

```

date Wed Feb 24 08:27:37 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/tmp25028
output in /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.out
scf guess from /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.f9
input data /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.d12
Fe-Cordierite: 4 Fe(2+) in primitive cell, total spin =16 (high-spin state)
CRYSTAL
1 0 0
C c c m
17.38668159 9.94452589 9.35377847
12
26 -1.636988018322E-01 5.000000000000E-01 2.500000000000E-01
13 2.500000000000E-01 2.500000000000E-01 2.499610859292E-01
13 4.938375209584E-02 3.073397793201E-01 0.000000000000E+00
14 0.000000000000E+00 -5.000000000000E-01 2.500000000000E-01
14 1.893673930670E-01 8.003763344749E-02 0.000000000000E+00
14 1.342110386244E-01 -2.322787287173E-01 0.000000000000E+00
8 2.440818529202E-01 -1.050115918706E-01 3.578554798738E-01
8 6.094323163264E-02 -4.156005949936E-01 3.488556545510E-01
8 -1.729878312451E-01 -3.023083019153E-01 3.574749661934E-01
8 4.330721679682E-02 -2.471825206532E-01 0.000000000000E+00
8 1.207792553935E-01 1.870144094163E-01 0.000000000000E+00
8 1.613867593376E-01 -7.499999417165E-02 0.000000000000E+00
FREQCALC
ANALYSIS
ENDFREQ
END
26 8 ! Fe(II)(2+) 86-4111G(41) (Fe_86-411d41G_towler_1992b with one additional sp, outer two sp and one
d reoptimized in Fe-Cordierite LDA/VWN)
0 0 8 2.0 1.0
316081.0 0.000227
45202.0 0.001929
9627.9 0.0111
2521.82 0.05
760.208 0.1705
262.994 0.3691
102.856 0.4034
42.9433 0.1434
0 1 6 8.0 1.0
797.99 -0.0052 0.00850
190.956 -0.0681 0.0609
63.6118 -0.1313 0.2116
25.3393 0.2522 0.3942
10.7282 0.642 0.3975
3.7566 0.2833 0.223
0 1 4 8.0 1.0
47.5075 0.012 -0.0217
17.3532 -0.2339 -0.083

```

6.9807	-0.8877	0.1988
3.0729	0.9954	1.2847
0 1 1	0.0	1.0
1.2936	1.0000	1.0000
0 1 1	0.0	1.0
0.567	1.0000	1.0000
0 1 1	0.0	1.0
0.248	1.0000	1.0000
0 3 4	6.0	1.0
29.0112	0.0574	
8.0431	0.2635	
2.7087	0.5236	
0.9412	0.5491	
0 3 1	0.0	1.0
0.278	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
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
SPIN
XLGRID
B3LYP
ENDDFT
MAXCYCLE
500
BIPOSIZE
7818200
EXCHSIZE
7876296

```

TOLINTEG
7 7 7 7 15
SCFDIR
GUESSP
SHRINK
4 4 4
SPINLOCK
16
500
FMIXING
80
BROYDEN
0.0001 50 2
ENDRUN
END hess guess from /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.opthess
geometry input from /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.gui
opt info from /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.optinfo
external geometry input found in /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.gui

*
*
* 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 *
*
*
* MAIN AUTHORS *
*
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EEEEEEEEEE STARTING DATE 24 02 2010 TIME 08:27:37.3
Fe-Cordierite: 4 Fe(2+) in primitive cell, total spin =16 (high-spin state)

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
17.38668	9.94453	9.35378	90.00000	90.00000	90.00000

NUMBER OF IRREDUCIBLE ATOMS IN THE CONVENTIONAL CELL: 12

INPUT COORDINATES

ATOM AT. N. COORDINATES

1	26	-1.636988018322E-01	5.000000000000E-01	2.500000000000E-01
2	13	2.500000000000E-01	2.500000000000E-01	2.499610859292E-01
3	13	4.938375209584E-02	3.073397793201E-01	0.000000000000E+00
4	14	0.000000000000E+00	-5.000000000000E-01	2.500000000000E-01
5	14	1.893673930670E-01	8.003763344749E-02	0.000000000000E+00
6	14	1.342110386244E-01	-2.322787287173E-01	0.000000000000E+00
7	8	2.440818529202E-01	-1.050115918706E-01	3.578554798738E-01
8	8	6.094323163264E-02	-4.156005949936E-01	3.488556545510E-01
9	8	-1.729878312451E-01	-3.023083019153E-01	3.574749661934E-01
10	8	4.330721679682E-02	-2.471825206532E-01	0.000000000000E+00
11	8	1.207792553935E-01	1.870144094163E-01	0.000000000000E+00
12	8	1.613867593376E-01	-7.499999417165E-02	0.000000000000E+00

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

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - PRIMITIVE CELL

A	B	C	ALPHA	BETA	GAMMA	VOLUME
10.01487	10.01487	9.35378	90.00000	90.00000	120.46414	808.644930

COORDINATES OF THE EQUIVALENT ATOMS (FRACTIONARY UNITS)

N. ATOM EQUIV AT. N. X Y Z

1	1	1	26	FE	3.36301198168E-01	-3.36301198168E-01	2.50000000000E-01
2	1	2	26	FE	-3.36301198168E-01	3.36301198168E-01	2.50000000000E-01
3	1	3	26	FE	-3.36301198168E-01	3.36301198168E-01	-2.50000000000E-01
4	1	4	26	FE	3.36301198168E-01	-3.36301198168E-01	-2.50000000000E-01
5	2	1	13	AL	-5.00000000000E-01	0.00000000000E+00	2.49961085929E-01
6	2	2	13	AL	0.00000000000E+00	5.00000000000E-01	2.50038914071E-01
7	2	3	13	AL	5.00000000000E-01	0.00000000000E+00	-2.49961085929E-01
8	2	4	13	AL	0.00000000000E+00	-5.00000000000E-01	-2.50038914071E-01
9	3	1	13	AL	3.56723531416E-01	2.57956027224E-01	0.00000000000E+00

10	3	2	13	AL	-3.56723531416E-01	-2.57956027224E-01	0.00000000000E+00
11	3	3	13	AL	-2.57956027224E-01	-3.56723531416E-01	-5.00000000000E-01
12	3	4	13	AL	2.57956027224E-01	3.56723531416E-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	2.69405026514E-01	-1.09329759620E-01	0.00000000000E+00
16	5	2	14	SI	-2.69405026514E-01	1.09329759620E-01	0.00000000000E+00
17	5	3	14	SI	1.09329759620E-01	-2.69405026514E-01	-5.00000000000E-01
18	5	4	14	SI	-1.09329759620E-01	2.69405026514E-01	-5.00000000000E-01
19	6	1	14	SI	-9.80676900929E-02	-3.66489767342E-01	0.00000000000E+00
20	6	2	14	SI	9.80676900929E-02	3.66489767342E-01	0.00000000000E+00
21	6	3	14	SI	3.66489767342E-01	9.80676900929E-02	-5.00000000000E-01
22	6	4	14	SI	-3.66489767342E-01	-9.80676900929E-02	-5.00000000000E-01
23	7	1	8	O	1.39070261050E-01	-3.49093444791E-01	3.57855479874E-01
24	7	2	8	O	-1.39070261050E-01	3.49093444791E-01	3.57855479874E-01
25	7	3	8	O	3.49093444791E-01	-1.39070261050E-01	1.42144520126E-01
26	7	4	8	O	-3.49093444791E-01	1.39070261050E-01	1.42144520126E-01
27	7	5	8	O	-1.39070261050E-01	3.49093444791E-01	-3.57855479874E-01
28	7	6	8	O	1.39070261050E-01	-3.49093444791E-01	-3.57855479874E-01
29	7	7	8	O	-3.49093444791E-01	1.39070261050E-01	-1.42144520126E-01
30	7	8	8	O	3.49093444791E-01	-1.39070261050E-01	-1.42144520126E-01
31	8	1	8	O	-3.54657363361E-01	-4.76543826626E-01	3.48855654551E-01
32	8	2	8	O	3.54657363361E-01	4.76543826626E-01	3.48855654551E-01
33	8	3	8	O	4.76543826626E-01	3.54657363361E-01	1.51144345449E-01
34	8	4	8	O	-4.76543826626E-01	-3.54657363361E-01	1.51144345449E-01
35	8	5	8	O	3.54657363361E-01	4.76543826626E-01	-3.48855654551E-01
36	8	6	8	O	-3.54657363361E-01	-4.76543826626E-01	-3.48855654551E-01
37	8	7	8	O	-4.76543826626E-01	-3.54657363361E-01	-1.51144345449E-01
38	8	8	8	O	4.76543826626E-01	3.54657363361E-01	-1.51144345449E-01
39	9	1	8	O	-4.75296133160E-01	-1.29320470670E-01	3.57474966193E-01
40	9	2	8	O	4.75296133160E-01	1.29320470670E-01	3.57474966193E-01
41	9	3	8	O	1.29320470670E-01	4.75296133160E-01	1.42525033807E-01
42	9	4	8	O	-1.29320470670E-01	-4.75296133160E-01	1.42525033807E-01
43	9	5	8	O	4.75296133160E-01	1.29320470670E-01	-3.57474966193E-01
44	9	6	8	O	-4.75296133160E-01	-1.29320470670E-01	-3.57474966193E-01
45	9	7	8	O	-1.29320470670E-01	-4.75296133160E-01	-1.42525033807E-01
46	9	8	8	O	1.29320470670E-01	4.75296133160E-01	-1.42525033807E-01
47	10	1	8	O	-2.03875303856E-01	-2.90489737450E-01	0.00000000000E+00
48	10	2	8	O	2.03875303856E-01	2.90489737450E-01	0.00000000000E+00
49	10	3	8	O	2.90489737450E-01	2.03875303856E-01	-5.00000000000E-01
50	10	4	8	O	-2.90489737450E-01	-2.03875303856E-01	-5.00000000000E-01
51	11	1	8	O	3.07793664810E-01	6.62351540228E-02	0.00000000000E+00
52	11	2	8	O	-3.07793664810E-01	-6.62351540228E-02	0.00000000000E+00
53	11	3	8	O	-6.62351540228E-02	-3.07793664810E-01	-5.00000000000E-01
54	11	4	8	O	6.62351540228E-02	3.07793664810E-01	-5.00000000000E-01

22 F 14 SI -3.664897673417E-01 -9.806769009290E-02 -5.000000000000E-01
23 T 8 O 1.390702610496E-01 -3.490934447908E-01 3.578554798738E-01
24 F 8 O -1.390702610496E-01 3.490934447908E-01 3.578554798738E-01
25 F 8 O 3.490934447908E-01 -1.390702610496E-01 1.421445201262E-01
26 F 8 O -3.490934447908E-01 1.390702610496E-01 1.421445201262E-01
27 F 8 O -1.390702610496E-01 3.490934447908E-01 -3.578554798738E-01
28 F 8 O 1.390702610496E-01 -3.490934447908E-01 -3.578554798738E-01
29 F 8 O -3.490934447908E-01 1.390702610496E-01 -1.421445201262E-01
30 F 8 O 3.490934447908E-01 -1.390702610496E-01 -1.421445201262E-01
31 T 8 O -3.546573633610E-01 -4.765438266262E-01 3.488556545510E-01
32 F 8 O 3.546573633610E-01 4.765438266262E-01 3.488556545510E-01
33 F 8 O 4.765438266262E-01 3.546573633610E-01 1.511443454490E-01
34 F 8 O -4.765438266262E-01 -3.546573633610E-01 1.511443454490E-01
35 F 8 O 3.546573633610E-01 4.765438266262E-01 -3.488556545510E-01
36 F 8 O -3.546573633610E-01 -4.765438266262E-01 -3.488556545510E-01
37 F 8 O -4.765438266262E-01 -3.546573633610E-01 -1.511443454490E-01
38 F 8 O 4.765438266262E-01 3.546573633610E-01 -1.511443454490E-01
39 T 8 O -4.752961331604E-01 -1.293204706702E-01 3.574749661934E-01
40 F 8 O 4.752961331604E-01 1.293204706702E-01 3.574749661934E-01
41 F 8 O 1.293204706702E-01 4.752961331604E-01 1.425250338066E-01
42 F 8 O -1.293204706702E-01 -4.752961331604E-01 1.425250338066E-01
43 F 8 O 4.752961331604E-01 1.293204706702E-01 -3.574749661934E-01
44 F 8 O -4.752961331604E-01 -1.293204706702E-01 -3.574749661934E-01
45 F 8 O -1.293204706702E-01 -4.752961331604E-01 -1.425250338066E-01
46 F 8 O 1.293204706702E-01 4.752961331604E-01 -1.425250338066E-01
47 T 8 O -2.038753038564E-01 -2.904897374500E-01 0.000000000000E+00
48 F 8 O 2.038753038564E-01 2.904897374500E-01 0.000000000000E+00
49 F 8 O 2.904897374500E-01 2.038753038564E-01 -5.000000000000E-01
50 F 8 O -2.904897374500E-01 -2.038753038564E-01 -5.000000000000E-01
51 T 8 O 3.077936648098E-01 6.623515402280E-02 0.000000000000E+00
52 F 8 O -3.077936648098E-01 -6.623515402280E-02 0.000000000000E+00
53 F 8 O -6.623515402280E-02 -3.077936648098E-01 -5.000000000000E-01
54 F 8 O 6.623515402280E-02 3.077936648098E-01 -5.000000000000E-01
55 T 8 O 8.638676516595E-02 -2.363867535093E-01 0.000000000000E+00
56 F 8 O -8.638676516595E-02 2.363867535093E-01 0.000000000000E+00
57 F 8 O 2.363867535092E-01 -8.638676516595E-02 -5.000000000000E-01
58 F 8 O -2.363867535092E-01 8.638676516595E-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

CRYSTALLOGRAPHIC CELL (VOLUME= 1617.28985991)
A B C ALPHA BETA GAMMA
17.38668159 9.94452589 9.35377847 90.000000 90.000000 90.000000

COORDINATES IN THE CRYSTALLOGRAPHIC CELL

ATOM X/A Y/B Z/C

1 T 26 FE -1.636988018322E-01 5.000000000000E-01 2.500000000000E-01
2 F 26 FE 1.636988018322E-01 5.000000000000E-01 2.500000000000E-01
3 F 26 FE 1.636988018322E-01 5.000000000000E-01 -2.500000000000E-01
4 F 26 FE -1.636988018322E-01 5.000000000000E-01 -2.500000000000E-01
5 T 13 AL 2.500000000000E-01 2.500000000000E-01 2.499610859292E-01

6 F 13 AL -2.500000000000E-01 2.500000000000E-01 2.500389140708E-01
7 F 13 AL 2.500000000000E-01 2.500000000000E-01 -2.499610859292E-01
8 F 13 AL -2.500000000000E-01 2.500000000000E-01 -2.500389140708E-01
9 T 13 AL 4.938375209584E-02 3.073397793201E-01 0.000000000000E+00
10 F 13 AL -4.938375209584E-02 -3.073397793201E-01 0.000000000000E+00
11 F 13 AL 4.938375209584E-02 -3.073397793201E-01 -5.000000000000E-01
12 F 13 AL -4.938375209584E-02 3.073397793201E-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 1.893673930670E-01 8.003763344749E-02 0.000000000000E+00
16 F 14 SI -1.893673930670E-01 -8.003763344749E-02 0.000000000000E+00
17 F 14 SI 1.893673930670E-01 -8.003763344749E-02 -5.000000000000E-01
18 F 14 SI -1.893673930670E-01 8.003763344749E-02 -5.000000000000E-01
19 T 14 SI 1.342110386244E-01 -2.322787287173E-01 0.000000000000E+00
20 F 14 SI -1.342110386244E-01 2.322787287173E-01 0.000000000000E+00
21 F 14 SI 1.342110386244E-01 2.322787287173E-01 -5.000000000000E-01
22 F 14 SI -1.342110386244E-01 -2.322787287173E-01 -5.000000000000E-01
23 T 8 O 2.440818529202E-01 -1.050115918706E-01 3.578554798738E-01
24 F 8 O -2.440818529202E-01 1.050115918706E-01 3.578554798738E-01
25 F 8 O 2.440818529202E-01 1.050115918706E-01 1.421445201262E-01
26 F 8 O -2.440818529202E-01 -1.050115918706E-01 1.421445201262E-01
27 F 8 O -2.440818529202E-01 1.050115918706E-01 -3.578554798738E-01
28 F 8 O 2.440818529202E-01 -1.050115918706E-01 -3.578554798738E-01
29 F 8 O -2.440818529202E-01 -1.050115918706E-01 -1.421445201262E-01
30 F 8 O 2.440818529202E-01 1.050115918706E-01 -1.421445201262E-01
31 T 8 O 6.094323163264E-02 -4.156005949936E-01 3.488556545510E-01
32 F 8 O -6.094323163264E-02 4.156005949936E-01 3.488556545510E-01
33 F 8 O 6.094323163264E-02 4.156005949936E-01 1.511443454490E-01
34 F 8 O -6.094323163264E-02 -4.156005949936E-01 1.511443454490E-01
35 F 8 O -6.094323163264E-02 4.156005949936E-01 -3.488556545510E-01
36 F 8 O 6.094323163264E-02 -4.156005949936E-01 -3.488556545510E-01
37 F 8 O -6.094323163264E-02 -4.156005949936E-01 -1.511443454490E-01
