0000	0.0000	0.0032
AT. 10	AL X	0.0000	0.0020	0.0000	-0.0007	0.0015	0.0000
	Y	0.0000	0.0000	0.0000	-0.0035	-0.0041	0.0000
	Z	0.0023	0.0000	-0.0004	0.0000	0.0000	0.0032
AT. 11	AL X	0.0000	-0.0020	0.0000	-0.0007	0.0015	0.0000
	Y	0.0000	0.0000	0.0000	0.0035	0.0041	0.0000
	Z	0.0023	0.0000	-0.0004	0.0000	0.0000	-0.0032
AT. 12	AL X	0.0000	-0.0020	0.0000	0.0007	0.0015	0.0000
	Y	0.0000	0.0000	0.0000	-0.0035	0.0041	0.0000
	Z	-0.0023	0.0000	-0.0004	0.0000	0.0000	-0.0032
AT. 13	SI X	0.0259	0.0000	0.0000	0.0000	0.0250	0.0000
	Y	0.0000	-0.0008	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	0.0198	0.0000	0.0000
AT. 14	SI X	-0.0259	0.0000	0.0000	0.0000	0.0250	0.0000
	Y	0.0000	-0.0008	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	-0.0198	0.0000	0.0000
AT. 15	SI X	0.0000	-0.0092	0.0000	0.0025	0.0003	0.0000
	Y	0.0000	-0.0025	0.0000	0.0035	-0.0029	0.0000
	Z	-0.0045	0.0000	-0.0112	0.0000	0.0000	0.0129
AT. 16	SI X	0.0000	-0.0092	0.0000	-0.0025	0.0003	0.0000
	Y	0.0000	-0.0025	0.0000	-0.0035	-0.0029	0.0000
	Z	0.0045	0.0000	-0.0112	0.0000	0.0000	0.0129
AT. 17	SI X	0.0000	0.0092	0.0000	-0.0025	0.0003	0.0000
	Y	0.0000	-0.0025	0.0000	0.0035	0.0029	0.0000
	Z	0.0045	0.0000	-0.0112	0.0000	0.0000	-0.0129
AT. 18	SI X	0.0000	0.0092	0.0000	0.0025	0.0003	0.0000
	Y	0.0000	-0.0025	0.0000	-0.0035	0.0029	0.0000
	Z	-0.0045	0.0000	-0.0112	0.0000	0.0000	-0.0129
AT. 19	SI X	0.0000	-0.0068	0.0000	0.0020	-0.0039	0.0000
	Y	0.0000	0.0069	0.0000	-0.0044	0.0001	0.0000
	Z	0.0049	0.0000	0.0127	0.0000	0.0000	0.0121
AT. 20	SI X	0.0000	-0.0068	0.0000	-0.0020	-0.0039	0.0000
	Y	0.0000	0.0069	0.0000	0.0044	0.0001	0.0000
	Z	-0.0049	0.0000	0.0127	0.0000	0.0000	0.0121
AT. 21	SI X	0.0000	0.0068	0.0000	-0.0020	-0.0039	0.0000
	Y	0.0000	0.0069	0.0000	-0.0044	-0.0001	0.0000
	Z	-0.0049	0.0000	0.0127	0.0000	0.0000	-0.0121
AT. 22	SI X	0.0000	0.0068	0.0000	0.0020	-0.0039	0.0000
	Y	0.0000	0.0069	0.0000	0.0044	-0.0001	0.0000
	Z	0.0049	0.0000	0.0127	0.0000	0.0000	-0.0121
AT. 23	O X	0.0039	-0.0085	-0.0076	0.0039	0.0029	-0.0077
	Y	-0.0009	0.0073	0.0074	-0.0040	-0.0009	0.0048
	Z	-0.0053	0.0148	0.0141	-0.0092	-0.0029	0.0143
AT. 24	O X	0.0039	-0.0085	0.0076	-0.0039	0.0029	0.0077
	Y	-0.0009	0.0073	-0.0074	0.0040	-0.0009	-0.0048
	Z	0.0053	-0.0148	0.0141	-0.0092	0.0029	0.0143
AT. 25	O X	0.0039	0.0085	0.0076	-0.0039	0.0029	-0.0077
	Y	0.0009	0.0073	0.0074	-0.0040	0.0009	-0.0048
	Z	0.0053	0.0148	0.0141	-0.0092	0.0029	-0.0143
AT. 26	O X	0.0039	0.0085	-0.0076	0.0039	0.0029	0.0077
	Y	0.0009	0.0073	-0.0074	0.0040	0.0009	0.0048