38 F 8 O 6.094323163264E-02 4.156005949936E-01 -1.511443454490E-01
39 T 8 O -1.729878312451E-01 -3.023083019153E-01 3.574749661934E-01
40 F 8 O 1.729878312451E-01 3.023083019153E-01 3.574749661934E-01
41 F 8 O -1.729878312451E-01 3.023083019153E-01 1.425250338066E-01
42 F 8 O 1.729878312451E-01 -3.023083019153E-01 1.425250338066E-01
43 F 8 O 1.729878312451E-01 3.023083019153E-01 -3.574749661934E-01
44 F 8 O -1.729878312451E-01 -3.023083019153E-01 -3.574749661934E-01
45 F 8 O 1.729878312451E-01 -3.023083019153E-01 -1.425250338066E-01
46 F 8 O -1.729878312451E-01 3.023083019153E-01 -1.425250338066E-01
47 T 8 O 4.330721679682E-02 -2.471825206532E-01 0.000000000000E+00
48 F 8 O -4.330721679682E-02 2.471825206532E-01 0.000000000000E+00
49 F 8 O 4.330721679682E-02 2.471825206532E-01 -5.000000000000E-01
50 F 8 O -4.330721679682E-02 -2.471825206532E-01 -5.000000000000E-01
51 T 8 O 1.207792553935E-01 1.870144094163E-01 0.000000000000E+00
52 F 8 O -1.207792553935E-01 -1.870144094163E-01 0.000000000000E+00
53 F 8 O 1.207792553935E-01 -1.870144094163E-01 -5.000000000000E-01
54 F 8 O -1.207792553935E-01 1.870144094163E-01 -5.000000000000E-01
55 T 8 O 1.613867593376E-01 -7.499999417165E-02 0.000000000000E+00
56 F 8 O -1.613867593376E-01 7.499999417165E-02 0.000000000000E+00
57 F 8 O 1.613867593376E-01 7.499999417165E-02 -5.000000000000E-01
58 F 8 O -1.613867593376E-01 -7.499999417165E-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
0.869334079500E+01	0.497226294500E+01	0.000000000000E+00
-0.869334079500E+01	0.497226294500E+01	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	0.935377847000E+01

CARTESIAN COORDINATES - PRIMITIVE CELL

* ATOM	X(ANGSTROM)	Y(ANGSTROM)	Z(ANGSTROM)
1 26 FE	-2.846178944121E+00	-4.972262945000E+00	2.338444617500E+00
2 26 FE	2.846178944121E+00	-4.972262945000E+00	2.338444617500E+00
3 26 FE	2.846178944121E+00	-4.972262945000E+00	-2.338444617500E+00
4 26 FE	-2.846178944121E+00	-4.972262945000E+00	-2.338444617500E+00
5 13 AL	4.346670397500E+00	2.486131472500E+00	2.338080623902E+00
6 13 AL	-4.346670397500E+00	2.486131472500E+00	2.338080611098E+00
7 13 AL	4.346670397500E+00	2.486131472500E+00	-2.338080623902E+00
8 13 AL	-4.346670397500E+00	2.486131472500E+00	-2.338080611098E+00
9 13 AL	8.586195734099E-01	3.056348392476E+00	0.000000000000E+00
10 13 AL	-8.586195734099E-01	-3.056348392476E+00	0.000000000000E+00
11 13 AL	8.586195734099E-01	-3.056348392476E+00	4.676889235000E+00
12 13 AL	-8.586195734099E-01	3.056348392476E+00	4.676889235000E+00
13 14 SI	0.000000000000E+00	4.972262945000E+00	2.338444617500E+00
14 14 SI	0.000000000000E+00	4.972262945000E+00	-2.338444617500E+00
15 14 SI	3.292470566784E+00	7.959363179929E-01	0.000000000000E+00
16 14 SI	-3.292470566784E+00	-7.959363179929E-01	0.000000000000E+00
17 14 SI	3.292470566784E+00	-7.959363179929E-01	4.676889235000E+00
18 14 SI	-3.292470566784E+00	7.959363179929E-01	4.676889235000E+00
19 14 SI	2.333484594426E+00	-2.309901831425E+00	0.000000000000E+00
20 14 SI	-2.333484594426E+00	2.309901831425E+00	0.000000000000E+00
21 14 SI	2.333484594426E+00	2.309901831425E+00	4.676889235000E+00
22 14 SI	-2.333484594426E+00	-2.309901831425E+00	4.676889235000E+00
23 8 O	4.243773458621E+00	-1.044290494107E+00	3.347300883015E+00
24 8 O	-4.243773458621E+00	1.044290494107E+00	3.347300883015E+00
25 8 O	4.243773458621E+00	1.044290494107E+00	1.329588351985E+00
26 8 O	-4.243773458621E+00	-1.044290494107E+00	1.329588351985E+00
27 8 O	-4.243773458621E+00	1.044290494107E+00	-3.347300883015E+00
28 8 O	4.243773458621E+00	-1.044290494107E+00	-3.347300883015E+00
29 8 O	-4.243773458621E+00	-1.044290494107E+00	-1.329588351985E+00
30 8 O	4.243773458621E+00	1.044290494107E+00	-1.329588351985E+00

31 8 O 1.059600563462E+00 -4.132950876813E+00 3.263118510677E+00
32 8 O -1.059600563462E+00 4.132950876813E+00 3.263118510677E+00
33 8 O 1.059600563462E+00 4.132950876813E+00 1.413770724323E+00
34 8 O -1.059600563462E+00 -4.132950876813E+00 1.413770724323E+00
35 8 O -1.059600563462E+00 4.132950876813E+00 -3.263118510677E+00
36 8 O 1.059600563462E+00 -4.132950876813E+00 -3.263118510677E+00
37 8 O -1.059600563462E+00 -4.132950876813E+00 -1.413770724323E+00
38 8 O 1.059600563462E+00 4.132950876813E+00 -1.413770724323E+00
39 8 O -3.007684340803E+00 -3.006312735159E+00 3.343741642344E+00
40 8 O 3.007684340803E+00 3.006312735159E+00 3.343741642344E+00
41 8 O -3.007684340803E+00 3.006312735159E+00 1.333147592656E+00
42 8 O 3.007684340803E+00 -3.006312735159E+00 1.333147592656E+00
43 8 O 3.007684340803E+00 3.006312735159E+00 -3.343741642344E+00
44 8 O -3.007684340803E+00 -3.006312735159E+00 -3.343741642344E+00
45 8 O 3.007684340803E+00 -3.006312735159E+00 -1.333147592656E+00
46 8 O -3.007684340803E+00 3.006312735159E+00 -1.333147592656E+00
47 8 O 7.529687889954E-01 -2.458112976191E+00 0.000000000000E+00
48 8 O -7.529687889954E-01 2.458112976191E+00 0.000000000000E+00
49 8 O 7.529687889954E-01 2.458112976191E+00 4.676889235000E+00
50 8 O -7.529687889954E-01 -2.458112976191E+00 4.676889235000E+00
51 8 O 2.099950456204E+00 1.859769636243E+00 0.000000000000E+00
52 8 O -2.099950456204E+00 -1.859769636243E+00 0.000000000000E+00
53 8 O 2.099950456204E+00 -1.859769636243E+00 4.676889235000E+00
54 8 O -2.099950456204E+00 1.859769636243E+00 4.676889235000E+00
55 8 O 2.805980197445E+00 -7.458393837898E-01 0.000000000000E+00
56 8 O -2.805980197445E+00 7.458393837898E-01 0.000000000000E+00
57 8 O 2.805980197445E+00 7.458393837898E-01 4.676889235000E+00
58 8 O -2.805980197445E+00 -7.458393837898E-01 4.676889235000E+00

LOCAL ATOMIC FUNCTIONS BASIS SET

ATOM X(AU) Y(AU) Z(AU) NO. TYPE EXPONENT S COEF P COEF D/F/G COEF

1 FE -5.378 -9.396 4.419
1 S
3.161E+05 2.270E-04 0.000E+00 0.000E+00
4.520E+04 1.929E-03 0.000E+00 0.000E+00
9.628E+03 1.110E-02 0.000E+00 0.000E+00
2.522E+03 5.000E-02 0.000E+00 0.000E+00
7.602E+02 1.705E-01 0.000E+00 0.000E+00
2.630E+02 3.691E-01 0.000E+00 0.000E+00
1.029E+02 4.034E-01 0.000E+00 0.000E+00
4.294E+01 1.434E-01 0.000E+00 0.000E+00
2- 5 SP
7.980E+02 -5.200E-03 8.500E-03 0.000E+00
1.910E+02 -6.810E-02 6.090E-02 0.000E+00
6.361E+01 -1.313E-01 2.116E-01 0.000E+00
2.534E+01 2.522E-01 3.942E-01 0.000E+00
1.073E+01 6.420E-01 3.975E-01 0.000E+00
3.757E+00 2.833E-01 2.230E-01 0.000E+00
6- 9 SP
4.751E+01 1.200E-02 -2.170E-02 0.000E+00
1.735E+01 -2.339E-01 -8.300E-02 0.000E+00

6.981E+00-8.877E-01 1.988E-01 0.000E+00
 3.073E+00 9.954E-01 1.285E+00 0.000E+00
 10- 13 SP
 1.294E+00 1.000E+00 1.000E+00 0.000E+00
 14- 17 SP
 5.670E-01 1.000E+00 1.000E+00 0.000E+00
 18- 21 SP
 2.480E-01 1.000E+00 1.000E+00 0.000E+00
 22- 26 D
 2.901E+01 0.000E+00 0.000E+00 5.740E-02
 8.043E+00 0.000E+00 0.000E+00 2.635E-01
 2.709E+00 0.000E+00 0.000E+00 5.236E-01
 9.412E-01 0.000E+00 0.000E+00 5.491E-01
 27- 31 D
 2.780E-01 0.000E+00 0.000E+00 1.000E+00
 2 FE 5.378 -9.396 4.419
 3 FE 5.378 -9.396 -4.419
 4 FE -5.378 -9.396 -4.419
 5 AL 8.214 4.698 4.418
 125 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
 126- 129 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
 130- 133 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
 134- 137 SP
 4.380E-01 1.000E+00 1.000E+00 0.000E+00
 138- 141 SP
 2.120E-01 1.000E+00 1.000E+00 0.000E+00
 142- 146 D
 5.820E-01 0.000E+00 0.000E+00 1.000E+00
 6 AL -8.214 4.698 4.420
 7 AL 8.214 4.698 -4.418
 8 AL -8.214 4.698 -4.420
 9 AL 1.623 5.776 0.000
 10 AL -1.623 -5.776 0.000
 11 AL 1.623 -5.776 8.838
 12 AL -1.623 5.776 8.838

13 SI 0.000 9.396 4.419
 301 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
 302- 305 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
 306- 309 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
 310- 313 SP
 3.440E-01 1.000E+00 1.000E+00 0.000E+00
 314- 317 SP
 1.300E-01 1.000E+00 1.000E+00 0.000E+00
 318- 322 D
 6.770E-01 0.000E+00 0.000E+00 1.000E+00
 14 SI 0.000 9.396 -4.419
 15 SI 6.222 1.504 0.000
 16 SI -6.222 -1.504 0.000
 17 SI 6.222 -1.504 8.838
 18 SI -6.222 1.504 8.838
 19 SI 4.410 -4.365 0.000
 20 SI -4.410 4.365 0.000
 21 SI 4.410 4.365 8.838
 22 SI -4.410 -4.365 8.838
 23 O 8.020 -1.973 6.325
 521 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
 522- 525 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
 526- 529 SP
 4.660E-01 1.000E+00 1.000E+00 0.000E+00
 530- 533 SP

1.950E-01 1.000E+00 1.000E+00 0.000E+00
534- 538 D

5.380E-01 0.000E+00 0.000E+00 1.000E+00

24 O -8.020 1.973 6.325
25 O 8.020 1.973 2.513
26 O -8.020 -1.973 2.513
27 O -8.020 1.973 -6.325
28 O 8.020 -1.973 -6.325
29 O -8.020 -1.973 -2.513
30 O 8.020 1.973 -2.513
31 O 2.002 -7.810 6.166
32 O -2.002 7.810 6.166
33 O 2.002 7.810 2.672
34 O -2.002 -7.810 2.672
35 O -2.002 7.810 -6.166
36 O 2.002 -7.810 -6.166
37 O -2.002 -7.810 -2.672
38 O 2.002 7.810 -2.672
39 O -5.684 -5.681 6.319
40 O 5.684 5.681 6.319
41 O -5.684 5.681 2.519
42 O 5.684 -5.681 2.519
43 O 5.684 5.681 -6.319
44 O -5.684 -5.681 -6.319
45 O 5.684 -5.681 -2.519
46 O -5.684 5.681 -2.519
47 O 1.423 -4.645 0.000
48 O -1.423 4.645 0.000
49 O 1.423 4.645 8.838
50 O -1.423 -4.645 8.838
51 O 3.968 3.514 0.000
52 O -3.968 -3.514 0.000
53 O 3.968 -3.514 8.838
54 O -3.968 3.514 8.838
55 O 5.303 -1.409 0.000
56 O -5.303 1.409 0.000
57 O 5.303 1.409 8.838
58 O -5.303 -1.409 8.838

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
INFORMATION **** GUESSP **** SCF GUESS FROM A PREVIOUS RUN DENSITY MATRIX
ALPHA-BETA ELECTRONS LOCKED TO 16 FOR 500 SCF CYCLES

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 320 COULOMB PENETRATION TOL (T2) 10** -7

NUMBER OF AO 1168 EXCHANGE OVERLAP TOL (T3) 10** -7

N. OF ELECTRONS PER CELL 636 EXCHANGE PSEUDO OVP (F(G)) (T4) 10**-7
CORE ELECTRONS PER CELL 324 EXCHANGE PSEUDO OVP (P(G)) (T5) 10**-15
N. OF SYMMETRY OPERATORS 8 POLE ORDER IN MONO ZONE 4

TYPE OF CALCULATION : UNRESTRICTED OPEN 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

SPIN POLARIZED DFT SELECTED
SPIN POLARIZATION - ALPHA-BETA = 16 FOR 500 CYCLES

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
SPIN POLARIZATION - ALPHA-BETA = 16 FOR 500 CYCLES
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
16.4280333	9.3962152	0.0000000	0.1912336	0.3343466	0.0000000
-16.4280333	9.3962152	0.0000000	-0.1912336	0.3343466	0.0000000
0.0000000	0.0000000	17.6760796	0.0000000	0.0000000	0.3554626

DISK SPACE FOR EIGENVECTORS (FTN 10) 49112064 REALS

SYMMETRY ADAPTION OF THE BLOCH FUNCTIONS ENABLED

DIMENSIONS P(G)= 2470752 F(G)= 399664 P(G),F(G) (IRR) 172555
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT TELAPSE 0.11 TCPU 0.02

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 FE	2	2.1631	4.0877	23 O	-1 0 0	25 O	-1 0 0
1 FE	2	2.1798	4.1191	32 O	-1-1 0	34 O	0 0 0
1 FE	2	2.2140	4.1838	39 O	0 0 0	41 O	-1-1 0
1 FE	1	2.8462	5.3785	13 SI	-1-1 0		
1 FE	2	2.9038	5.4875	5 AL	-1 0 0	6 AL	-1-1 0
1 FE	2	3.5536	6.7154	15 SI	-1 0 0	17 SI	-1 0 0
5 AL	2	1.7535	3.3137	39 O	1 0 0	40 O	0 0 0
5 AL	2	1.7625	3.3307	25 O	0 0 0	26 O	1 0 0
5 AL	2	2.9038	5.4875	1 FE	1 0 0	2 FE	1 1 0
5 AL	2	3.0716	5.8045	15 SI	0 0 0	16 SI	1 0 0
5 AL	2	3.0910	5.8411	21 SI	0 0 0	22 SI	1 0 0
5 AL	2	3.2973	6.2310	57 O	0 0 0	58 O	1 0 0
9 AL	1	1.7190	3.2485	48 O	0 0 0		
9 AL	1	1.7242	3.2582	51 O	0 0 0		
9 AL	2	1.7884	3.3795	33 O	0 0 0	38 O	0 0 0
9 AL	2	3.1427	5.9388	13 SI	0 0 0	14 SI	0 0 0
9 AL	1	3.2782	6.1949	20 SI	0 0 0		
9 AL	1	3.3216	6.2769	15 SI	0 0 0		
13 SI	4	1.6377	3.0949	31 O	1 1 0	32 O	0 0 0
				34 O	1 1 0		
13 SI	2	2.8462	5.3785	1 FE	1 1 0	2 FE	1 1 0
13 SI	4	3.1427	5.9388	9 AL	0 0 0	10 AL	1 1 0
				12 AL	0 0 0		
13 SI	4	3.5151	6.6427	47 O	1 1 0	48 O	0 0 0
				50 O	1 1 0		
13 SI	4	3.7312	7.0509	39 O	1 1 0	40 O	0 0 0
				42 O	1 1 0		
13 SI	4	3.9883	7.5367	35 O	0 0 1	36 O	1 1 1
				37 O	1 1 0		
				38 O	0 0 0		
15 SI	1	1.5981	3.0199	51 O	0 0 0		
15 SI	1	1.6167	3.0551	55 O	0 0 0		
15 SI	2	1.6536	3.1249	25 O	0 0 0	30 O	0 0 0
15 SI	2	3.0716	5.8045	5 AL	0 0 0	7 AL	0 0 0
15 SI	1	3.2505	6.1426	19 SI	0 0 0		
15 SI	1	3.3216	6.2769	9 AL	0 0 0		
19 SI	1	1.5874	2.9998	47 O	0 0 0		
19 SI	1	1.6339	3.0876	55 O	0 0 0		
19 SI	2	1.6483	3.1148	42 O	0 0 0	45 O	0 0 0
19 SI	2	3.0910	5.8411	6 AL	0-1 0	8 AL	0-1 0
19 SI	1	3.2505	6.1426	15 SI	0 0 0		
19 SI	1	3.2782	6.1949	10 AL	0 0 0		
23 O	1	1.6536	3.1249	17 SI	0 0 0		
23 O	1	1.7625	3.3307	6 AL	0-1 0		
23 O	1	2.1631	4.0877	1 FE	1 0 0		
23 O	1	2.6430	4.9945	41 O	0-1 0		

23 O 1 2.6512 5.0100 53 O 0 0 0
23 O 1 2.6532 5.0139 57 O 0 0 0

31 O 1 1.6377 3.0949 13 SI -1-1 0
31 O 1 1.7884 3.3795 11 AL 0 0 0
31 O 1 2.1798 4.1191 2 FE 0 0 0
31 O 1 2.4976 4.7197 33 O -1-1 0
31 O 1 2.7035 5.1088 32 O -1-1 0
31 O 1 2.8127 5.3152 34 O 0 0 0

39 O 1 1.6483 3.1148 22 SI 0 0 0
39 O 1 1.7535 3.3137 5 AL -1 0 0
39 O 1 2.2140 4.1838 1 FE 0 0 0
39 O 1 2.6321 4.9739 58 O 0 0 0
39 O 1 2.6430 4.9945 25 O -1 0 0
39 O 1 2.6663 5.0386 44 O 0 0 1

47 O 1 1.5874 2.9998 19 SI 0 0 0
47 O 1 1.7190 3.2485 10 AL 0 0 0