	Z	-0.0053	-0.0148	0.0141	-0.0092	-0.0029	-0.0143
AT. 27	O X	-0.0039	-0.0085	-0.0076	-0.0039	0.0029	-0.0077
	Y	0.0009	0.0073	0.0074	0.0040	-0.0009	0.0048
	Z	0.0053	0.0148	0.0141	0.0092	-0.0029	0.0143
AT. 28	O X	-0.0039	-0.0085	0.0076	0.0039	0.0029	0.0077
	Y	0.0009	0.0073	-0.0074	-0.0040	-0.0009	-0.0048
	Z	-0.0053	-0.0148	0.0141	0.0092	0.0029	0.0143
AT. 29	O X	-0.0039	0.0085	0.0076	0.0039	0.0029	-0.0077
	Y	-0.0009	0.0073	0.0074	0.0040	0.0009	-0.0048
	Z	-0.0053	0.0148	0.0141	0.0092	0.0029	-0.0143
AT. 30	O X	-0.0039	0.0085	-0.0076	-0.0039	0.0029	0.0077
	Y	-0.0009	0.0073	-0.0074	-0.0040	0.0009	0.0048
	Z	0.0053	-0.0148	0.0141	0.0092	-0.0029	-0.0143
AT. 31	O X	-0.0107	0.0017	-0.0017	-0.0071	-0.0104	0.0002
	Y	-0.0132	0.0006	-0.0016	-0.0091	-0.0121	0.0026
	Z	-0.0145	0.0010	-0.0011	-0.0137	-0.0153	0.0040
AT. 32	O X	-0.0107	0.0017	0.0017	0.0071	-0.0104	-0.0002
	Y	-0.0132	0.0006	0.0016	0.0091	-0.0121	-0.0026
	Z	0.0145	-0.0010	-0.0011	-0.0137	0.0153	0.0040
AT. 33	O X	-0.0107	-0.0017	0.0017	0.0071	-0.0104	0.0002
	Y	0.0132	0.0006	-0.0016	-0.0091	0.0121	-0.0026
	Z	0.0145	0.0010	-0.0011	-0.0137	0.0153	-0.0040
AT. 34	O X	-0.0107	-0.0017	-0.0017	-0.0071	-0.0104	-0.0002
	Y	0.0132	0.0006	0.0016	0.0091	0.0121	0.0026
	Z	-0.0145	-0.0010	-0.0011	-0.0137	-0.0153	-0.0040
AT. 35	O X	0.0107	0.0017	-0.0017	0.0071	-0.0104	0.0002
	Y	0.0132	0.0006	-0.0016	0.0091	-0.0121	0.0026
	Z	0.0145	0.0010	-0.0011	0.0137	-0.0153	0.0040
AT. 36	O X	0.0107	0.0017	0.0017	-0.0071	-0.0104	-0.0002
	Y	0.0132	0.0006	0.0016	-0.0091	-0.0121	-0.0026
	Z	-0.0145	-0.0010	-0.0011	0.0137	0.0153	0.0040
AT. 37	O X	0.0107	-0.0017	0.0017	-0.0071	-0.0104	0.0002
	Y	-0.0132	0.0006	-0.0016	0.0091	0.0121	-0.0026
	Z	-0.0145	0.0010	-0.0011	0.0137	0.0153	-0.0040
AT. 38	O X	0.0107	-0.0017	-0.0017	0.0071	-0.0104	-0.0002
	Y	-0.0132	0.0006	0.0016	-0.0091	0.0121	0.0026
	Z	0.0145	-0.0010	-0.0011	0.0137	-0.0153	-0.0040
AT. 39	O X	-0.0025	-0.0101	-0.0099	-0.0064	0.0009	0.0085
	Y	-0.0028	-0.0051	-0.0039	-0.0022	0.0001	0.0042
	Z	-0.0056	-0.0150	-0.0152	-0.0108	0.0005	0.0139
AT. 40	O X	-0.0025	-0.0101	0.0099	0.0064	0.0009	-0.0085
	Y	-0.0028	-0.0051	0.0039	0.0022	0.0001	-0.0042
	Z	0.0056	0.0150	-0.0152	-0.0108	-0.0005	0.0139
AT. 41	O X	-0.0025	0.0101	0.0099	0.0064	0.0009	0.0085
	Y	0.0028	-0.0051	-0.0039	-0.0022	-0.0001	-0.0042
	Z	0.0056	-0.0150	-0.0152	-0.0108	-0.0005	-0.0139
AT. 42	O X	-0.0025	0.0101	-0.0099	-0.0064	0.0009	-0.0085
	Y	0.0028	-0.0051	0.0039	0.0022	-0.0001	0.0042
	Z	-0.0056	0.0150	-0.0152	-0.0108	0.0005	-0.0139
AT. 43	O X	0.0025	-0.0101	-0.0099	0.0064	0.0009	0.0085
	Y	0.0028	-0.0051	-0.0039	0.0022	0.0001	0.0042
	Z	0.0056	-0.0150	-0.0152	0.0108	0.0005	0.0139
AT. 44	O X	0.0025	-0.0101	0.0099	-0.0064	0.0009	-0.0085
	Y	0.0028	-0.0051	0.0039	-0.0022	0.0001	-0.0042

	Z	-0.0056	0.0150	-0.0152	0.0108	-0.0005	0.0139
AT. 45	O X	0.0025	0.0101	0.0099	-0.0064	0.0009	0.0085
	Y	-0.0028	-0.0051	-0.0039	0.0022	-0.0001	-0.0042
	Z	-0.0056	-0.0150	-0.0152	0.0108	-0.0005	-0.0139
AT. 46	O X	0.0025	0.0101	-0.0099	0.0064	0.0009	-0.0085
	Y	-0.0028	-0.0051	0.0039	-0.0022	-0.0001	0.0042
	Z	0.0056	0.0150	-0.0152	0.0108	0.0005	-0.0139
AT. 47	O X	0.0000	0.0012	0.0000	0.0043	0.0075	0.0000
	Y	0.0000	-0.0002	0.0000	0.0004	0.0007	0.0000
	Z	0.0004	0.0000	-0.0001	0.0000	0.0000	-0.0012
AT. 48	O X	0.0000	0.0012	0.0000	-0.0043	0.0075	0.0000
	Y	0.0000	-0.0002	0.0000	-0.0004	0.0007	0.0000
	Z	-0.0004	0.0000	-0.0001	0.0000	0.0000	-0.0012
AT. 49	O X	0.0000	-0.0012	0.0000	-0.0043	0.0075	0.0000
	Y	0.0000	-0.0002	0.0000	0.0004	-0.0007	0.0000
	Z	-0.0004	0.0000	-0.0001	0.0000	0.0000	0.0012
AT. 50	O X	0.0000	-0.0012	0.0000	0.0043	0.0075	0.0000
	Y	0.0000	-0.0002	0.0000	-0.0004	-0.0007	0.0000
	Z	0.0004	0.0000	-0.0001	0.0000	0.0000	0.0012
AT. 51	O X	0.0000	0.0026	0.0000	0.0046	-0.0079	0.0000
	Y	0.0000	-0.0023	0.0000	-0.0037	0.0061	0.0000
	Z	-0.0012	0.0000	0.0012	0.0000	0.0000	-0.0020
AT. 52	O X	0.0000	0.0026	0.0000	-0.0046	-0.0079	0.0000
	Y	0.0000	-0.0023	0.0000	0.0037	0.0061	0.0000
	Z	0.0012	0.0000	0.0012	0.0000	0.0000	-0.0020
AT. 53	O X	0.0000	-0.0026	0.0000	-0.0046	-0.0079	0.0000
	Y	0.0000	-0.0023	0.0000	-0.0037	-0.0061	0.0000
	Z	0.0012	0.0000	0.0012	0.0000	0.0000	0.0020
AT. 54	O X	0.0000	-0.0026	0.0000	0.0046	-0.0079	0.0000
	Y	0.0000	-0.0023	0.0000	0.0037	-0.0061	0.0000
	Z	-0.0012	0.0000	0.0012	0.0000	0.0000	0.0020
AT. 55	O X	0.0000	-0.0004	0.0000	-0.0002	0.0004	0.0000
	Y	0.0000	-0.0002	0.0000	-0.0001	0.0004	0.0000
	Z	0.0001	0.0000	-0.0009	0.0000	0.0000	-0.0019
AT. 56	O X	0.0000	-0.0004	0.0000	0.0002	0.0004	0.0000
	Y	0.0000	-0.0002	0.0000	0.0001	0.0004	0.0000
	Z	-0.0001	0.0000	-0.0009	0.0000	0.0000	-0.0019
AT. 57	O X	0.0000	0.0004	0.0000	0.0002	0.0004	0.0000
	Y	0.0000	-0.0002	0.0000	-0.0001	-0.0004	0.0000
	Z	-0.0001	0.0000	-0.0009	0.0000	0.0000	0.0019
AT. 58	O X	0.0000	0.0004	0.0000	-0.0002	0.0004	0.0000
	Y	0.0000	-0.0002	0.0000	0.0001	-0.0004	0.0000
	Z	0.0001	0.0000	-0.0009	0.0000	0.0000	0.0019

FREQ(CM\*\*-1) 1128.96 1130.74 1149.64 1156.64 1170.01 1175.56

AT. 1 MG	X	0.0005	0.0000	0.0000	0.0003	0.0000	0.0008
	Y	0.0000	0.0001	0.0007	0.0000	0.0008	0.0000
	Z	0.0000	0.0001	-0.0009	0.0000	0.0009	0.0000
AT. 2 MG	X	-0.0005	0.0000	0.0000	0.0003	0.0000	0.0008
	Y	0.0000	-0.0001	0.0007	0.0000	0.0008	0.0000
	Z	0.0000	0.0001	0.0009	0.0000	-0.0009	0.0000
AT. 3 MG	X	-0.0005	0.0000	0.0000	0.0003	0.0000	0.0008
	Y	0.0000	-0.0001	0.0007	0.0000	0.0008	0.0000

	Z	0.0000	-0.0001	-0.0009	0.0000	0.0009	0.0000
AT. 4	MG X	0.0005	0.0000	0.0000	0.0003	0.0000	0.0008
	Y	0.0000	0.0001	0.0007	0.0000	0.0008	0.0000
	Z	0.0000	-0.0001	0.0009	0.0000	-0.0009	0.0000
AT. 5	AL X	0.0000	0.0000	0.0006	0.0012	0.0024	-0.0010
	Y	0.0000	0.0000	-0.0021	0.0014	0.0001	0.0036
	Z	0.0003	0.0003	0.0000	0.0000	0.0000	0.0000
AT. 6	AL X	0.0000	0.0000	-0.0006	0.0012	-0.0024	-0.0010
	Y	0.0000	0.0000	-0.0021	-0.0014	0.0001	-0.0036
	Z	-0.0003	0.0003	0.0000	0.0000	0.0000	0.0000
AT. 7	AL X	0.0000	0.0000	0.0006	0.0012	0.0024	-0.0010
	Y	0.0000	0.0000	-0.0021	0.0014	0.0001	0.0036
	Z	-0.0003	-0.0003	0.0000	0.0000	0.0000	0.0000
AT. 8	AL X	0.0000	0.0000	-0.0006	0.0012	-0.0024	-0.0010
	Y	0.0000	0.0000	-0.0021	-0.0014	0.0001	-0.0036
	Z	0.0003	-0.0003	0.0000	0.0000	0.0000	0.0000
AT. 9	AL X	-0.0060	0.0058	0.0053	-0.0063	0.0044	-0.0011
	Y	0.0022	-0.0021	-0.0030	0.0018	0.0017	0.0018
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0060	-0.0058	0.0053	-0.0063	0.0044	-0.0011
	Y	-0.0022	0.0021	-0.0030	0.0018	0.0017	0.0018
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	-0.0060	-0.0058	-0.0053	-0.0063	-0.0044	-0.0011
	Y	-0.0022	-0.0021	-0.0030	-0.0018	0.0017	-0.0018
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0060	0.0058	-0.0053	-0.0063	-0.0044	-0.0011
	Y	0.0022	0.0021	-0.0030	-0.0018	0.0017	-0.0018
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0037	0.0000	0.0004
	Y	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000
	Z	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0037	0.0000	0.0004
	Y	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000
	Z	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	-0.0075	0.0080	0.0083	-0.0066	-0.0012	-0.0029
	Y	0.0095	-0.0095	-0.0050	0.0106	-0.0083	-0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0075	-0.0080	0.0083	-0.0066	-0.0012	-0.0029
	Y	-0.0095	0.0095	-0.0050	0.0106	-0.0083	-0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	-0.0075	-0.0080	-0.0083	-0.0066	0.0012	-0.0029
	Y	-0.0095	-0.0095	-0.0050	-0.0106	-0.0083	0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0075	0.0080	-0.0083	-0.0066	0.0012	-0.0029
	Y	0.0095	0.0095	-0.0050	-0.0106	-0.0083	0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	0.0078	-0.0074	0.0046	-0.0045	0.0057	-0.0062
	Y	0.0016	-0.0015	0.0054	-0.0015	-0.0043	-0.0085
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	-0.0078	0.0074	0.0046	-0.0045	0.0057	-0.0062
	Y	-0.0016	0.0015	0.0054	-0.0015	-0.0043	-0.0085
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0078	0.0074	-0.0046	-0.0045	-0.0057	-0.0062
	Y	-0.0016	-0.0015	0.0054	0.0015	-0.0043	0.0085