47 O 1 2.6733 5.0519 55 O 0 0 0
47 O 2 2.6761 5.0571 42 O 0 0 0 45 O 0 0 0
47 O 2 2.8442 5.3747 34 O 0 0 0 37 O 0 0 0
47 O 1 2.9150 5.5085 52 O 0 0 0

51 O 1 1.5981 3.0199 15 SI 0 0 0
51 O 1 1.7242 3.2582 9 AL 0 0 0
51 O 2 2.6512 5.0100 25 O 0 0 0 30 O 0 0 0
51 O 1 2.6996 5.1014 55 O 0 0 0
51 O 2 2.8720 5.4273 33 O 0 0 0 38 O 0 0 0
51 O 1 2.9150 5.5085 48 O 0 0 0

55 O 1 1.6167 3.0551 15 SI 0 0 0
55 O 1 1.6339 3.0876 19 SI 0 0 0
55 O 2 2.6321 4.9739 42 O 0 0 0 45 O 0 0 0
55 O 2 2.6532 5.0139 25 O 0 0 0 30 O 0 0 0
55 O 1 2.6733 5.0519 47 O 0 0 0
55 O 1 2.6996 5.1014 51 O 0 0 0

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM TELAPSE 0.56 TCPU 0.26
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE 0.68 TCPU 0.32

* *
* *
* 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. *

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*
* 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 FE 55.934900  2 FE 55.934900  3 FE 55.934900  4 FE 55.934900
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

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STEP SIZE          0.0030
USE OF RESIDUAL SYMMETRY AFTER DISPLACEMENT

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

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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 1019 RMAX 209.02652 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)= 2470752 F(G)= 399664 P(G),F(G) (IRR) 172555
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT TELAPSE 0.70 TCPU 0.34

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM TELAPSE 1.09 TCPU 0.58

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE 1.15 TCPU 0.64

INFORMATION **** EXCBUF **** EXCH. BIPO BUFFER: WORDS USED = 6609672

DFT PARAMETERS

ATOM	ELECTRONS	NET CHARGE	R(ANGSTROM)
1 26 FE	24.0000	2.0000	0.78000000
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= 196833

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MAKEGRID TELAPSE 43.49 TCPU 33.71

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)

Fe-Cordierite: 4 Fe(2+) in primitive cell, total spin =16 (high-spin state)

CRYSTAL - SCF - TYPE OF CALCULATION : UNRESTRICTED OPEN 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

INFORMATION FROM INTEGRAL EVALUATION

RESTART FROM A PREVIOUS DENSITY MATRIX - DEP ACTIVE

NUMBER OF COUPLE SETS (NEW, OLD, FOUND): 6082 6081 6081

NUMBER OF IRREDUCIBLE G VECTORS : 11466 11466 11462

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SDIK TELAPSE 82.34 TCPU 65.02

CHARGE NORMALIZATION FACTOR 1.00000004

SUMMED SPIN DENSITY 16.00009065

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 83.33 TCPU 65.90

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 706.13 TCPU 572.33

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 726.06 TCPU 587.83

NUMERICALLY INTEGRATED DENSITY 326.0000107467 309.9999228971

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 908.43 TCPU 736.51

CYC 0 ETOT(AU) -1.260077623010E+04 DETOT -1.26E+04 tst 0.00E+00 PX 1.00E+00

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 1763.26 TCPU 1441.84

INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.0000000E+00

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 1835.16 TCPU 1499.63

CHARGE NORMALIZATION FACTOR 1.00000000

SUMMED SPIN DENSITY 16.00000000

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 1836.17 TCPU 1500.51

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 2458.30 TCPU 2008.64

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 2477.03 TCPU 2024.25

NUMERICALLY INTEGRATED DENSITY 325.9999654231 309.9999682240

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 2652.46 TCPU 2171.28

CYC 1 ETOT(AU) -1.260077596159E+04 DETOT 2.69E-04 tst 0.00E+00 PX 4.06E-03

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 2898.14 TCPU 2371.51

INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.0000000E+00

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 2967.76 TCPU 2429.59

CHARGE NORMALIZATION FACTOR 1.00000000

SUMMED SPIN DENSITY 16.00000000

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD TELAPSE 2968.64 TCPU 2430.48

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX TELAPSE 3596.38 TCPU 2941.52

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3 TELAPSE 3614.65 TCPU 2957.00

NUMERICALLY INTEGRATED DENSITY 325.9999654225 309.9999682234

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT TELAPSE 3787.12 TCPU 3102.34

CYC 2 ETOT(AU) -1.260077596335E+04 DETOT -1.77E-06 tst 5.37E-10 PX 1.34E-03

MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 8.294671175641E+02

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK TELAPSE 4037.77 TCPU 3302.33

INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.0000000E+00

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG TELAPSE 4106.76 TCPU 3360.98

CHARGE NORMALIZATION FACTOR 1.00000000

```

SUMMED SPIN DENSITY      16.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD  TELAPSE  4107.70 TCPU  3361.87
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX  TELAPSE  4734.25 TCPU  3870.26
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3  TELAPSE  4753.98 TCPU  3885.83
NUMERICALLY INTEGRATED DENSITY  325.9999654216  309.9999682228
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT  TELAPSE  4941.24 TCPU  4038.02
CYC  3 ETOT(AU) -1.260077596487E+04 DETOT -1.52E-06 tst 4.69E-09 PX 4.13E-03
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 8.871460064837E+02
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK    TELAPSE  5244.62 TCPU  4286.42
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.0000000E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG    TELAPSE  5318.75 TCPU  4347.16
CHARGE NORMALIZATION FACTOR  1.00000000
SUMMED SPIN DENSITY      16.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD  TELAPSE  5319.63 TCPU  4348.04
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX  TELAPSE  5949.33 TCPU  4864.90
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3  TELAPSE  5968.11 TCPU  4880.45
NUMERICALLY INTEGRATED DENSITY  325.9999654213  309.9999682221
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT  TELAPSE  6160.37 TCPU  5033.15
CYC  4 ETOT(AU) -1.260077596466E+04 DETOT 2.09E-07 tst 1.03E-09 PX 8.29E-04
MODIFIED BROYDEN: MIX%= 50 W0= 1.000000000000E-04 W= 5.189535838252E+02
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK    TELAPSE  6419.83 TCPU  5249.24
INSULATING STATE - TOP OF VALENCE BANDS (A.U.) -1.0000000E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG    TELAPSE  6495.07 TCPU  5307.93
CHARGE NORMALIZATION FACTOR  1.00000000
SUMMED SPIN DENSITY      16.00000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD  TELAPSE  6495.95 TCPU  5308.81
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLX  TELAPSE  7121.17 TCPU  5825.41
::: PSEUDO TOTAL ENERGY      -1.1880288479857E+04
::: VIRIAL COEFFICIENT          1.0279687671314E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3  TELAPSE  7138.08 TCPU  5840.93
NUMERICALLY INTEGRATED DENSITY  325.9999654214  309.9999682225
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT  TELAPSE  7327.94 TCPU  5995.28
CYC  5 ETOT(AU) -1.260077596463E+04 DETOT 3.12E-08 tst 9.81E-10 PX 8.29E-04

== SCF ENDED - CONVERGENCE ON ENERGY    E(AU) -1.2600775964630E+04 CYCLES  5

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

TOTAL ENERGY(DFT)(AU)( 5) -1.2600775964630E+04 DE 3.1E-08 tester 9.8E-10
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EDFT    TELAPSE  7327.95 TCPU  5995.29

*****
*                                *
*          FORCE CALCULATION          *
*****

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFG  TELAPSE  7921.90 TCPU  6481.32
INFORMATION **** EXCPOG **** EXCH. BIPO BUFFER LENGTH (WORDS) = 26438688
INFORMATION **** GENPOG **** BIPO BUFFER LENGTH (WORDS) = 2651400
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELXG  TELAPSE  11846.96 TCPU  10264.62

CARTESIAN FORCES (ANALYTICAL)
ATOM      X      Y      Z

```

1	26	2.202427399345E-06	4.163336342344E-14	-2.375877272698E-14
2	26	-2.202427368037E-06	5.218048215738E-14	-1.576516694968E-14
3	26	-2.202427348941E-06	2.486899575160E-14	1.110223024625E-14
4	26	2.202427367370E-06	6.017408793468E-14	2.148281552650E-14
5	13	1.998401444325E-14	-3.042011087473E-14	-3.308841722061E-05
6	13	-1.554312234475E-14	7.882583474839E-15	3.308841718486E-05
7	13	2.264854970235E-14	-1.842970220878E-14	3.308841719729E-05
8	13	-8.160139230995E-15	9.880984919164E-15	-3.308841718686E-05
9	13	-1.788173420492E-05	-9.525331687854E-06	-2.582554803492E-15
10	13	1.788173419603E-05	9.525331687854E-06	-2.270258653339E-15
11	13	-1.788173419648E-05	9.525331705618E-06	-1.601720905691E-15
12	13	1.788173419914E-05	-9.525331709170E-06	-2.073103907246E-15
13	14	-1.805500193797E-14	1.817990202824E-14	-9.992007221626E-15
14	14	-9.478529072737E-15	1.867950238932E-14	-7.771561172376E-16
15	14	-9.442625259481E-06	7.862175253948E-06	-5.922411833151E-16
16	14	9.442625266587E-06	-7.862175263718E-06	-2.434559254856E-15
17	14	-9.442625255929E-06	-7.862175270379E-06	6.644434737531E-15
18	14	9.442625252376E-06	7.862175271711E-06	1.031206327290E-14
19	14	1.805803581689E-05	8.068366010860E-07	-1.779666565381E-14
20	14	-1.805803582400E-05	-8.068366081915E-07	-7.897964615456E-15
21	14	1.805803579558E-05	-8.068366401659E-07	-4.846587618977E-16
22	14	-1.805803579025E-05	8.068366241787E-07	-2.987056324780E-15
23	8	1.123047754348E-05	1.565391154390E-05	9.928072223053E-06
24	8	-1.123047754703E-05	-1.565391156721E-05	9.928072208121E-06
25	8	1.123047754348E-05	-1.565391155345E-05	-9.928072187970E-06
26	8	-1.123047751062E-05	1.565391155345E-05	-9.928072213672E-06
27	8	-1.123047753637E-05	-1.565391157410E-05	-9.928072221888E-06
28	8	1.123047750973E-05	1.565391156677E-05	-9.928072225857E-06
29	8	-1.123047751062E-05	1.565391155744E-05	9.928072216669E-06
30	8	1.123047754170E-05	-1.565391155811E-05	9.928072184862E-06
31	8	5.645356124628E-06	-7.481273412324E-06	4.326418213019E-06
32	8	-5.645356116635E-06	7.481273422982E-06	4.326418219236E-06
33	8	5.645356087824E-06	7.481273410548E-06	-4.326418238332E-06
34	8	-5.645356123574E-06	-7.481273406995E-06	-4.326418227230E-06
35	8	-5.645356102202E-06	7.481273422982E-06	-4.326418235223E-06
36	8	5.645356113193E-06	-7.481273412324E-06	-4.326418227230E-06
37	8	-5.645356120354E-06	-7.481273382126E-06	4.326418240552E-06
38	8	5.645356096262E-06	7.481273391008E-06	4.326418254319E-06
39	8	-5.764883725945E-06	-1.133990416502E-05	8.235679368918E-06
40	8	5.764883732162E-06	1.133990414948E-05	8.235679391233E-06
41	8	-5.764883733939E-06	1.133990412994E-05	-8.235679398561E-06
42	8	5.764883714399E-06	-1.133990415836E-05	-8.235679386903E-06
43	8	5.764883747261E-06	1.133990414592E-05	-8.235679379465E-06
44	8	-5.764883733050E-06	-1.133990417168E-05	-8.235679358370E-06
45	8	5.764883696635E-06	-1.133990413349E-05	8.235679416213E-06
46	8	-5.764883714399E-06	1.133990410018E-05	8.235679425650E-06
47	8	-1.951215985230E-06	-1.123432067196E-05	8.932275113556E-16
48	8	1.951215981677E-06	1.123432067018E-05	2.865882225231E-15
49	8	-1.951216001217E-06	1.123432066485E-05	1.624054638312E-16
50	8	1.951215999441E-06	-1.123432067018E-05	-1.160990039234E-16
51	8	2.447565491082E-05	1.165646530410E-05	-8.785184902342E-16
52	8	-2.447565490904E-05	-1.165646532630E-05	-1.061625268991E-15
53	8	2.447565490016E-05	-1.165646532009E-05	-3.419780052045E-15
54	8	-2.447565490371E-05	1.165646530854E-05	-3.305116153070E-16

47 O DX 1 * 5.6692E-03 -1.260077595426E+04 4 1.0367E-05 2
47 O DY 1 * 5.6692E-03 -1.260077596282E+04 4 1.8089E-06 2
47 O DZ 1 * 5.6692E-03 -1.260077596256E+04 4 2.0681E-06 1
51 O DX 1 * 5.6692E-03 -1.260077595880E+04 4 5.8254E-06 2
51 O DY 1 * 5.6692E-03 -1.260077595854E+04 4 6.0936E-06 2
51 O DZ 1 * 5.6692E-03 -1.260077596261E+04 4 2.0244E-06 1
55 O DX 1 * 5.6692E-03 -1.260077596208E+04 4 2.5496E-06 2
55 O DY 1 * 5.6692E-03 -1.260077595432E+04 4 1.0315E-05 2
55 O DZ 1 * 5.6692E-03 -1.260077596241E+04 4 2.2232E-06 1

GCALCO - MAX INDICES DIRECT LATTICE VECTOR 15 15 14
NO.OF VECTORS CREATED 6999 STARS 1019 RMAX 209.02652 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)= 2470752 F(G)= 399664 P(G),F(G) (IRR) 172555
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 43

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT TELAPSE 1736818.52 TCPU 1729000.94

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 23

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM TELAPSE 1736818.84 TCPU 1729001.19

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE 1736818.90 TCPU 1729001.24

+++ 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

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

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.