	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	-0.0078	-0.0074	-0.0046	-0.0045	-0.0057	-0.0062
	Y	0.0016	0.0015	0.0054	0.0015	-0.0043	0.0085
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	-0.0001	0.0004	-0.0014	-0.0006	0.0008	-0.0016
	Y	-0.0005	-0.0012	0.0020	0.0011	-0.0010	0.0032
	Z	-0.0002	-0.0012	0.0029	0.0009	-0.0010	0.0028
AT. 24	O X	0.0001	-0.0004	-0.0014	-0.0006	0.0008	-0.0016
	Y	0.0005	0.0012	0.0020	0.0011	-0.0010	0.0032
	Z	-0.0002	-0.0012	-0.0029	-0.0009	0.0010	-0.0028
AT. 25	O X	-0.0001	-0.0004	0.0014	-0.0006	-0.0008	-0.0016
	Y	0.0005	-0.0012	0.0020	-0.0011	-0.0010	-0.0032
	Z	0.0002	-0.0012	0.0029	-0.0009	-0.0010	-0.0028
AT. 26	O X	0.0001	0.0004	0.0014	-0.0006	-0.0008	-0.0016
	Y	-0.0005	0.0012	0.0020	-0.0011	-0.0010	-0.0032
	Z	0.0002	-0.0012	-0.0029	0.0009	0.0010	0.0028
AT. 27	O X	0.0001	-0.0004	-0.0014	-0.0006	0.0008	-0.0016
	Y	0.0005	0.0012	0.0020	0.0011	-0.0010	0.0032
	Z	0.0002	0.0012	0.0029	0.0009	-0.0010	0.0028
AT. 28	O X	-0.0001	0.0004	-0.0014	-0.0006	0.0008	-0.0016
	Y	-0.0005	-0.0012	0.0020	0.0011	-0.0010	0.0032
	Z	0.0002	0.0012	-0.0029	-0.0009	0.0010	-0.0028
AT. 29	O X	0.0001	0.0004	0.0014	-0.0006	-0.0008	-0.0016
	Y	-0.0005	0.0012	0.0020	-0.0011	-0.0010	-0.0032
	Z	-0.0002	0.0012	0.0029	-0.0009	-0.0010	-0.0028
AT. 30	O X	-0.0001	-0.0004	0.0014	-0.0006	-0.0008	-0.0016
	Y	0.0005	-0.0012	0.0020	-0.0011	-0.0010	-0.0032
	Z	-0.0002	0.0012	-0.0029	0.0009	0.0010	0.0028
AT. 31	O X	-0.0008	-0.0015	-0.0015	-0.0020	-0.0002	-0.0008
	Y	-0.0005	-0.0014	-0.0018	-0.0021	-0.0002	0.0010
	Z	-0.0004	-0.0018	-0.0017	-0.0023	0.0002	0.0009
AT. 32	O X	0.0008	0.0015	-0.0015	-0.0020	-0.0002	-0.0008
	Y	0.0005	0.0014	-0.0018	-0.0021	-0.0002	0.0010
	Z	-0.0004	-0.0018	0.0017	0.0023	-0.0002	-0.0009
AT. 33	O X	-0.0008	0.0015	0.0015	-0.0020	0.0002	-0.0008
	Y	0.0005	-0.0014	-0.0018	0.0021	-0.0002	-0.0010
	Z	0.0004	-0.0018	-0.0017	0.0023	0.0002	-0.0009
AT. 34	O X	0.0008	-0.0015	0.0015	-0.0020	0.0002	-0.0008
	Y	-0.0005	0.0014	-0.0018	0.0021	-0.0002	-0.0010
	Z	0.0004	-0.0018	0.0017	-0.0023	-0.0002	0.0009
AT. 35	O X	0.0008	0.0015	-0.0015	-0.0020	-0.0002	-0.0008
	Y	0.0005	0.0014	-0.0018	-0.0021	-0.0002	0.0010
	Z	0.0004	0.0018	-0.0017	-0.0023	0.0002	0.0009
AT. 36	O X	-0.0008	-0.0015	-0.0015	-0.0020	-0.0002	-0.0008
	Y	-0.0005	-0.0014	-0.0018	-0.0021	-0.0002	0.0010
	Z	0.0004	0.0018	0.0017	0.0023	-0.0002	-0.0009
AT. 37	O X	0.0008	-0.0015	0.0015	-0.0020	0.0002	-0.0008
	Y	-0.0005	0.0014	-0.0018	0.0021	-0.0002	-0.0010
	Z	-0.0004	0.0018	-0.0017	0.0023	0.0002	-0.0009
AT. 38	O X	-0.0008	0.0015	0.0015	-0.0020	0.0002	-0.0008
	Y	0.0005	-0.0014	-0.0018	0.0021	-0.0002	-0.0010
	Z	-0.0004	0.0018	0.0017	-0.0023	-0.0002	0.0009
AT. 39	O X	-0.0002	0.0005	-0.0011	-0.0022	-0.0024	0.0013
	Y	0.0010	0.0010	-0.0003	-0.0021	-0.0012	0.0001