```
1 CM*(-1) = 0.2194746E+06 HARTREE
1 THZ    = 0.2997925E-01 CM*(-1)
```

MODES		EIGV	FREQUENCIES		IRREP	IR	INTENS	RAMAN
		(HARTREE**2)	(CM**-1)	(THZ)	(KM/MOL)			
1-	1	-0.1094E-08	-7.2578	-0.2176	(B3U)	A (0.00)	I
2-	2	-0.6461E-09	-5.5787	-0.1672	(B2U)	A (0.00)	I
3-	3	-0.6248E-09	-5.4859	-0.1645	(B1U)	A (0.00)	I
4-	4	0.1032E-06	70.4923	2.1133	(AG)	I (0.00)	A
5-	5	0.2230E-06	103.6443	3.1072	(B3G)	I (0.00)	A
6-	6	0.2304E-06	105.3429	3.1581	(B2G)	I (0.00)	A
7-	7	0.2898E-06	118.1593	3.5423	(B3G)	I (0.00)	A
8-	8	0.2920E-06	118.6015	3.5556	(B1U)	A (0.00)	I
9-	9	0.3127E-06	122.7388	3.6796	(AU)	I (0.00)	I
10-	10	0.3677E-06	133.0892	3.9899	(B1G)	I (0.00)	A
11-	11	0.3720E-06	133.8530	4.0128	(B3G)	I (0.00)	A
12-	12	0.3814E-06	135.5509	4.0637	(B2G)	I (0.00)	A
13-	13	0.3841E-06	136.0226	4.0779	(B3U)	A (0.00)	I
14-	14	0.4305E-06	144.0073	4.3172	(B3U)	A (0.00)	I
15-	15	0.4328E-06	144.3834	4.3285	(B1G)	I (0.00)	A
16-	16	0.4864E-06	153.0618	4.5887	(B1U)	A (0.00)	I
17-	17	0.4906E-06	153.7312	4.6087	(B2G)	I (0.00)	A
18-	18	0.5195E-06	158.1825	4.7422	(B3G)	I (0.00)	A
19-	19	0.5483E-06	162.5180	4.8722	(B3G)	I (0.00)	A
20-	20	0.5673E-06	165.3010	4.9556	(B2U)	A (0.00)	I
21-	21	0.5700E-06	165.7035	4.9677	(B3U)	A (0.00)	I
22-	22	0.5766E-06	166.6530	4.9961	(AG)	I (0.00)	A
23-	23	0.6101E-06	171.4278	5.1393	(B2U)	A (0.00)	I
24-	24	0.6151E-06	172.1242	5.1602	(B3U)	A (0.00)	I
25-	25	0.6167E-06	172.3543	5.1671	(B1G)	I (0.00)	A
26-	26	0.7223E-06	186.5308	5.5921	(B2U)	A (0.00)	I
27-	27	0.7397E-06	188.7611	5.6589	(B1U)	A (0.00)	I

28- 28	0.7878E-06	194.7977	5.8399	(AU)	I (0.00)	I
29- 29	0.7948E-06	195.6692	5.8660	(B1U)	A (0.00)	I
30- 30	0.8438E-06	201.6106	6.0441	(B2G)	I (0.00)	A
31- 31	0.8507E-06	202.4235	6.0685	(B3U)	A (0.00)	I
32- 32	0.8848E-06	206.4417	6.1890	(B3G)	I (0.00)	A
33- 33	0.9032E-06	208.5857	6.2532	(B2G)	I (0.00)	A
34- 34	0.9330E-06	211.9944	6.3554	(B1G)	I (0.00)	A
35- 35	0.9467E-06	213.5509	6.4021	(AU)	I (0.00)	I
36- 36	0.9503E-06	213.9480	6.4140	(B2G)	I (0.00)	A
37- 37	0.9707E-06	216.2314	6.4825	(B1U)	A (0.00)	I
38- 38	0.1064E-05	226.3372	6.7854	(B1G)	I (0.00)	A
39- 39	0.1091E-05	229.2872	6.8739	(AG)	I (0.00)	A
40- 40	0.1124E-05	232.6488	6.9746	(AU)	I (0.00)	I
41- 41	0.1145E-05	234.8967	7.0420	(B1U)	A (0.00)	I
42- 42	0.1188E-05	239.2380	7.1722	(B3G)	I (0.00)	A
43- 43	0.1264E-05	246.7710	7.3980	(AU)	I (0.00)	I
44- 44	0.1280E-05	248.3205	7.4445	(B3G)	I (0.00)	A
45- 45	0.1359E-05	255.8635	7.6706	(B1U)	A (0.00)	I
46- 46	0.1384E-05	258.1838	7.7402	(B2G)	I (0.00)	A
47- 47	0.1385E-05	258.3214	7.7443	(B1G)	I (0.00)	A
48- 48	0.1395E-05	259.1907	7.7703	(B2U)	A (0.00)	I
49- 49	0.1468E-05	265.9237	7.9722	(AG)	I (0.00)	A
50- 50	0.1520E-05	270.5700	8.1115	(AU)	I (0.00)	I
51- 51	0.1523E-05	270.8399	8.1196	(B3U)	A (0.00)	I
52- 52	0.1568E-05	274.8147	8.2387	(B2U)	A (0.00)	I
53- 53	0.1602E-05	277.7820	8.3277	(B3G)	I (0.00)	A
54- 54	0.1761E-05	291.2635	8.7319	(B3U)	A (0.00)	I
55- 55	0.1769E-05	291.9101	8.7512	(B1G)	I (0.00)	A
56- 56	0.1820E-05	296.0870	8.8765	(AG)	I (0.00)	A
57- 57	0.1845E-05	298.0790	8.9362	(B2G)	I (0.00)	A
58- 58	0.1846E-05	298.2172	8.9403	(B1G)	I (0.00)	A
59- 59	0.1857E-05	299.1024	8.9669	(AU)	I (0.00)	I
60- 60	0.1911E-05	303.4037	9.0958	(B2U)	A (0.00)	I
61- 61	0.1950E-05	306.5112	9.1890	(AG)	I (0.00)	A
62- 62	0.2037E-05	313.2403	9.3907	(B1G)	I (0.00)	A
63- 63	0.2078E-05	316.3823	9.4849	(B2U)	A (0.00)	I
64- 64	0.2092E-05	317.4798	9.5178	(B3G)	I (0.00)	A
65- 65	0.2267E-05	330.4602	9.9069	(B2G)	I (0.00)	A
66- 66	0.2276E-05	331.1200	9.9267	(B1U)	A (0.00)	I
67- 67	0.2342E-05	335.8797	10.0694	(AG)	I (0.00)	A
68- 68	0.2382E-05	338.7122	10.1543	(B3G)	I (0.00)	A
69- 69	0.2423E-05	341.6278	10.2417	(B3U)	A (0.00)	I
70- 70	0.2455E-05	343.9053	10.3100	(AG)	I (0.00)	A
71- 71	0.2474E-05	345.2044	10.3490	(B2U)	A (0.00)	I
72- 72	0.2484E-05	345.8928	10.3696	(B2G)	I (0.00)	A
73- 73	0.2569E-05	351.7664	10.5457	(B1G)	I (0.00)	A
74- 74	0.2661E-05	358.0155	10.7330	(B3U)	A (0.00)	I
75- 75	0.2938E-05	376.2070	11.2784	(AU)	I (0.00)	I
76- 76	0.2951E-05	377.0055	11.3023	(B2U)	A (0.00)	I
77- 77	0.2953E-05	377.1484	11.3066	(B3U)	A (0.00)	I
78- 78	0.2978E-05	378.7692	11.3552	(B1U)	A (0.00)	I
79- 79	0.3018E-05	381.2955	11.4310	(AG)	I (0.00)	A
80- 80	0.3376E-05	403.2462	12.0890	(B2G)	I (0.00)	A
81- 81	0.3467E-05	408.6723	12.2517	(B2U)	A (0.00)	I

82-	82	0.3620E-05	417.5955	12.5192	(B2U)	A (0.00)	I
83-	83	0.3782E-05	426.7957	12.7950	(B1G)	I (0.00)	A
84-	84	0.3802E-05	427.9522	12.8297	(B3U)	A (0.00)	I
85-	85	0.3950E-05	436.2161	13.0774	(B3U)	A (0.00)	I
86-	86	0.3957E-05	436.5616	13.0878	(AG)	I (0.00)	A
87-	87	0.4423E-05	461.5804	13.8378	(AU)	I (0.00)	I
88-	88	0.4445E-05	462.7091	13.8717	(B2U)	A (0.00)	I
89-	89	0.4470E-05	464.0440	13.9117	(B1G)	I (0.00)	A
90-	90	0.4653E-05	473.4070	14.1924	(B3G)	I (0.00)	A
91-	91	0.4713E-05	476.4626	14.2840	(B2G)	I (0.00)	A
92-	92	0.4780E-05	479.8656	14.3860	(AU)	I (0.00)	I
93-	93	0.4958E-05	488.7125	14.6512	(B3G)	I (0.00)	A
94-	94	0.4985E-05	490.0286	14.6907	(B1U)	A (0.00)	I
95-	95	0.5019E-05	491.6714	14.7399	(B3U)	A (0.00)	I
96-	96	0.5072E-05	494.2937	14.8186	(AG)	I (0.00)	A
97-	97	0.5155E-05	498.3314	14.9396	(B1G)	I (0.00)	A
98-	98	0.5211E-05	501.0119	15.0200	(B1U)	A (0.00)	I
99-	99	0.5233E-05	502.0545	15.0512	(B3G)	I (0.00)	A
100-	100	0.5327E-05	506.5659	15.1865	(B1U)	A (0.00)	I
101-	101	0.5361E-05	508.1876	15.2351	(B3U)	A (0.00)	I
102-	102	0.5464E-05	513.0459	15.3807	(B2G)	I (0.00)	A
103-	103	0.6011E-05	538.0712	16.1310	(B2U)	A (0.00)	I
104-	104	0.6378E-05	554.2582	16.6162	(AU)	I (0.00)	I
105-	105	0.6603E-05	563.9712	16.9074	(B1G)	I (0.00)	A
106-	106	0.6669E-05	566.7789	16.9916	(AG)	I (0.00)	A
107-	107	0.6804E-05	572.4861	17.1627	(B2U)	A (0.00)	I
108-	108	0.7025E-05	581.7146	17.4394	(B1G)	I (0.00)	A
109-	109	0.7050E-05	582.7550	17.4706	(B3U)	A (0.00)	I
110-	110	0.7114E-05	585.3647	17.5488	(AU)	I (0.00)	I
111-	111	0.7150E-05	586.8646	17.5938	(B1U)	A (0.00)	I
112-	112	0.7383E-05	596.3557	17.8783	(B3U)	A (0.00)	I
113-	113	0.7499E-05	601.0271	18.0183	(B1G)	I (0.00)	A
114-	114	0.7557E-05	603.3458	18.0879	(AG)	I (0.00)	A
115-	115	0.7657E-05	607.2965	18.2063	(B1U)	A (0.00)	I
116-	116	0.7859E-05	615.2574	18.4450	(B3G)	I (0.00)	A
117-	117	0.8292E-05	632.0105	18.9472	(AU)	I (0.00)	I
118-	118	0.8324E-05	633.2301	18.9838	(AG)	I (0.00)	A
119-	119	0.9218E-05	666.3637	19.9771	(B3G)	I (0.00)	A
120-	120	0.9264E-05	668.0074	20.0264	(B3U)	A (0.00)	I
121-	121	0.9460E-05	675.0406	20.2372	(AG)	I (0.00)	A
122-	122	0.9712E-05	683.9874	20.5054	(B2G)	I (0.00)	A
123-	123	0.9981E-05	693.3792	20.7870	(B2U)	A (0.00)	I
124-	124	0.1017E-04	699.9955	20.9853	(B1G)	I (0.00)	A
125-	125	0.1023E-04	701.9296	21.0433	(AU)	I (0.00)	I
126-	126	0.1031E-04	704.8068	21.1296	(B1U)	A (0.00)	I
127-	127	0.1042E-04	708.4184	21.2378	(B2U)	A (0.00)	I
128-	128	0.1061E-04	714.8734	21.4314	(AG)	I (0.00)	A
129-	129	0.1114E-04	732.6340	21.9638	(B1G)	I (0.00)	A
130-	130	0.1149E-04	743.9264	22.3024	(B3G)	I (0.00)	A
131-	131	0.1150E-04	744.1759	22.3098	(AG)	I (0.00)	A
132-	132	0.1171E-04	751.1454	22.5188	(B2G)	I (0.00)	A
133-	133	0.1185E-04	755.4451	22.6477	(B3U)	A (0.00)	I
134-	134	0.1188E-04	756.3146	22.6737	(B1G)	I (0.00)	A
135-	135	0.1212E-04	764.0901	22.9068	(B2U)	A (0.00)	I

[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]

MODE	FRQ(CM**-1)	IRREP	TYP	A	B	LONG	C	ANG	PEC
1	-7.2578	(B3U)							
2	-5.5787	(B2U)							
3	-5.4859	(B1U)							
4	70.4923	(AG)							
	(?)	51 O	9 AL(0.0)	48 O (1.0)		0.0			
	(?)	10 AL	52 O (0.0)	16 SI(1.0)		0.0			
	(?)	11 AL	53 O (0.0)	17 SI(1.0)		0.0			
	(?)	12 AL	54 O (0.0)	18 SI(1.0)		0.0			
5	103.6443	(B3G)							
	(B)	32 O	1 FE(0.2)	25 O (0.8)		0.0			
	(B)	34 O	1 FE(0.2)	23 O (0.8)		0.0			
	(B)	31 O	2 FE(0.2)	26 O (0.8)		0.0			
	(B)	33 O	2 FE(0.2)	24 O (0.8)		0.0			
	(B)	36 O	3 FE(0.2)	29 O (0.8)		0.0			
	(B)	38 O	3 FE(0.2)	27 O (0.8)		0.0			
	(B)	35 O	4 FE(0.2)	30 O (0.8)		0.0			
	(B)	37 O	4 FE(0.2)	28 O (0.8)		0.0			
6	105.3429	(B2G)							
	(B)	5 AL	1 FE(0.0)	6 AL(1.0)		0.0			
	(B)	6 AL	1 FE(0.0)	5 AL(1.0)		0.0			
	(B)	5 AL	2 FE(0.0)	6 AL(1.0)		0.0			
	(B)	6 AL	2 FE(0.0)	5 AL(1.0)		0.0			
	(B)	7 AL	3 FE(0.0)	8 AL(1.0)		0.0			
	(B)	8 AL	3 FE(0.0)	7 AL(1.0)		0.0			
	(B)	7 AL	4 FE(0.0)	8 AL(1.0)		0.0			
	(B)	8 AL	4 FE(0.0)	7 AL(1.0)		0.0			
7	118.1593	(B3G)							
	(B)	5 AL	1 FE(0.0)	25 O (1.0)		0.0			
	(B)	6 AL	1 FE(0.0)	23 O (1.0)		0.0			
	(B)	5 AL	2 FE(0.0)	26 O (1.0)		0.0			
	(B)	6 AL	2 FE(0.0)	24 O (1.0)		0.0			
	(B)	7 AL	3 FE(0.0)	29 O (1.0)		0.0			
	(B)	8 AL	3 FE(0.0)	27 O (1.0)		0.0			
	(B)	7 AL	4 FE(0.0)	30 O (1.0)		0.0			
	(B)	8 AL	4 FE(0.0)	28 O (1.0)		0.0			
8	118.6015	(B1U)							
	(O)	32 O	1 FE(0.0)	39 O (0.5)		0.0			
	(O)	34 O	1 FE(0.0)	41 O (0.5)		0.0			
	(O)	31 O	2 FE(0.0)	40 O (0.5)		0.0			
	(O)	33 O	2 FE(0.0)	42 O (0.5)		0.0			
	(O)	36 O	3 FE(0.0)	43 O (0.5)		0.0			
	(O)	38 O	3 FE(0.0)	45 O (0.5)		0.0			
	(O)	35 O	4 FE(0.0)	44 O (0.5)		0.0			
	(O)	37 O	4 FE(0.0)	46 O (0.5)		0.0			
	(O)	48 O	9 AL(0.0)	38 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)	36 O (0.7)		0.0			
	(O)	49 O	12 AL(0.0)	32 O (0.7)		0.0			
9	122.7388	(AU)							
	(O)	5 AL	1 FE(0.0)	25 O (0.6)		0.0			
	(O)	6 AL	1 FE(0.0)	23 O (0.6)		0.0			
	(O)	39 O	1 FE(0.0)	23 O (0.5)		0.0			
	(O)	41 O	1 FE(0.0)	25 O (0.5)		0.0			

	(O)	5 AL	2 FE(0.0)	26 O (0.6)	0.0
	(O)	6 AL	2 FE(0.0)	24 O (0.6)	0.0
	(O)	40 O	2 FE(0.0)	24 O (0.5)	-0.1
	(O)	42 O	2 FE(0.0)	26 O (0.5)	0.0
	(O)	3 FE	7 AL(0.0)	29 O (0.6)	0.0
	(O)	8 AL	3 FE(0.0)	27 O (0.6)	0.0
	(O)	43 O	3 FE(0.0)	27 O (0.5)	0.0
	(O)	45 O	3 FE(0.0)	29 O (0.5)	0.0
	(O)	7 AL	4 FE(0.0)	30 O (0.6)	0.0
	(O)	8 AL	4 FE(0.0)	28 O (0.6)	0.0
	(O)	44 O	4 FE(0.0)	28 O (0.5)	0.0
	(O)	46 O	4 FE(0.0)	30 O (0.5)	0.0
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	46 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)	44 O (0.7)	0.0
10	133.0892 (B1G)				
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0
	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
11	133.8530 (B3G)				
	(B)	23 O	1 FE(0.1)	32 O (0.9)	0.0
	(B)	25 O	1 FE(0.1)	34 O (0.9)	0.0
	(B)	24 O	2 FE(0.1)	31 O (0.9)	0.0
	(B)	26 O	2 FE(0.1)	33 O (0.9)	0.0
	(B)	27 O	3 FE(0.1)	36 O (0.9)	0.0
	(B)	29 O	3 FE(0.1)	38 O (0.9)	0.0
	(B)	28 O	4 FE(0.1)	35 O (0.9)	0.0
	(B)	30 O	4 FE(0.1)	37 O (0.9)	0.0
12	135.5509 (B2G)				
	(B)	39 O	1 FE(0.0)	34 O (0.9)	0.0
	(B)	41 O	1 FE(0.0)	32 O (0.9)	0.0
	(B)	40 O	2 FE(0.0)	33 O (0.9)	0.0
	(B)	42 O	2 FE(0.0)	31 O (0.9)	0.0
	(B)	43 O	3 FE(0.0)	38 O (0.9)	0.0
	(B)	45 O	3 FE(0.0)	36 O (0.9)	0.0
	(B)	44 O	4 FE(0.0)	37 O (0.9)	0.0
	(B)	46 O	4 FE(0.0)	35 O (0.9)	0.0
	(O)	33 O	9 AL(0.0)	48 O (0.8)	0.0
	(O)	38 O	9 AL(0.0)	48 O (0.8)	0.0
	(O)	51 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	34 O	10 AL(0.0)	47 O (0.8)	0.0
	(O)	37 O	10 AL(0.0)	47 O (0.8)	0.0
	(O)	52 O	10 AL(0.0)	37 O (0.7)	0.0
	(O)	31 O	11 AL(0.0)	50 O (0.8)	0.0
	(O)	36 O	11 AL(0.0)	50 O (0.8)	0.0
	(O)	53 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	32 O	12 AL(0.0)	49 O (0.8)	0.0
	(O)	35 O	12 AL(0.0)	49 O (0.8)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
	(B)	25 O	15 SI(0.0)	30 O (0.9)	0.0
	(B)	30 O	15 SI(0.0)	25 O (0.9)	0.0
	(B)	26 O	16 SI(0.0)	29 O (0.9)	0.0

	(B)	29 O	16 SI(0.0)	26 O (0.9)	0.0
	(B)	23 O	17 SI(0.0)	28 O (0.9)	0.0
	(B)	28 O	17 SI(0.0)	23 O (0.9)	0.0
	(B)	24 O	18 SI(0.0)	27 O (0.9)	0.0
	(B)	27 O	18 SI(0.0)	24 O (0.9)	0.0
13	136.0226	(B3U)			
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
	(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
	(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0
14	144.0073	(B3U)			
	(O)	1 FE	5 AL(0.0)	26 O (0.8)	0.0
	(O)	1 FE	6 AL(0.0)	24 O (0.8)	0.0
	(O)	23 O	1 FE(0.1)	32 O (0.6)	0.0
	(O)	25 O	1 FE(0.1)	34 O (0.6)	0.0
	(O)	39 O	1 FE(0.0)	23 O (0.6)	0.0
	(O)	41 O	1 FE(0.0)	25 O (0.6)	0.0
	(O)	2 FE	5 AL(0.0)	25 O (0.8)	0.0
	(O)	2 FE	6 AL(0.0)	23 O (0.8)	0.0
	(O)	24 O	2 FE(0.1)	31 O (0.6)	0.0
	(O)	26 O	2 FE(0.1)	33 O (0.6)	0.0
	(O)	40 O	2 FE(0.0)	24 O (0.6)	-0.1
	(O)	42 O	2 FE(0.0)	26 O (0.6)	0.0
	(O)	3 FE	7 AL(0.0)	30 O (0.8)	0.0
	(O)	3 FE	8 AL(0.0)	28 O (0.8)	0.0
	(O)	27 O	3 FE(0.1)	36 O (0.6)	0.0
	(O)	29 O	3 FE(0.1)	38 O (0.6)	0.0
	(O)	43 O	3 FE(0.0)	27 O (0.6)	0.0
	(O)	45 O	3 FE(0.0)	29 O (0.6)	0.0
	(O)	4 FE	7 AL(0.0)	29 O (0.8)	0.0
	(O)	4 FE	8 AL(0.0)	27 O (0.8)	0.0
	(O)	28 O	4 FE(0.1)	35 O (0.6)	0.0
	(O)	30 O	4 FE(0.1)	37 O (0.6)	0.0
	(O)	44 O	4 FE(0.0)	28 O (0.6)	0.0
	(O)	46 O	4 FE(0.0)	30 O (0.6)	0.0
15	144.3834	(B1G)			
	(O)	1 FE	5 AL(0.0)	26 O (0.6)	0.0
	(O)	1 FE	6 AL(0.0)	24 O (0.6)	0.0
	(O)	2 FE	5 AL(0.0)	25 O (0.6)	0.0
	(O)	2 FE	6 AL(0.0)	23 O (0.6)	0.0
	(O)	3 FE	7 AL(0.0)	30 O (0.6)	0.0
	(O)	3 FE	8 AL(0.0)	28 O (0.6)	0.0
	(O)	4 FE	7 AL(0.0)	29 O (0.6)	0.0
	(O)	4 FE	8 AL(0.0)	27 O (0.6)	0.0
16	153.0618	(B1U)			
	(O)	1 FE	5 AL(0.0)	26 O (0.6)	0.0
	(O)	1 FE	6 AL(0.0)	24 O (0.6)	0.0
	(O)	1 FE	32 O (0.2)	12 AL(0.6)	0.0
	(O)	1 FE	34 O (0.2)	10 AL(0.6)	0.0
	(O)	2 FE	5 AL(0.0)	25 O (0.6)	0.0
	(O)	2 FE	6 AL(0.0)	23 O (0.6)	0.0
	(O)	2 FE	31 O (0.2)	11 AL(0.6)	0.0
	(O)	2 FE	33 O (0.2)	9 AL(0.6)	0.0
	(O)	3 FE	7 AL(0.0)	30 O (0.6)	0.0

	(O)	3 FE	8 AL(0.0)	28 O (0.6)	0.0
	(O)	3 FE	36 O (0.2)	11 AL(0.6)	0.0
	(O)	3 FE	38 O (0.2)	9 AL(0.6)	0.0
	(O)	4 FE	7 AL(0.0)	29 O (0.6)	0.0
	(O)	4 FE	8 AL(0.0)	27 O (0.6)	0.0
	(O)	4 FE	35 O (0.2)	12 AL(0.6)	0.0
	(O)	4 FE	37 O (0.2)	10 AL(0.6)	0.0
17	153.7312	(B2G)			
	(B)	32 O	1 FE(0.0)	39 O (0.9)	0.0
	(B)	34 O	1 FE(0.0)	41 O (0.9)	0.0
	(B)	31 O	2 FE(0.0)	40 O (0.9)	0.0
	(B)	33 O	2 FE(0.0)	42 O (0.9)	0.0
	(B)	36 O	3 FE(0.0)	43 O (0.9)	0.0
	(B)	38 O	3 FE(0.0)	45 O (0.9)	0.0
	(B)	35 O	4 FE(0.0)	44 O (0.9)	0.0
	(B)	37 O	4 FE(0.0)	46 O (0.9)	0.0
	(O)	33 O	9 AL(0.0)	38 O (0.8)	0.0
	(O)	38 O	9 AL(0.0)	33 O (0.8)	0.0
	(O)	34 O	10 AL(0.0)	37 O (0.8)	0.0
	(O)	37 O	10 AL(0.0)	34 O (0.8)	0.0
	(O)	31 O	11 AL(0.0)	36 O (0.8)	0.0
	(O)	36 O	11 AL(0.0)	31 O (0.8)	0.0
	(O)	32 O	12 AL(0.0)	35 O (0.8)	0.0
	(O)	35 O	12 AL(0.0)	32 O (0.8)	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
18	158.1825	(B3G)			
	(B)	39 O	1 FE(0.1)	23 O (0.9)	0.0
	(B)	41 O	1 FE(0.1)	25 O (0.9)	0.0
	(B)	40 O	2 FE(0.1)	24 O (0.9)	-0.1
	(B)	42 O	2 FE(0.1)	26 O (0.9)	0.0
	(B)	43 O	3 FE(0.1)	27 O (0.9)	0.0
	(B)	45 O	3 FE(0.1)	29 O (0.9)	0.0
	(B)	44 O	4 FE(0.1)	28 O (0.9)	0.0
	(B)	46 O	4 FE(0.1)	30 O (0.9)	0.0
19	162.5180	(B3G)			
	(O)	23 O	1 FE(0.2)	32 O (0.7)	0.0
	(O)	25 O	1 FE(0.2)	34 O (0.7)	0.0
	(B)	32 O	1 FE(0.0)	39 O (0.9)	0.0
	(B)	34 O	1 FE(0.0)	41 O (0.9)	0.0
	(S)	39 O	1 FE(0.6)	23 O (0.4)	0.0
	(S)	41 O	1 FE(0.6)	25 O (0.4)	0.0
	(O)	24 O	2 FE(0.2)	31 O (0.7)	0.0
	(O)	26 O	2 FE(0.2)	33 O (0.7)	0.0
	(B)	31 O	2 FE(0.0)	40 O (0.9)	0.0
	(B)	33 O	2 FE(0.0)	42 O (0.9)	0.0
	(S)	40 O	2 FE(0.6)	24 O (0.4)	0.0
	(S)	42 O	2 FE(0.6)	26 O (0.4)	0.0

	(O)	27 O	3 FE(0.2)	36 O (0.7)	0.0
	(O)	29 O	3 FE(0.2)	38 O (0.7)	0.0
	(B)	36 O	3 FE(0.0)	43 O (0.9)	0.0
	(B)	38 O	3 FE(0.0)	45 O (0.9)	0.0
	(S)	43 O	3 FE(0.6)	27 O (0.4)	0.0
	(S)	45 O	3 FE(0.6)	29 O (0.4)	0.0
	(O)	28 O	4 FE(0.2)	35 O (0.7)	0.0
	(O)	30 O	4 FE(0.2)	37 O (0.7)	0.0
	(B)	35 O	4 FE(0.0)	44 O (0.9)	0.0
	(B)	37 O	4 FE(0.0)	46 O (0.9)	0.0
	(S)	44 O	4 FE(0.6)	28 O (0.4)	0.0
	(S)	46 O	4 FE(0.6)	30 O (0.4)	0.0
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	46 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)	44 O (0.7)	0.0
20	165.3010 (B2U)				
	(B)	5 AL	1 FE(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	1 FE(0.0)	5 AL(1.0)	0.0
	(B)	5 AL	2 FE(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	2 FE(0.0)	5 AL(1.0)	0.0
	(B)	7 AL	3 FE(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	3 FE(0.0)	7 AL(1.0)	0.0
	(B)	7 AL	4 FE(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	4 FE(0.0)	7 AL(1.0)	0.0
21	165.7035 (B3U)				
	(B)	32 O	1 FE(0.0)	5 AL(0.9)	0.0
	(B)	34 O	1 FE(0.0)	6 AL(0.9)	0.0
	(B)	31 O	2 FE(0.0)	5 AL(0.9)	0.0
	(B)	33 O	2 FE(0.0)	6 AL(0.9)	0.0
	(B)	36 O	3 FE(0.0)	7 AL(0.9)	0.0
	(B)	38 O	3 FE(0.0)	8 AL(0.9)	0.0
	(B)	35 O	4 FE(0.0)	7 AL(0.9)	0.0
	(B)	37 O	4 FE(0.0)	8 AL(0.9)	0.0
22	166.6530 (AG)				
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0
	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
	(B)	55 O	19 SI(0.0)	47 O (1.0)	0.0
	(B)	56 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	57 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	58 O	22 SI(0.0)	50 O (1.0)	0.0
23	171.4278 (B2U)				
	(B)	39 O	1 FE(0.3)	34 O (0.7)	0.0
	(B)	41 O	1 FE(0.3)	32 O (0.7)	0.0
	(B)	40 O	2 FE(0.3)	33 O (0.7)	0.0
	(B)	42 O	2 FE(0.3)	31 O (0.7)	0.0
	(B)	43 O	3 FE(0.3)	38 O (0.7)	0.0
	(B)	45 O	3 FE(0.3)	36 O (0.7)	0.0
	(B)	44 O	4 FE(0.3)	37 O (0.7)	0.0
	(B)	46 O	4 FE(0.3)	35 O (0.7)	0.0
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0

	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
24	172.1242 (B3U)				
	(B)	32 O	1 FE(0.1)	5 AL(0.8)	0.0
	(B)	34 O	1 FE(0.1)	6 AL(0.8)	0.0
	(B)	31 O	2 FE(0.1)	5 AL(0.8)	0.0
	(B)	33 O	2 FE(0.1)	6 AL(0.8)	0.0
	(B)	36 O	3 FE(0.1)	7 AL(0.8)	0.0
	(B)	38 O	3 FE(0.1)	8 AL(0.8)	0.0
	(B)	35 O	4 FE(0.1)	7 AL(0.8)	0.0
	(B)	37 O	4 FE(0.1)	8 AL(0.8)	0.0
25	172.3543 (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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0
26	186.5308 (B2U)				
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
	(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
	(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0
	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
	(B)	19 SI	47 O (0.0)	10 AL(1.0)	0.0
	(B)	55 O	19 SI(0.0)	47 O (1.0)	0.0
	(B)	48 O	20 SI(0.0)	56 O (1.0)	0.0
	(B)	56 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	21 SI	49 O (0.0)	12 AL(1.0)	0.0
	(B)	57 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	22 SI	50 O (0.0)	11 AL(1.0)	0.0
	(B)	58 O	22 SI(0.0)	50 O (1.0)	0.0
27	188.7611 (B1U)				
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	29 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)	27 O (0.7)	0.0
28	194.7977 (AU)				
	(O)	51 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	37 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
29	195.6692 (B1U)				
	(B)	23 O	1 FE(0.0)	32 O (1.0)	0.0
	(B)	25 O	1 FE(0.0)	34 O (1.0)	0.0
	(O)	39 O	1 FE(0.2)	23 O (0.6)	0.0
	(O)	41 O	1 FE(0.2)	25 O (0.6)	0.0
	(B)	24 O	2 FE(0.0)	31 O (1.0)	0.0
	(B)	26 O	2 FE(0.0)	33 O (1.0)	0.0
	(O)	40 O	2 FE(0.2)	24 O (0.6)	-0.1
	(O)	42 O	2 FE(0.2)	26 O (0.6)	0.0
	(B)	27 O	3 FE(0.0)	36 O (1.0)	0.0
	(B)	29 O	3 FE(0.0)	38 O (1.0)	0.0

	(O)	43 O	3 FE(0.2)	27 O (0.6)	0.0
	(O)	45 O	3 FE(0.2)	29 O (0.6)	0.0
	(B)	28 O	4 FE(0.0)	35 O (1.0)	0.0
	(B)	30 O	4 FE(0.0)	37 O (1.0)	0.0
	(O)	44 O	4 FE(0.2)	28 O (0.6)	0.0
	(O)	46 O	4 FE(0.2)	30 O (0.6)	0.0
30		201.6106 (B2G)			
	(O)	39 O	1 FE(0.0)	23 O (0.8)	0.0
	(O)	41 O	1 FE(0.0)	25 O (0.8)	0.0
	(O)	40 O	2 FE(0.0)	24 O (0.8)	-0.1
	(O)	42 O	2 FE(0.0)	26 O (0.8)	0.0
	(O)	43 O	3 FE(0.0)	27 O (0.8)	0.0