	Z	0.0007	0.0012	-0.0006	-0.0028	-0.0026	0.0019
AT. 40	O X	0.0002	-0.0005	-0.0011	-0.0022	-0.0024	0.0013
	Y	-0.0010	-0.0010	-0.0003	-0.0021	-0.0012	0.0001
	Z	0.0007	0.0012	0.0006	0.0028	0.0026	-0.0019
AT. 41	O X	-0.0002	-0.0005	0.0011	-0.0022	0.0024	0.0013
	Y	-0.0010	0.0010	-0.0003	0.0021	-0.0012	-0.0001
	Z	-0.0007	0.0012	-0.0006	0.0028	-0.0026	-0.0019
AT. 42	O X	0.0002	0.0005	0.0011	-0.0022	0.0024	0.0013
	Y	0.0010	-0.0010	-0.0003	0.0021	-0.0012	-0.0001
	Z	-0.0007	0.0012	0.0006	-0.0028	0.0026	0.0019
AT. 43	O X	0.0002	-0.0005	-0.0011	-0.0022	-0.0024	0.0013
	Y	-0.0010	-0.0010	-0.0003	-0.0021	-0.0012	0.0001
	Z	-0.0007	-0.0012	-0.0006	-0.0028	-0.0026	0.0019
AT. 44	O X	-0.0002	0.0005	-0.0011	-0.0022	-0.0024	0.0013
	Y	0.0010	0.0010	-0.0003	-0.0021	-0.0012	0.0001
	Z	-0.0007	-0.0012	0.0006	0.0028	0.0026	-0.0019
AT. 45	O X	0.0002	0.0005	0.0011	-0.0022	0.0024	0.0013
	Y	0.0010	-0.0010	-0.0003	0.0021	-0.0012	-0.0001
	Z	0.0007	-0.0012	-0.0006	0.0028	-0.0026	-0.0019
AT. 46	O X	-0.0002	-0.0005	0.0011	-0.0022	0.0024	0.0013
	Y	-0.0010	0.0010	-0.0003	0.0021	-0.0012	-0.0001
	Z	0.0007	-0.0012	0.0006	-0.0028	0.0026	0.0019
AT. 47	O X	-0.0174	0.0160	-0.0095	0.0163	-0.0234	0.0060
	Y	-0.0028	0.0026	-0.0019	0.0037	-0.0046	0.0005
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	0.0174	-0.0160	-0.0095	0.0163	-0.0234	0.0060
	Y	0.0028	-0.0026	-0.0019	0.0037	-0.0046	0.0005
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	-0.0174	-0.0160	0.0095	0.0163	0.0234	0.0060
	Y	0.0028	0.0026	-0.0019	-0.0037	-0.0046	-0.0005
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	0.0174	0.0160	0.0095	0.0163	0.0234	0.0060
	Y	-0.0028	-0.0026	-0.0019	-0.0037	-0.0046	-0.0005
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	0.0214	-0.0216	-0.0223	0.0209	-0.0021	0.0037
	Y	-0.0190	0.0192	0.0211	-0.0194	0.0017	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	-0.0214	0.0216	-0.0223	0.0209	-0.0021	0.0037
	Y	0.0190	-0.0192	0.0211	-0.0194	0.0017	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	0.0214	0.0216	0.0223	0.0209	0.0021	0.0037
	Y	0.0190	0.0192	0.0211	0.0194	0.0017	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	-0.0214	-0.0216	0.0223	0.0209	0.0021	0.0037
	Y	-0.0190	-0.0192	0.0211	0.0194	0.0017	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	-0.0029	0.0031	-0.0041	-0.0030	0.0087	0.0104
	Y	-0.0093	0.0095	-0.0143	-0.0075	0.0257	0.0324
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56	O X	0.0029	-0.0031	-0.0041	-0.0030	0.0087	0.0104
	Y	0.0093	-0.0095	-0.0143	-0.0075	0.0257	0.0324
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57	O X	-0.0029	-0.0031	0.0041	-0.0030	-0.0087	0.0104
	Y	0.0093	0.0095	-0.0143	0.0075	0.0257	-0.0324



	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	0.0029	0.0031	0.0041	-0.0030	-0.0087	0.0104
	Y	-0.0093	-0.0095	-0.0143	0.0075	0.0257	-0.0324
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

FREQ(CM\*\*-1) 1176.13 1176.76 1190.96 1194.94 1209.86 1212.61

AT. 1 MG	X	0.0000	0.0010	0.0000	0.0005	0.0015	0.0000
	Y	-0.0008	0.0000	-0.0007	0.0000	0.0000	-0.0017
	Z	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
AT. 2 MG	X	0.0000	-0.0010	0.0000	0.0005	-0.0015	0.0000
	Y	0.0008	0.0000	-0.0007	0.0000	0.0000	0.0017
	Z	0.0000	0.0000	-0.0003	0.0000	0.0000	0.0000
AT. 3 MG	X	0.0000	-0.0010	0.0000	0.0005	-0.0015	0.0000
	Y	0.0008	0.0000	-0.0007	0.0000	0.0000	0.0017
	Z	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000
AT. 4 MG	X	0.0000	0.0010	0.0000	0.0005	0.0015	0.0000
	Y	-0.0008	0.0000	-0.0007	0.0000	0.0000	-0.0017
	Z	0.0000	0.0000	-0.0003	0.0000	0.0000	0.0000
AT. 5 AL	X	0.0000	0.0000	-0.0010	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	-0.0015	0.0000	0.0000
	Z	0.0011	0.0032	0.0000	0.0000	-0.0006	-0.0010
AT. 6 AL	X	0.0000	0.0000	0.0010	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	0.0015	0.0000	0.0000
	Z	0.0011	-0.0032	0.0000	0.0000	0.0006	-0.0010
AT. 7 AL	X	0.0000	0.0000	-0.0010	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	-0.0015	0.0000	0.0000
	Z	-0.0011	-0.0032	0.0000	0.0000	0.0006	0.0010
AT. 8 AL	X	0.0000	0.0000	0.0010	0.0020	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	0.0015	0.0000	0.0000
	Z	-0.0011	0.0032	0.0000	0.0000	-0.0006	0.0010
AT. 9 AL	X	-0.0025	-0.0042	0.0013	-0.0033	0.0013	-0.0038
	Y	0.0025	0.0013	0.0011	-0.0025	0.0034	-0.0017
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10 AL	X	0.0025	0.0042	0.0013	-0.0033	-0.0013	0.0038
	Y	-0.0025	-0.0013	0.0011	-0.0025	-0.0034	0.0017
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11 AL	X	0.0025	-0.0042	-0.0013	-0.0033	0.0013	0.0038
	Y	0.0025	-0.0013	0.0011	0.0025	-0.0034	-0.0017
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12 AL	X	-0.0025	0.0042	-0.0013	-0.0033	-0.0013	-0.0038
	Y	-0.0025	0.0013	0.0011	0.0025	0.0034	0.0017
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 13 SI	X	0.0000	0.0000	0.0000	-0.0079	0.0000	0.0000
	Y	0.0000	0.0000	-0.0052	0.0000	0.0000	0.0000
	Z	-0.0035	0.0000	0.0000	0.0000	0.0000	0.0044
AT. 14 SI	X	0.0000	0.0000	0.0000	-0.0079	0.0000	0.0000
	Y	0.0000	0.0000	-0.0052	0.0000	0.0000	0.0000
	Z	0.0035	0.0000	0.0000	0.0000	0.0000	-0.0044
AT. 15 SI	X	-0.0061	-0.0043	-0.0046	0.0067	-0.0055	0.0007
	Y	-0.0037	-0.0074	0.0079	-0.0024	0.0054	-0.0087
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16 SI	X	0.0061	0.0043	-0.0046	0.0067	0.0055	-0.0007
	Y	0.0037	0.0074	0.0079	-0.0024	-0.0054	0.0087