	(O)	45 O	3 FE(0.0)	29 O (0.8)	0.0
	(O)	44 O	4 FE(0.0)	28 O (0.8)	0.0
	(O)	46 O	4 FE(0.0)	30 O (0.8)	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)	0.1
	(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
31		202.4235 (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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0
32		206.4417 (B3G)			
	(O)	51 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	37 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
33		208.5857 (B2G)			
	(O)	47 O	19 SI(0.0)	45 O (0.8)	-0.1
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	48 O	20 SI(0.0)	46 O (0.8)	0.0
	(O)	56 O	20 SI(0.0)	46 O (0.7)	0.0
	(O)	49 O	21 SI(0.0)	40 O (0.8)	0.0
	(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)	44 O (0.7)	0.0
34		211.9944 (B1G)			
	(S)	5 AL	1 FE(0.7)	32 O (0.3)	0.0
	(S)	6 AL	1 FE(0.7)	34 O (0.3)	0.0
	(B)	23 O	1 FE(0.0)	5 AL(0.9)	0.0
	(B)	25 O	1 FE(0.0)	6 AL(0.9)	0.0
	(S)	39 O	1 FE(1.0)		0.0
	(S)	41 O	1 FE(1.0)		0.0
	(S)	5 AL	2 FE(0.7)	31 O (0.3)	0.0
	(S)	6 AL	2 FE(0.7)	33 O (0.3)	0.0
	(B)	24 O	2 FE(0.0)	5 AL(0.9)	0.0
	(B)	26 O	2 FE(0.0)	6 AL(0.9)	0.0
	(S)	40 O	2 FE(1.0)		0.0

	(S)	42 O	2 FE(1.0)	0.0
	(S)	7 AL	3 FE(0.7) 36 O (0.3)	0.0
	(S)	8 AL	3 FE(0.7) 38 O (0.3)	0.0
	(B)	27 O	3 FE(0.0) 7 AL(0.9)	0.0
	(B)	29 O	3 FE(0.0) 8 AL(0.9)	0.0
	(S)	43 O	3 FE(1.0)	0.0
	(S)	45 O	3 FE(1.0)	0.0
	(S)	7 AL	4 FE(0.7) 35 O (0.3)	0.0
	(S)	8 AL	4 FE(0.7) 37 O (0.3)	0.0
	(B)	28 O	4 FE(0.0) 7 AL(0.9)	0.0
	(B)	30 O	4 FE(0.0) 8 AL(0.9)	0.0
	(S)	44 O	4 FE(1.0)	0.0
	(S)	46 O	4 FE(1.0)	0.0
35	213.5509 (AU)			
	(O)	55 O	15 SI(0.0) 25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0) 29 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) 27 O (0.7)	0.0
36	213.9480 (B2G)			
	(O)	51 O	9 AL(0.0) 38 O (0.7)	0.0
	(O)	52 O	10 AL(0.0) 37 O (0.7)	0.0
	(O)	53 O	11 AL(0.0) 36 O (0.7)	0.0
	(O)	54 O	12 AL(0.0) 32 O (0.7)	0.0
	(O)	51 O	15 SI(0.0) 25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0) 29 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
37	216.2314 (B1U)			
	(O)	51 O	9 AL(0.0) 38 O (0.7)	0.0
	(O)	52 O	10 AL(0.0) 37 O (0.7)	0.0
	(O)	53 O	11 AL(0.0) 36 O (0.7)	0.0
	(O)	54 O	12 AL(0.0) 32 O (0.7)	0.0
38	226.3372 (B1G)			
	(S)	23 O	1 FE(0.7) 5 AL(0.3)	0.0
	(S)	25 O	1 FE(0.7) 6 AL(0.3)	0.0
	(S)	24 O	2 FE(0.7) 5 AL(0.3)	0.0
	(S)	26 O	2 FE(0.7) 6 AL(0.3)	0.0
	(S)	27 O	3 FE(0.7) 7 AL(0.3)	0.0
	(S)	29 O	3 FE(0.7) 8 AL(0.3)	0.0
	(S)	28 O	4 FE(0.7) 7 AL(0.3)	0.0
	(S)	30 O	4 FE(0.7) 8 AL(0.3)	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)	17 SI	53 O (0.0) 11 AL(1.0)	0.0
	(B)	18 SI	54 O (0.0) 12 AL(1.0)	0.0
39	229.2872 (AG)			
	(B)	5 AL	1 FE(0.2) 32 O (0.7)	0.0
	(B)	6 AL	1 FE(0.2) 34 O (0.7)	0.0
	(B)	39 O	1 FE(0.0) 41 O (1.0)	0.0
	(B)	41 O	1 FE(0.0) 39 O (1.0)	0.0
	(B)	5 AL	2 FE(0.2) 31 O (0.7)	0.0
	(B)	6 AL	2 FE(0.2) 33 O (0.7)	0.0
	(B)	40 O	2 FE(0.0) 42 O (1.0)	0.0
	(B)	42 O	2 FE(0.0) 40 O (1.0)	0.0

	(B)	7 AL	3 FE(0.2)	36 O (0.7)	0.0
	(B)	8 AL	3 FE(0.2)	38 O (0.7)	0.0
	(B)	43 O	3 FE(0.0)	45 O (1.0)	0.0
	(B)	45 O	3 FE(0.0)	43 O (1.0)	0.0
	(B)	7 AL	4 FE(0.2)	35 O (0.7)	0.0
	(B)	8 AL	4 FE(0.2)	37 O (0.7)	0.0
	(B)	44 O	4 FE(0.0)	46 O (1.0)	0.0
	(B)	46 O	4 FE(0.0)	44 O (1.0)	0.0
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
	(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
	(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0
40	232.6488 (AU)				
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	29 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
41	234.8967 (B1U)				
	(B)	23 O	1 FE(0.2)	34 O (0.8)	0.0
	(B)	25 O	1 FE(0.2)	32 O (0.8)	0.0
	(B)	24 O	2 FE(0.2)	33 O (0.8)	0.0
	(B)	26 O	2 FE(0.2)	31 O (0.8)	0.0
	(B)	27 O	3 FE(0.2)	38 O (0.8)	0.0
	(B)	29 O	3 FE(0.2)	36 O (0.8)	0.0
	(B)	28 O	4 FE(0.2)	37 O (0.8)	0.0
	(B)	30 O	4 FE(0.2)	35 O (0.8)	0.0
42	239.2380 (B3G)				
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	29 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
43	246.7710 (AU)				
	(B)	39 O	1 FE(0.0)	34 O (0.9)	0.0
	(B)	41 O	1 FE(0.0)	32 O (0.9)	-0.1
	(B)	40 O	2 FE(0.0)	33 O (0.9)	-0.1
	(B)	42 O	2 FE(0.0)	31 O (0.9)	0.0
	(B)	43 O	3 FE(0.0)	38 O (0.9)	0.0
	(B)	45 O	3 FE(0.0)	36 O (0.9)	0.0
	(B)	44 O	4 FE(0.0)	37 O (0.9)	0.0
	(B)	46 O	4 FE(0.0)	35 O (0.9)	0.0
44	248.3205 (B3G)				
	(O)	39 O	1 FE(0.0)	23 O (0.8)	0.0
	(O)	41 O	1 FE(0.0)	25 O (0.8)	0.0
	(O)	40 O	2 FE(0.0)	24 O (0.8)	-0.1
	(O)	42 O	2 FE(0.0)	26 O (0.8)	0.0
	(O)	43 O	3 FE(0.0)	27 O (0.8)	0.0
	(O)	45 O	3 FE(0.0)	29 O (0.8)	0.0
	(O)	44 O	4 FE(0.0)	28 O (0.8)	0.0
	(O)	46 O	4 FE(0.0)	30 O (0.8)	0.0
45	255.8635 (B1U)				
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	46 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)	44 O (0.7)	0.0

46 258.1838 (B2G)

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

47 258.3214 (B1G)

(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0

48 259.1907 (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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0

49 265.9237 (AG)

(B)	55 O	19 SI(0.0)	47 O (1.0)	0.0
(B)	56 O	20 SI(0.0)	48 O (1.0)	0.0
(B)	57 O	21 SI(0.0)	49 O (1.0)	0.0
(B)	58 O	22 SI(0.0)	50 O (1.0)	0.0

50 270.5700 (AU)

(B)	23 O	1 FE(0.0)	32 O (0.9)	0.0
(B)	25 O	1 FE(0.0)	34 O (0.9)	0.0
(B)	24 O	2 FE(0.0)	31 O (0.9)	0.0
(B)	26 O	2 FE(0.0)	33 O (0.9)	0.0
(B)	27 O	3 FE(0.0)	36 O (0.9)	0.0
(B)	29 O	3 FE(0.0)	38 O (0.9)	0.0
(B)	28 O	4 FE(0.0)	35 O (0.9)	0.0
(B)	30 O	4 FE(0.0)	37 O (0.9)	0.0

51 270.8399 (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)	50 O	11 AL(0.0)	53 O (1.0)	0.0
(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0
(B)	19 SI	47 O (0.0)	10 AL(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

52 274.8147 (B2U)

(B)	32 O	1 FE(0.0)	39 O (1.0)	0.0
(B)	34 O	1 FE(0.0)	41 O (1.0)	0.0
(B)	31 O	2 FE(0.0)	40 O (1.0)	0.0
(B)	33 O	2 FE(0.0)	42 O (1.0)	0.0
(B)	36 O	3 FE(0.0)	43 O (1.0)	0.0
(B)	38 O	3 FE(0.0)	45 O (1.0)	0.0
(B)	35 O	4 FE(0.0)	44 O (1.0)	0.0
(B)	37 O	4 FE(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
53	277.7820	(B3G)			
	(O)	51 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	52 O	10 AL(0.0)	37 O (0.7)	0.0
	(O)	53 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	54 O	12 AL(0.0)	32 O (0.7)	0.0
54	291.2635	(B3U)			
	(S)	5 AL	1 FE(1.0)		0.0
	(S)	6 AL	1 FE(1.0)		0.0
	(B)	23 O	1 FE(0.5)	39 O (0.5)	0.0
	(B)	25 O	1 FE(0.5)	41 O (0.5)	0.0
	(S)	1 FE	39 O (0.7)	22 SI(0.3)	0.0
	(S)	1 FE	41 O (0.7)	20 SI(0.3)	0.0
	(S)	5 AL	2 FE(1.0)		0.0
	(S)	6 AL	2 FE(1.0)		0.0
	(B)	24 O	2 FE(0.5)	40 O (0.5)	0.0
	(B)	26 O	2 FE(0.5)	42 O (0.5)	0.0
	(S)	2 FE	40 O (0.7)	21 SI(0.3)	0.0
	(S)	2 FE	42 O (0.7)	19 SI(0.3)	0.0
	(S)	7 AL	3 FE(1.0)		0.0
	(S)	8 AL	3 FE(1.0)		0.0
	(B)	27 O	3 FE(0.5)	43 O (0.5)	0.0
	(B)	29 O	3 FE(0.5)	45 O (0.5)	0.0
	(S)	3 FE	43 O (0.7)	21 SI(0.3)	0.0
	(S)	3 FE	45 O (0.7)	19 SI(0.3)	0.0
	(S)	7 AL	4 FE(1.0)		0.0
	(S)	8 AL	4 FE(1.0)		0.0
	(B)	28 O	4 FE(0.5)	44 O (0.5)	0.0
	(B)	30 O	4 FE(0.5)	46 O (0.5)	0.0
	(S)	4 FE	44 O (0.7)	22 SI(0.3)	0.0
	(S)	4 FE	46 O (0.7)	20 SI(0.3)	0.0
55	291.9101	(B1G)			
	(B)	32 O	1 FE(0.1)	39 O (0.8)	0.0
	(B)	34 O	1 FE(0.1)	41 O (0.8)	0.0
	(B)	31 O	2 FE(0.1)	40 O (0.8)	0.0
	(B)	33 O	2 FE(0.1)	42 O (0.8)	0.0
	(B)	36 O	3 FE(0.1)	43 O (0.8)	0.0
	(B)	38 O	3 FE(0.1)	45 O (0.8)	0.0
	(B)	35 O	4 FE(0.1)	44 O (0.8)	0.0
	(B)	37 O	4 FE(0.1)	46 O (0.8)	0.0
56	296.0870	(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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0
57	298.0790	(B2G)			
	(B)	5 AL	1 FE(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	1 FE(0.0)	5 AL(1.0)	0.0
	(B)	5 AL	2 FE(0.0)	6 AL(1.0)	0.0
	(B)	6 AL	2 FE(0.0)	5 AL(1.0)	0.0

	(B)	7 AL	3 FE(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	3 FE(0.0)	7 AL(1.0)	0.0
	(B)	7 AL	4 FE(0.0)	8 AL(1.0)	0.0
	(B)	8 AL	4 FE(0.0)	7 AL(1.0)	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)	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)	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)	45 O	8 AL(0.0)	28 O (1.0)	0.0
	(B)	46 O	8 AL(0.0)	27 O (1.0)	0.0
58	298.2172 (B1G)				
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0
	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
	(B)	55 O	19 SI(0.0)	47 O (1.0)	0.0
	(B)	56 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	57 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	58 O	22 SI(0.0)	50 O (1.0)	0.0
59	299.1024 (AU)				
	(B)	32 O	1 FE(0.0)	39 O (0.9)	0.0
	(B)	34 O	1 FE(0.0)	41 O (0.9)	0.0
	(B)	31 O	2 FE(0.0)	40 O (0.9)	0.0
	(B)	33 O	2 FE(0.0)	42 O (0.9)	0.0
	(B)	36 O	3 FE(0.0)	43 O (0.9)	0.0
	(B)	38 O	3 FE(0.0)	45 O (0.9)	0.0
	(B)	35 O	4 FE(0.0)	44 O (0.9)	0.0
	(B)	37 O	4 FE(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
60	303.4037 (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
61	306.5112 (AG)				
	(B)	23 O	1 FE(0.2)	32 O (0.7)	0.0
	(B)	25 O	1 FE(0.2)	34 O (0.7)	0.0
	(B)	24 O	2 FE(0.2)	31 O (0.7)	0.0
	(B)	26 O	2 FE(0.2)	33 O (0.7)	0.0
	(B)	27 O	3 FE(0.2)	36 O (0.7)	0.0
	(B)	29 O	3 FE(0.2)	38 O (0.7)	0.0

	(B)	28 O	4 FE(0.2)	35 O (0.7)	0.0
	(B)	30 O	4 FE(0.2)	37 O (0.7)	0.0
62	313.2403 (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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(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)	17 SI	53 O (0.0)	11 AL(1.0)	0.0
	(B)	18 SI	54 O (0.0)	12 AL(1.0)	0.0
63	316.3823 (B2U)				
	(S)	1 FE	32 O (0.6)	12 AL(0.4)	0.0
	(S)	1 FE	34 O (0.6)	10 AL(0.4)	0.0