	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	0.0061	-0.0043	0.0046	0.0067	-0.0055	-0.0007
	Y	-0.0037	0.0074	0.0079	0.0024	-0.0054	-0.0087
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	-0.0061	0.0043	0.0046	0.0067	0.0055	0.0007
	Y	0.0037	-0.0074	0.0079	0.0024	0.0054	0.0087
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0074	-0.0015	0.0117	-0.0108	-0.0129	0.0103
	Y	-0.0072	-0.0065	0.0039	0.0012	-0.0015	-0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0074	0.0015	0.0117	-0.0108	0.0129	-0.0103
	Y	0.0072	0.0065	0.0039	0.0012	0.0015	0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0074	-0.0015	-0.0117	-0.0108	-0.0129	-0.0103
	Y	-0.0072	0.0065	0.0039	-0.0012	0.0015	-0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	-0.0074	0.0015	-0.0117	-0.0108	0.0129	0.0103
	Y	0.0072	-0.0065	0.0039	-0.0012	-0.0015	0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0011	-0.0013	-0.0018	-0.0021	0.0002	-0.0004
	Y	-0.0005	0.0012	0.0009	-0.0006	0.0001	0.0015
	Z	-0.0016	0.0022	0.0017	0.0012	-0.0008	0.0011
AT. 24	O X	-0.0011	0.0013	-0.0018	-0.0021	-0.0002	0.0004
	Y	0.0005	-0.0012	0.0009	-0.0006	-0.0001	-0.0015
	Z	-0.0016	0.0022	-0.0017	-0.0012	-0.0008	0.0011
AT. 25	O X	-0.0011	-0.0013	0.0018	-0.0021	0.0002	0.0004
	Y	-0.0005	-0.0012	0.0009	0.0006	-0.0001	0.0015
	Z	-0.0016	-0.0022	0.0017	-0.0012	0.0008	0.0011
AT. 26	O X	0.0011	0.0013	0.0018	-0.0021	-0.0002	-0.0004
	Y	0.0005	0.0012	0.0009	0.0006	0.0001	-0.0015
	Z	-0.0016	-0.0022	-0.0017	0.0012	0.0008	0.0011
AT. 27	O X	-0.0011	0.0013	-0.0018	-0.0021	-0.0002	0.0004
	Y	0.0005	-0.0012	0.0009	-0.0006	-0.0001	-0.0015
	Z	0.0016	-0.0022	0.0017	0.0012	0.0008	-0.0011
AT. 28	O X	0.0011	-0.0013	-0.0018	-0.0021	0.0002	-0.0004
	Y	-0.0005	0.0012	0.0009	-0.0006	0.0001	0.0015
	Z	0.0016	-0.0022	-0.0017	-0.0012	0.0008	-0.0011
AT. 29	O X	0.0011	0.0013	0.0018	-0.0021	-0.0002	-0.0004
	Y	0.0005	0.0012	0.0009	0.0006	0.0001	-0.0015
	Z	0.0016	0.0022	0.0017	-0.0012	-0.0008	-0.0011
AT. 30	O X	-0.0011	-0.0013	0.0018	-0.0021	0.0002	0.0004
	Y	-0.0005	-0.0012	0.0009	0.0006	-0.0001	0.0015
	Z	0.0016	0.0022	-0.0017	0.0012	-0.0008	-0.0011
AT. 31	O X	0.0003	0.0005	0.0011	0.0033	0.0012	-0.0012
	Y	0.0014	0.0004	0.0042	0.0035	-0.0006	-0.0025
	Z	0.0024	0.0004	0.0034	0.0039	-0.0006	-0.0030
AT. 32	O X	-0.0003	-0.0005	0.0011	0.0033	-0.0012	0.0012
	Y	-0.0014	-0.0004	0.0042	0.0035	0.0006	0.0025
	Z	0.0024	0.0004	-0.0034	-0.0039	-0.0006	-0.0030
AT. 33	O X	-0.0003	0.0005	-0.0011	0.0033	0.0012	0.0012
	Y	0.0014	-0.0004	0.0042	-0.0035	0.0006	-0.0025
	Z	0.0024	-0.0004	0.0034	-0.0039	0.0006	-0.0030
AT. 34	O X	0.0003	-0.0005	-0.0011	0.0033	-0.0012	-0.0012
	Y	-0.0014	0.0004	0.0042	-0.0035	-0.0006	0.0025