	(S)	2 FE	31 O (0.6)	11 AL(0.4)	0.0
	(S)	2 FE	33 O (0.6)	9 AL(0.4)	0.0
	(S)	3 FE	36 O (0.6)	11 AL(0.4)	0.0
	(S)	3 FE	38 O (0.6)	9 AL(0.4)	0.0
	(S)	4 FE	35 O (0.6)	12 AL(0.4)	0.0
	(S)	4 FE	37 O (0.6)	10 AL(0.4)	0.0
64	317.4798 (B3G)				
	(B)	5 AL	1 FE(0.4)	6 AL(0.6)	0.0
	(B)	6 AL	1 FE(0.4)	5 AL(0.6)	0.0
	(B)	5 AL	2 FE(0.4)	6 AL(0.6)	0.0
	(B)	6 AL	2 FE(0.4)	5 AL(0.6)	0.0
	(B)	7 AL	3 FE(0.4)	8 AL(0.6)	0.0
	(B)	8 AL	3 FE(0.4)	7 AL(0.6)	0.0
	(B)	7 AL	4 FE(0.4)	8 AL(0.6)	0.0
	(B)	8 AL	4 FE(0.4)	7 AL(0.6)	0.0
	(O)	48 O	9 AL(0.0)	38 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)	36 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
65	330.4602 (B2G)				
	(B)	32 O	1 FE(0.5)	25 O (0.5)	0.0
	(B)	34 O	1 FE(0.5)	23 O (0.5)	0.0
	(B)	31 O	2 FE(0.5)	26 O (0.5)	0.0
	(B)	33 O	2 FE(0.5)	24 O (0.5)	0.0
	(B)	36 O	3 FE(0.5)	29 O (0.5)	0.0
	(B)	38 O	3 FE(0.5)	27 O (0.5)	0.0
	(B)	35 O	4 FE(0.5)	30 O (0.5)	0.0
	(B)	37 O	4 FE(0.5)	28 O (0.5)	0.0
66	331.1200 (B1U)				
	(O)	48 O	9 AL(0.0)	38 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)	36 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
67	335.8797 (AG)				
	(B)	55 O	15 SI(0.0)	51 O (1.0)	0.0
	(B)	56 O	16 SI(0.0)	52 O (1.0)	0.0
	(B)	57 O	17 SI(0.0)	53 O (1.0)	0.0
	(B)	58 O	18 SI(0.0)	54 O (1.0)	0.0
68	338.7122 (B3G)				
	(S)	5 AL	1 FE(1.0)		0.0

	(S)	6 AL	1 FE(1.0)	0.0
	(S)	5 AL	2 FE(1.0)	0.0
	(S)	6 AL	2 FE(1.0)	0.0
	(S)	7 AL	3 FE(1.0)	0.0
	(S)	8 AL	3 FE(1.0)	0.0
	(S)	7 AL	4 FE(1.0)	0.0
	(S)	8 AL	4 FE(1.0)	0.0
	(O)	48 O	9 AL(0.0) 38 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) 36 O (0.7)	0.0
	(O)	49 O	12 AL(0.0) 32 O (0.7)	0.0
	(O)	47 O	19 SI(0.0) 45 O (0.8)	-0.1
	(O)	48 O	20 SI(0.0) 46 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
69	341.6278	(B3U)		
	(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)	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
70	343.9053	(AG)		
	(B)	25 O	5 AL(0.0) 26 O (0.9)	0.0
	(B)	26 O	5 AL(0.0) 25 O (0.9)	0.0
	(B)	23 O	6 AL(0.0) 24 O (0.9)	0.0
	(B)	24 O	6 AL(0.0) 23 O (0.9)	0.0
	(B)	29 O	7 AL(0.0) 30 O (0.9)	0.0
	(B)	30 O	7 AL(0.0) 29 O (0.9)	0.0
	(B)	27 O	8 AL(0.0) 28 O (0.9)	0.0
	(B)	28 O	8 AL(0.0) 27 O (0.9)	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
	(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
71	345.2044	(B2U)		
	(S)	1 FE	32 O (0.5) 12 AL(0.5)	0.0
	(S)	1 FE	34 O (0.5) 10 AL(0.5)	0.0
	(S)	2 FE	31 O (0.5) 11 AL(0.5)	0.0
	(S)	2 FE	33 O (0.5) 9 AL(0.5)	0.0

	(S)	3 FE	36 O (0.5)	11 AL(0.5)	0.0
	(S)	3 FE	38 O (0.5)	9 AL(0.5)	0.0
	(S)	4 FE	35 O (0.5)	12 AL(0.5)	0.0
	(S)	4 FE	37 O (0.5)	10 AL(0.5)	0.0
72	345.8928 (B2G)				
	(S)	5 AL	1 FE(1.0)		0.0
	(S)	6 AL	1 FE(1.0)		0.0
	(S)	5 AL	2 FE(1.0)		0.0
	(S)	6 AL	2 FE(1.0)		0.0
	(S)	7 AL	3 FE(1.0)		0.0
	(S)	8 AL	3 FE(1.0)		0.0
	(S)	7 AL	4 FE(1.0)		0.0
	(S)	8 AL	4 FE(1.0)		0.0
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	29 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)	27 O (0.7)	0.0
73	351.7664 (B1G)				
	(B)	23 O	1 FE(0.0)	32 O (0.9)	0.0
	(B)	25 O	1 FE(0.0)	34 O (0.9)	0.0
	(B)	39 O	1 FE(0.1)	23 O (0.8)	0.0
	(B)	41 O	1 FE(0.1)	25 O (0.8)	0.0
	(B)	24 O	2 FE(0.0)	31 O (0.9)	0.0
	(B)	26 O	2 FE(0.0)	33 O (0.9)	0.0
	(B)	40 O	2 FE(0.1)	24 O (0.8)	-0.1
	(B)	42 O	2 FE(0.1)	26 O (0.8)	0.0
	(B)	27 O	3 FE(0.0)	36 O (0.9)	0.0
	(B)	29 O	3 FE(0.0)	38 O (0.9)	0.0
	(B)	43 O	3 FE(0.1)	27 O (0.8)	0.0
	(B)	45 O	3 FE(0.1)	29 O (0.8)	0.0
	(B)	28 O	4 FE(0.0)	35 O (0.9)	0.0
	(B)	30 O	4 FE(0.0)	37 O (0.9)	0.0
	(B)	44 O	4 FE(0.1)	28 O (0.8)	0.0
	(B)	46 O	4 FE(0.1)	30 O (0.8)	0.0
	(B)	25 O	15 SI(0.0)	30 O (0.9)	0.0
	(B)	30 O	15 SI(0.0)	25 O (0.9)	0.0
	(B)	26 O	16 SI(0.0)	29 O (0.9)	0.0
	(B)	29 O	16 SI(0.0)	26 O (0.9)	0.0
	(B)	23 O	17 SI(0.0)	28 O (0.9)	0.0
	(B)	28 O	17 SI(0.0)	23 O (0.9)	0.0
	(B)	24 O	18 SI(0.0)	27 O (0.9)	0.0
	(B)	27 O	18 SI(0.0)	24 O (0.9)	0.0
74	358.0155 (B3U)				
	(O)	33 O	9 AL(0.0)	51 O (0.8)	0.0
	(O)	38 O	9 AL(0.0)	51 O (0.8)	0.0
	(O)	34 O	10 AL(0.0)	52 O (0.8)	0.0
	(O)	37 O	10 AL(0.0)	52 O (0.8)	0.0
	(O)	31 O	11 AL(0.0)	53 O (0.8)	0.0
	(O)	36 O	11 AL(0.0)	53 O (0.8)	0.0
	(O)	32 O	12 AL(0.0)	54 O (0.8)	0.0
	(O)	35 O	12 AL(0.0)	54 O (0.8)	0.0
75	376.2070 (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)	0.0
	(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
76		377.0055 (B2U)			
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
	(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
	(B)	49 O	12 AL(0.0)	54 O (1.0)	0.0
77		377.1484 (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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0
78		378.7692 (B1U)			
	(B)	25 O	5 AL(0.0)	26 O (0.9)	0.0
	(B)	26 O	5 AL(0.0)	25 O (0.9)	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)	23 O	6 AL(0.0)	24 O (0.9)	0.0
	(B)	24 O	6 AL(0.0)	23 O (0.9)	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)	29 O	7 AL(0.0)	30 O (0.9)	0.0
	(B)	30 O	7 AL(0.0)	29 O (0.9)	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)	27 O	8 AL(0.0)	28 O (0.9)	0.0
	(B)	28 O	8 AL(0.0)	27 O (0.9)	0.0
	(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
79		381.2955 (AG)			
	(B)	32 O	1 FE(0.0)	39 O (1.0)	0.0
	(B)	34 O	1 FE(0.0)	41 O (1.0)	0.0
	(B)	31 O	2 FE(0.0)	40 O (1.0)	0.0
	(B)	33 O	2 FE(0.0)	42 O (1.0)	0.0
	(B)	36 O	3 FE(0.0)	43 O (1.0)	0.0
	(B)	38 O	3 FE(0.0)	45 O (1.0)	0.0
	(B)	35 O	4 FE(0.0)	44 O (1.0)	0.0
	(B)	37 O	4 FE(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
	(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
80	403.2462	(B2G)			
	(O)	48 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.1
	(O)	50 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.1
81	408.6723	(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)	11 AL	53 O (0.0)	17 SI(1.0)	0.0
	(B)	12 AL	54 O (0.0)	18 SI(1.0)	0.0
	(B)	55 O	19 SI(0.0)	47 O (1.0)	0.0
	(B)	56 O	20 SI(0.0)	48 O (1.0)	0.0
	(B)	57 O	21 SI(0.0)	49 O (1.0)	0.0
	(B)	58 O	22 SI(0.0)	50 O (1.0)	0.0
82	417.5955	(B2U)			
	(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
83	426.7957	(B1G)			
	(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
	(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
	(B)	43 O	7 AL(0.0)	44 O (0.9)	0.1
	(B)	44 O	7 AL(0.0)	43 O (0.9)	0.0
	(B)	45 O	8 AL(0.0)	46 O (0.9)	0.0
	(B)	46 O	8 AL(0.0)	45 O (0.9)	0.0
84	427.9522	(B3U)			
	(B)	19 SI	47 O (0.0)	10 AL(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
85	436.2161	(B3U)			
	(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)	-0.1
86	436.5616 (AG)				
	(B)	33 O	9 AL(0.0)	38 O (0.9)	0.0
	(B)	38 O	9 AL(0.0)	33 O (0.9)	0.0
	(B)	48 O	9 AL(0.0)	51 O (1.0)	0.0
	(B)	34 O	10 AL(0.0)	37 O (0.9)	0.0
	(B)	37 O	10 AL(0.0)	34 O (0.9)	0.0
	(B)	10 AL	47 O (0.0)	19 SI(1.0)	0.0
	(B)	31 O	11 AL(0.0)	36 O (0.9)	0.0
	(B)	36 O	11 AL(0.0)	31 O (0.9)	0.0
	(B)	50 O	11 AL(0.0)	53 O (1.0)	0.0
	(B)	32 O	12 AL(0.0)	35 O (0.9)	0.0
	(B)	35 O	12 AL(0.0)	32 O (0.9)	0.0
	(B)	49 O	12 AL(0.0)	54 O (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	461.5804 (AU)				
	(O)	48 O	9 AL(0.0)	38 O (0.7)	0.0
	(O)	47 O	10 AL(0.0)	34 O (0.7)	0.1
	(O)	50 O	11 AL(0.0)	36 O (0.7)	0.0
	(O)	49 O	12 AL(0.0)	32 O (0.7)	0.0
88	462.7091 (B2U)				
	(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

89 464.0440 (B1G)
 (B) 46 O 8 AL(0.0) 27 O (0.9) 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
 (B) 19 SI 47 O (0.0) 10 AL(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
 90 473.4070 (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
 91 476.4626 (B2G)
 (O) 47 O 19 SI(0.0) 45 O (0.8) -0.1
 (O) 55 O 19 SI(0.0) 45 O (0.7) 0.0
 (O) 48 O 20 SI(0.0) 46 O (0.8) 0.0
 (O) 56 O 20 SI(0.0) 46 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) 44 O (0.7) 0.0
 92 479.8656 (AU)
 (B) 5 AL 39 O (0.0) 22 SI(0.9) 0.0
 (B) 5 AL 40 O (0.0) 21 SI(0.9) 0.0
 (B) 6 AL 41 O (0.0) 20 SI(0.9) 0.0
 (B) 6 AL 42 O (0.0) 19 SI(0.9) 0.0
 (B) 7 AL 43 O (0.0) 21 SI(0.9) 0.0
 (B) 7 AL 44 O (0.0) 22 SI(0.9) 0.0
 (B) 8 AL 45 O (0.0) 19 SI(0.9) 0.1
 (B) 8 AL 46 O (0.0) 20 SI(0.9) 0.0
 93 488.7125 (B3G)
 (O) 51 O 15 SI(0.0) 25 O (0.7) 0.0
 (O) 52 O 16 SI(0.0) 29 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
 94 490.0286 (B1U)
 (O) 55 O 19 SI(0.0) 45 O (0.7) 0.0
 (O) 56 O 20 SI(0.0) 46 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) 44 O (0.7) 0.0
 95 491.6714 (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
96	494.2937 (AG)				
	(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
97	498.3314 (B1G)				
	(B)	23 O	1 FE(0.5)	5 AL(0.5)	0.0
	(B)	25 O	1 FE(0.5)	6 AL(0.5)	0.0
	(B)	24 O	2 FE(0.5)	5 AL(0.5)	0.0
	(B)	26 O	2 FE(0.5)	6 AL(0.5)	0.0
	(B)	27 O	3 FE(0.5)	7 AL(0.5)	0.0
	(B)	29 O	3 FE(0.5)	8 AL(0.5)	0.0
	(B)	28 O	4 FE(0.5)	7 AL(0.5)	0.0
	(B)	30 O	4 FE(0.5)	8 AL(0.5)	0.0
	(B)	25 O	5 AL(0.0)	26 O (0.9)	0.0
	(B)	26 O	5 AL(0.0)	25 O (0.9)	0.0
	(B)	23 O	6 AL(0.0)	24 O (0.9)	0.0
	(B)	24 O	6 AL(0.0)	23 O (0.9)	0.0
	(B)	29 O	7 AL(0.0)	30 O (0.9)	0.0
	(B)	30 O	7 AL(0.0)	29 O (0.9)	0.0
	(B)	27 O	8 AL(0.0)	28 O (0.9)	0.0
	(B)	28 O	8 AL(0.0)	27 O (0.9)	0.0
98	501.0119 (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)	0.1
	(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	502.0545 (B3G)				
	(O)	55 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	29 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)	27 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	46 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)	44 O (0.7)	0.0