	Z	0.0024	-0.0004	-0.0034	0.0039	0.0006	-0.0030
AT. 35	O X	-0.0003	-0.0005	0.0011	0.0033	-0.0012	0.0012
	Y	-0.0014	-0.0004	0.0042	0.0035	0.0006	0.0025
	Z	-0.0024	-0.0004	0.0034	0.0039	0.0006	0.0030
AT. 36	O X	0.0003	0.0005	0.0011	0.0033	0.0012	-0.0012
	Y	0.0014	0.0004	0.0042	0.0035	-0.0006	-0.0025
	Z	-0.0024	-0.0004	-0.0034	-0.0039	0.0006	0.0030
AT. 37	O X	0.0003	-0.0005	-0.0011	0.0033	-0.0012	-0.0012
	Y	-0.0014	0.0004	0.0042	-0.0035	-0.0006	0.0025
	Z	-0.0024	0.0004	0.0034	-0.0039	-0.0006	0.0030
AT. 38	O X	-0.0003	0.0005	-0.0011	0.0033	0.0012	0.0012
	Y	0.0014	-0.0004	0.0042	-0.0035	0.0006	-0.0025
	Z	-0.0024	0.0004	-0.0034	0.0039	-0.0006	0.0030
AT. 39	O X	0.0003	-0.0023	0.0013	-0.0008	-0.0017	-0.0007
	Y	0.0013	-0.0016	0.0011	0.0013	0.0000	0.0008
	Z	0.0009	-0.0036	0.0017	0.0005	-0.0010	-0.0002
AT. 40	O X	-0.0003	0.0023	0.0013	-0.0008	0.0017	0.0007
	Y	-0.0013	0.0016	0.0011	0.0013	0.0000	-0.0008
	Z	0.0009	-0.0036	-0.0017	-0.0005	-0.0010	-0.0002
AT. 41	O X	-0.0003	-0.0023	-0.0013	-0.0008	-0.0017	0.0007
	Y	0.0013	0.0016	0.0011	-0.0013	0.0000	0.0008
	Z	0.0009	0.0036	0.0017	-0.0005	0.0010	-0.0002
AT. 42	O X	0.0003	0.0023	-0.0013	-0.0008	0.0017	-0.0007
	Y	-0.0013	-0.0016	0.0011	-0.0013	0.0000	-0.0008
	Z	0.0009	0.0036	-0.0017	0.0005	0.0010	-0.0002
AT. 43	O X	-0.0003	0.0023	0.0013	-0.0008	0.0017	0.0007
	Y	-0.0013	0.0016	0.0011	0.0013	0.0000	-0.0008
	Z	-0.0009	0.0036	0.0017	0.0005	0.0010	0.0002
AT. 44	O X	0.0003	-0.0023	0.0013	-0.0008	-0.0017	-0.0007
	Y	0.0013	-0.0016	0.0011	0.0013	0.0000	0.0008
	Z	-0.0009	0.0036	-0.0017	-0.0005	0.0010	0.0002
AT. 45	O X	0.0003	0.0023	-0.0013	-0.0008	0.0017	-0.0007
	Y	-0.0013	-0.0016	0.0011	-0.0013	0.0000	-0.0008
	Z	-0.0009	-0.0036	0.0017	-0.0005	-0.0010	0.0002
AT. 46	O X	-0.0003	-0.0023	-0.0013	-0.0008	-0.0017	0.0007
	Y	0.0013	0.0016	0.0011	-0.0013	0.0000	0.0008
	Z	-0.0009	-0.0036	-0.0017	0.0005	-0.0010	0.0002
AT. 47	O X	0.0095	-0.0074	-0.0228	0.0284	0.0277	-0.0272
	Y	0.0010	-0.0019	-0.0030	0.0044	0.0046	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	-0.0095	0.0074	-0.0228	0.0284	-0.0277	0.0272
	Y	-0.0010	0.0019	-0.0030	0.0044	-0.0046	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	-0.0095	-0.0074	0.0228	0.0284	0.0277	0.0272
	Y	0.0010	0.0019	-0.0030	-0.0044	-0.0046	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	0.0095	0.0074	0.0228	0.0284	-0.0277	-0.0272
	Y	-0.0010	-0.0019	-0.0030	-0.0044	0.0046	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	0.0128	0.0067	0.0115	-0.0116	0.0138	-0.0066
	Y	-0.0114	-0.0063	-0.0092	0.0101	-0.0117	0.0059
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	-0.0128	-0.0067	0.0115	-0.0116	-0.0138	0.0066
	Y	0.0114	0.0063	-0.0092	0.0101	0.0117	-0.0059

	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	-0.0128	0.0067	-0.0115	-0.0116	0.0138	0.0066
	Y	-0.0114	0.0063	-0.0092	-0.0101	0.0117	0.0059
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	0.0128	-0.0067	-0.0115	-0.0116	-0.0138	-0.0066
	Y	0.0114	-0.0063	-0.0092	-0.0101	-0.0117	-0.0059
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	0.0088	0.0102	-0.0051	-0.0022	0.0005	0.0047
	Y	0.0283	0.0322	-0.0166	-0.0047	0.0004	0.0163
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56	O X	-0.0088	-0.0102	-0.0051	-0.0022	-0.0005	-0.0047
	Y	-0.0283	-0.0322	-0.0166	-0.0047	-0.0004	-0.0163
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57	O X	-0.0088	0.0102	0.0051	-0.0022	0.0005	-0.0047
	Y	0.0283	-0.0322	-0.0166	0.0047	-0.0004	0.0163
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58	O X	0.0088	-0.0102	0.0051	-0.0022	-0.0005	0.0047
	Y	-0.0283	0.0322	-0.0166	0.0047	0.0004	-0.0163
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

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# VIBRATIONAL TEMPERATURES (K) [MODE NUMBER;IRREP]

## TO MODES

135.8 [ 4;B2G]	142.7 [ 5;B3G]	163.7 [ 6;B1U]	168.7 [ 7;AU ]
170.9 [ 8;B3G]	184.1 [ 9;B1G]	188.2 [ 10;B3U]	191.2 [ 11;B2G]
191.6 [ 12;AG ]	193.4 [ 13;B3G]	226.4 [ 14;B2U]	232.4 [ 15;B2G]
233.4 [ 16;AG ]	241.4 [ 17;B3U]	243.9 [ 18;B1G]	249.3 [ 19;B2U]
251.0 [ 20;B3U]	252.4 [ 21;B1U]	254.7 [ 22;B3G]	265.3 [ 23;B3G]
266.9 [ 24;AU ]	271.2 [ 25;B1G]	272.7 [ 26;B2G]	275.8 [ 27;B3U]
277.7 [ 28;B1U]	278.4 [ 29;B2U]	281.4 [ 30;AU ]	288.2 [ 31;B1U]
291.8 [ 32;B2G]	306.6 [ 33;B3G]	310.8 [ 34;AU ]	318.0 [ 35;B2G]
351.0 [ 36;B3G]	352.0 [ 37;AG ]	352.4 [ 38;B3U]	353.5 [ 39;B1G]
356.1 [ 40;B1U]	359.4 [ 41;B1G]	363.5 [ 42;B1U]	367.0 [ 43;B2U]
374.2 [ 44;B2G]	382.3 [ 45;B3G]	382.9 [ 46;AG ]	384.3 [ 47;AU ]
384.9 [ 48;B2U]	390.7 [ 49;B1G]	390.8 [ 50;B3U]	414.6 [ 51;B2G]
420.9 [ 52;B1U]	427.7 [ 53;B1G]	428.4 [ 54;AG ]	428.7 [ 55;B3G]
429.0 [ 56;B2U]	429.2 [ 57;AU ]	435.4 [ 58;B1G]	440.6 [ 59;B3G]
452.6 [ 60;AG ]	463.5 [ 61;AU ]	470.5 [ 62;B2U]	474.8 [ 63;AG ]
475.0 [ 64;B2G]	477.0 [ 65;B3U]	489.9 [ 66;B3U]	492.3 [ 67;B1U]
492.6 [ 68;B1G]	516.0 [ 69;B3U]	516.3 [ 70;B1G]	517.5 [ 71;B2U]
522.3 [ 72;AG ]	523.4 [ 73;B2U]	532.8 [ 74;B1U]	533.0 [ 75;AG ]
534.6 [ 76;AU ]	544.3 [ 77;B3G]	546.4 [ 78;B3U]	555.0 [ 79;B2G]
572.2 [ 80;B2G]	582.9 [ 81;B2U]	589.7 [ 82;B3U]	600.2 [ 83;B2U]
610.5 [ 84;B1G]	620.8 [ 85;B3U]	626.4 [ 86;AG ]	646.7 [ 87;B2U]
662.9 [ 88;B2G]	664.8 [ 89;B1G]	670.0 [ 90;B3G]	672.7 [ 91;AU ]
684.5 [ 92;AU ]	688.4 [ 93;B3G]	700.7 [ 94;B1U]	704.8 [ 95;AG ]
712.1 [ 96;B3G]	715.5 [ 97;B1G]	716.7 [ 98;B1U]	717.0 [ 99;B3U]
719.6 [ 100;B2G]	721.4 [ 101;B3U]	732.7 [ 102;B1U]	766.5 [ 103;B2U]
778.7 [ 104;AU ]	800.1 [ 105;B1G]	808.9 [ 106;AG ]	821.8 [ 107;B2U]
822.6 [ 108;B1U]	825.3 [ 109;B1G]	829.3 [ 110;AU ]	836.0 [ 111;B3U]
843.0 [ 112;AG ]	864.9 [ 113;B3U]	867.1 [ 114;B1G]	894.9 [ 115;AU ]
900.5 [ 116;B1U]	907.9 [ 117;B3G]	915.4 [ 118;AG ]	955.3 [ 119;B3G]

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total 715120

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-rw-r--r-- 1 dtoebbens dtoebbens      0 Mar 16 08:18 ERROR
-rw-r--r-- 1 dtoebbens dtoebbens 7882378 Mar 29 19:27 FREQINFO.DAT
-rw-r--r-- 1 dtoebbens dtoebbens 643365 Mar 29 19:27 OPTHESS.DAT
-rw-r--r-- 1 dtoebbens dtoebbens 510707 Mar 29 19:27 SCFOUT.LOG
-rw-r--r-- 1 dtoebbens dtoebbens 637673760 Mar 29 12:07 fort.10
-rw-r--r-- 1 dtoebbens dtoebbens 18911392 Mar 29 11:59 fort.11
-rw-r--r-- 1 dtoebbens dtoebbens 86844 Mar 29 08:10 fort.12
-rw-r--r-- 1 dtoebbens dtoebbens 18825576 Mar 16 11:35 fort.13
-rw-r--r-- 1 dtoebbens dtoebbens 12552 Mar 29 19:27 fort.19
-rw-r--r-- 1 dtoebbens dtoebbens 4489028 Mar 16 11:35 fort.20
-rw-r--r-- 1 dtoebbens dtoebbens 9455688 Mar 29 11:59 fort.71
-rw-r--r-- 1 dtoebbens dtoebbens 9455688 Mar 29 11:59 fort.72
-rw-r--r-- 1 dtoebbens dtoebbens 30992 Mar 29 19:27 fort.8
-rw-r--r-- 1 dtoebbens dtoebbens 4489028 Mar 16 11:35 fort.9
-rw-r--r-- 1 dtoebbens dtoebbens 9528904 Mar 29 10:59 fort.95
-rw-r--r-- 1 dtoebbens dtoebbens 9455688 Mar 29 08:10 fort.96
```

wave function binary file /home/dtoebbens/CRYSTAL/test\_cases/Cordierite-B3LYP-FREQ.f9

Mon Mar 29 19:27:43 CEST 2010

file SCFOUT.LOG saved as /home/dtoebbens/CRYSTAL/test\_cases/Cordierite-B3LYP-FREQ.SCFLOG

file fort.20 saved as /home/dtoebbens/CRYSTAL/test\_cases/Cordierite-B3LYP-FREQ.f20

file OPTHESS.DAT saved as /home/dtoebbens/CRYSTAL/test\_cases/Cordierite-B3LYP-FREQ.opthess

file FREQINFO.DAT saved as /home/dtoebbens/CRYSTAL/test\_cases/Cordierite-B3LYP-FREQ.freqinfo

/home/dtoebbens/scr/tmp2639 removed