100	506.5659 (B1U)				
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	29 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	508.1876	(B3U)			
	(B)	33 O	9 AL(0.1)	48 O (0.9)	0.0
	(B)	38 O	9 AL(0.1)	48 O (0.9)	0.0
	(B)	34 O	10 AL(0.1)	47 O (0.9)	0.0
	(B)	37 O	10 AL(0.1)	47 O (0.9)	0.0
	(B)	31 O	11 AL(0.1)	50 O (0.9)	0.0
	(B)	36 O	11 AL(0.1)	50 O (0.9)	0.0
	(B)	32 O	12 AL(0.1)	49 O (0.9)	0.0
	(B)	35 O	12 AL(0.1)	49 O (0.9)	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
102	513.0459	(B2G)			
	(O)	51 O	15 SI(0.0)	25 O (0.7)	0.0
	(O)	52 O	16 SI(0.0)	29 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	538.0712	(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 (0.8)	0.0
	(B)	30 O	15 SI(0.0)	55 O (0.8)	0.0
	(B)	26 O	16 SI(0.0)	56 O (0.8)	0.0
	(B)	29 O	16 SI(0.0)	56 O (0.8)	0.0
	(B)	23 O	17 SI(0.0)	57 O (0.8)	0.0
	(B)	28 O	17 SI(0.0)	57 O (0.8)	0.0
	(B)	24 O	18 SI(0.0)	58 O (0.8)	0.0
	(B)	27 O	18 SI(0.0)	58 O (0.8)	0.0
104	554.2582	(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)	29 O (0.7)	0.0
	(O)	56 O	16 SI(0.0)	29 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)	27 O (0.7)	0.0
	(O)	55 O	19 SI(0.0)	45 O (0.7)	0.0
	(O)	56 O	20 SI(0.0)	46 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)	44 O (0.7)	0.0
105	563.9712	(B1G)			

(S)	32 O	1 FE(0.7)	5 AL(0.3)	0.0
(S)	34 O	1 FE(0.7)	6 AL(0.3)	0.0
(S)	31 O	2 FE(0.7)	5 AL(0.3)	0.0
(S)	33 O	2 FE(0.7)	6 AL(0.3)	0.0
(S)	36 O	3 FE(0.7)	7 AL(0.3)	0.0
(S)	38 O	3 FE(0.7)	8 AL(0.3)	0.0
(S)	35 O	4 FE(0.7)	7 AL(0.3)	0.0
(S)	37 O	4 FE(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

106 566.7789 (AG)

(S)	23 O	1 FE(0.7)	5 AL(0.3)	0.0
(S)	25 O	1 FE(0.7)	6 AL(0.3)	0.0
(S)	24 O	2 FE(0.7)	5 AL(0.3)	0.0
(S)	26 O	2 FE(0.7)	6 AL(0.3)	0.0
(S)	27 O	3 FE(0.7)	7 AL(0.3)	0.0
(S)	29 O	3 FE(0.7)	8 AL(0.3)	0.0
(S)	28 O	4 FE(0.7)	7 AL(0.3)	0.0
(S)	30 O	4 FE(0.7)	8 AL(0.3)	0.0
(S)	51 O	9 AL(0.7)	48 O (0.3)	0.0
(S)	10 AL	52 O (0.7)	16 SI(0.3)	0.0
(S)	11 AL	53 O (0.7)	17 SI(0.3)	0.0
(S)	12 AL	54 O (0.7)	18 SI(0.3)	0.0

107 572.4861 (B2U)

(B)	39 O	5 AL(0.1)	25 O (0.9)	0.0
(B)	40 O	5 AL(0.1)	26 O (0.9)	0.0
(B)	41 O	6 AL(0.1)	23 O (0.9)	0.0
(B)	42 O	6 AL(0.1)	24 O (0.9)	0.0
(B)	43 O	7 AL(0.1)	29 O (0.9)	0.0
(B)	44 O	7 AL(0.1)	30 O (0.9)	0.0
(B)	45 O	8 AL(0.1)	27 O (0.9)	0.0
(B)	46 O	8 AL(0.1)	28 O (0.9)	0.0
(S)	48 O	9 AL(0.5)	51 O (0.5)	0.0
(S)	10 AL	47 O (0.5)	19 SI(0.5)	0.0
(S)	50 O	11 AL(0.5)	53 O (0.5)	0.0
(S)	49 O	12 AL(0.5)	54 O (0.5)	0.0
(B)	15 SI	25 O (0.0)	5 AL(1.0)	0.0
(B)	15 SI	30 O (0.0)	7 AL(1.0)	0.0
(B)	16 SI	26 O (0.0)	5 AL(1.0)	0.0
(B)	16 SI	29 O (0.0)	7 AL(1.0)	0.0

	(B)	17 SI	23 O (0.0)	6 AL(1.0)	0.0
	(B)	17 SI	28 O (0.0)	8 AL(1.0)	0.0
	(B)	18 SI	24 O (0.0)	6 AL(1.0)	0.0
	(B)	18 SI	27 O (0.0)	8 AL(1.0)	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
108	581.7146	(B1G)			
	(S)	39 O	1 FE(0.7)	41 O (0.3)	0.0
	(S)	41 O	1 FE(0.7)	39 O (0.3)	-0.1
	(S)	40 O	2 FE(0.7)	42 O (0.3)	0.0
	(S)	42 O	2 FE(0.7)	40 O (0.3)	0.0
	(S)	43 O	3 FE(0.7)	45 O (0.3)	0.0
	(S)	45 O	3 FE(0.7)	43 O (0.3)	0.0
	(S)	44 O	4 FE(0.7)	46 O (0.3)	0.0
	(S)	46 O	4 FE(0.7)	44 O (0.3)	0.0
	(O)	25 O	15 SI(0.0)	55 O (0.7)	0.0
	(O)	30 O	15 SI(0.0)	55 O (0.7)	0.0
	(B)	51 O	15 SI(0.0)	55 O (1.0)	0.0
	(O)	26 O	16 SI(0.0)	56 O (0.7)	0.0
	(O)	29 O	16 SI(0.0)	56 O (0.7)	0.0
	(B)	16 SI	52 O (0.0)	10 AL(1.0)	0.0
	(O)	23 O	17 SI(0.0)	57 O (0.7)	0.0
	(O)	28 O	17 SI(0.0)	57 O (0.7)	0.0
	(B)	17 SI	53 O (0.0)	11 AL(1.0)	0.0
	(O)	24 O	18 SI(0.0)	58 O (0.7)	0.0
	(O)	27 O	18 SI(0.0)	58 O (0.7)	0.0
	(B)	18 SI	54 O (0.0)	12 AL(1.0)	0.0
109	582.7550	(B3U)			
	(B)	5 AL	25 O (0.1)	15 SI(0.9)	0.0
	(B)	5 AL	26 O (0.1)	16 SI(0.9)	0.0
	(B)	6 AL	23 O (0.1)	17 SI(0.9)	0.0
	(B)	6 AL	24 O (0.1)	18 SI(0.9)	0.0
	(B)	7 AL	29 O (0.1)	16 SI(0.9)	0.0
	(B)	7 AL	30 O (0.1)	15 SI(0.9)	0.0
	(B)	8 AL	27 O (0.1)	18 SI(0.9)	0.0
	(B)	8 AL	28 O (0.1)	17 SI(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)	17 SI	53 O (0.1)	11 AL(0.9)	0.0
	(B)	18 SI	54 O (0.1)	12 AL(0.9)	0.0
110	585.3647	(AU)			
	(B)	33 O	9 AL(0.4)	51 O (0.6)	0.0
	(B)	38 O	9 AL(0.4)	51 O (0.6)	0.0
	(B)	34 O	10 AL(0.4)	52 O (0.6)	0.0
	(B)	37 O	10 AL(0.4)	52 O (0.6)	0.0
	(B)	31 O	11 AL(0.4)	53 O (0.6)	0.0
	(B)	36 O	11 AL(0.4)	53 O (0.6)	0.0
	(B)	32 O	12 AL(0.4)	54 O (0.6)	0.0

	(B)	35 O	12 AL(0.4)	54 O (0.6)	0.0
111	586.8646	(B1U)			
	(B)	23 O	1 FE(0.4)	39 O (0.6)	0.0
	(B)	25 O	1 FE(0.4)	41 O (0.6)	0.0
	(B)	24 O	2 FE(0.4)	40 O (0.6)	0.0
	(B)	26 O	2 FE(0.4)	42 O (0.6)	0.0
	(B)	27 O	3 FE(0.4)	43 O (0.6)	0.0
	(B)	29 O	3 FE(0.4)	45 O (0.6)	0.0
	(B)	28 O	4 FE(0.4)	44 O (0.6)	0.0
	(B)	30 O	4 FE(0.4)	46 O (0.6)	0.0
	(B)	25 O	15 SI(0.2)	55 O (0.8)	0.0
	(B)	30 O	15 SI(0.2)	55 O (0.8)	0.0
	(B)	26 O	16 SI(0.2)	56 O (0.8)	0.0
	(B)	29 O	16 SI(0.2)	56 O (0.8)	0.0
	(B)	23 O	17 SI(0.2)	57 O (0.8)	0.0
	(B)	28 O	17 SI(0.2)	57 O (0.8)	0.0
	(B)	24 O	18 SI(0.2)	58 O (0.8)	0.0
	(B)	27 O	18 SI(0.2)	58 O (0.8)	0.0
	(B)	42 O	19 SI(0.1)	47 O (0.8)	0.0
	(B)	45 O	19 SI(0.1)	47 O (0.8)	0.0
	(B)	41 O	20 SI(0.1)	48 O (0.8)	0.0
	(B)	46 O	20 SI(0.1)	48 O (0.8)	0.0
	(B)	40 O	21 SI(0.1)	49 O (0.8)	0.0
	(B)	43 O	21 SI(0.1)	49 O (0.8)	0.0
	(B)	39 O	22 SI(0.1)	50 O (0.8)	0.0
	(B)	44 O	22 SI(0.1)	50 O (0.8)	0.0
112	596.3557	(B3U)			
	(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
113	601.0271	(B1G)			
	(S)	33 O	9 AL(0.5)	38 O (0.5)	0.0
	(S)	38 O	9 AL(0.5)	33 O (0.5)	0.0
	(S)	34 O	10 AL(0.5)	37 O (0.5)	0.0
	(S)	37 O	10 AL(0.5)	34 O (0.5)	0.0
	(S)	31 O	11 AL(0.5)	36 O (0.5)	0.0
	(S)	36 O	11 AL(0.5)	31 O (0.5)	0.0
	(S)	32 O	12 AL(0.5)	35 O (0.5)	0.0
	(S)	35 O	12 AL(0.5)	32 O (0.5)	0.0
114	603.3458	(AG)			
	(S)	32 O	1 FE(0.9)		0.0
	(S)	34 O	1 FE(0.9)		0.0
	(S)	31 O	2 FE(0.9)		0.0
	(S)	33 O	2 FE(0.9)		0.0
	(S)	36 O	3 FE(0.9)		0.0
	(S)	38 O	3 FE(0.9)		0.0
	(S)	35 O	4 FE(0.9)		0.0
	(S)	37 O	4 FE(0.9)		0.0
	(B)	9 AL	33 O (0.4)	13 SI(0.6)	0.0

	(B)	9 AL	38 O (0.4)	14 SI(0.6)	0.0
	(B)	10 AL	34 O (0.4)	13 SI(0.6)	0.0
	(B)	10 AL	37 O (0.4)	14 SI(0.6)	0.0
	(B)	11 AL	31 O (0.4)	13 SI(0.6)	0.0
	(B)	11 AL	36 O (0.4)	14 SI(0.6)	0.0
	(B)	12 AL	32 O (0.4)	13 SI(0.6)	0.0
	(B)	12 AL	35 O (0.4)	14 SI(0.6)	0.0
	(B)	13 SI	31 O (0.1)	11 AL(0.9)	0.0
	(B)	13 SI	32 O (0.1)	12 AL(0.9)	0.0
	(B)	13 SI	33 O (0.1)	9 AL(0.9)	0.0
	(B)	13 SI	34 O (0.1)	10 AL(0.9)	0.0
	(B)	14 SI	35 O (0.1)	12 AL(0.9)	0.0
	(B)	14 SI	36 O (0.1)	11 AL(0.9)	0.0
	(B)	14 SI	37 O (0.1)	10 AL(0.9)	0.0
	(B)	14 SI	38 O (0.1)	9 AL(0.9)	0.0
115	607.2965	(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)	0.1
116	615.2574	(B3G)			
	(S)	33 O	9 AL(0.7)	38 O (0.3)	0.1
	(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
117	632.0105	(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
118	633.2301	(AG)			
	(B)	33 O	9 AL(0.2)	48 O (0.8)	0.0
	(B)	38 O	9 AL(0.2)	48 O (0.8)	0.0
	(B)	34 O	10 AL(0.2)	47 O (0.8)	0.0
	(B)	37 O	10 AL(0.2)	47 O (0.8)	0.0
	(B)	31 O	11 AL(0.2)	50 O (0.8)	0.0
	(B)	36 O	11 AL(0.2)	50 O (0.8)	0.0
	(B)	32 O	12 AL(0.2)	49 O (0.8)	0.0
	(B)	35 O	12 AL(0.2)	49 O (0.8)	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)	17 SI	53 O (0.0)	11 AL(1.0)	0.0

119 666.3637 (B3G)
 (B) 18 SI 54 O (0.0) 12 AL(1.0) 0.0
 (S) 25 O 5 AL(0.6) 26 O (0.3) 0.0
 (S) 26 O 5 AL(0.6) 25 O (0.3) 0.0
 (S) 23 O 6 AL(0.6) 24 O (0.3) 0.0
 (S) 24 O 6 AL(0.6) 23 O (0.3) 0.0
 (S) 29 O 7 AL(0.6) 30 O (0.3) 0.0
 (S) 30 O 7 AL(0.6) 29 O (0.3) 0.0
 (S) 27 O 8 AL(0.6) 28 O (0.3) 0.0
 (S) 28 O 8 AL(0.6) 27 O (0.3) 0.0
 120 668.0074 (B3U)
 (S) 48 O 9 AL(0.7) 51 O (0.3) 0.0
 (S) 10 AL 47 O (0.7) 19 SI(0.3) 0.0
 (S) 50 O 11 AL(0.7) 53 O (0.3) 0.0
 (S) 49 O 12 AL(0.7) 54 O (0.3) 0.0
 121 675.0406 (AG)
 (B) 48 O 9 AL(0.2) 51 O (0.8) 0.0
 (B) 10 AL 47 O (0.2) 19 SI(0.8) 0.0
 (B) 50 O 11 AL(0.2) 53 O (0.8) 0.0
 (B) 49 O 12 AL(0.2) 54 O (0.8) 0.0
 (B) 42 O 19 SI(0.1) 55 O (0.8) -0.1
 (B) 45 O 19 SI(0.1) 55 O (0.8) 0.0
 (B) 19 SI 47 O (0.0) 10 AL(1.0) 0.0
 (B) 41 O 20 SI(0.1) 56 O (0.8) 0.0
 (B) 46 O 20 SI(0.1) 56 O (0.8) 0.0
 (B) 48 O 20 SI(0.0) 56 O (1.0) 0.0
 (B) 40 O 21 SI(0.1) 57 O (0.8) -0.1
 (B) 43 O 21 SI(0.1) 57 O (0.8) 0.0
 (B) 21 SI 49 O (0.0) 12 AL(1.0) 0.0
 (B) 39 O 22 SI(0.1) 58 O (0.8) 0.0
 (B) 44 O 22 SI(0.1) 58 O (0.8) 0.0
 (B) 22 SI 50 O (0.0) 11 AL(1.0) 0.0
 122 683.9874 (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
 123 693.3792 (B2U)
 (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) 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) 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) 45 O 8 AL(0.8) 46 O (0.2) 0.0
 (S) 46 O 8 AL(0.8) 45 O (0.2) 0.0
 (O) 42 O 19 SI(0.1) 45 O (0.6) 0.0
 (O) 45 O 19 SI(0.1) 42 O (0.6) 0.0
 (B) 19 SI 47 O (0.2) 10 AL(0.8) 0.0
 (B) 55 O 19 SI(0.1) 47 O (0.9) 0.0

(O)	41 O	20 SI(0.1)	46 O (0.6)	0.0
(O)	46 O	20 SI(0.1)	41 O (0.6)	0.0
(B)	48 O	20 SI(0.2)	56 O (0.8)	0.0
(B)	56 O	20 SI(0.1)	48 O (0.9)	0.0
(O)	40 O	21 SI(0.1)	43 O (0.6)	-0.1
(O)	43 O	21 SI(0.1)	40 O (0.6)	0.0
(B)	21 SI	49 O (0.2)	12 AL(0.8)	0.0
(B)	57 O	21 SI(0.1)	49 O (0.9)	0.0
(O)	39 O	22 SI(0.1)	44 O (0.6)	0.0
(O)	44 O	22 SI(0.1)	39 O (0.6)	0.0
(B)	22 SI	50 O (0.2)	11 AL(0.8)	0.0
(B)	58 O	22 SI(0.1)	50 O (0.9)	0.0

124 699.9955 (B1G)

(B)	9 AL	33 O (0.1)	2 FE(0.9)	0.0
(B)	9 AL	38 O (0.1)	3 FE(0.9)	0.0
(S)	48 O	9 AL(1.0)		0.0
(B)	10 AL	34 O (0.1)	1 FE(0.9)	0.0
(B)	10 AL	37 O (0.1)	4 FE(0.9)	0.0
(S)	47 O	10 AL(1.0)		0.1
(B)	11 AL	31 O (0.1)	2 FE(0.9)	0.0
(B)	11 AL	36 O (0.1)	3 FE(0.9)	0.0
(S)	50 O	11 AL(1.0)		-0.1
(B)	12 AL	32 O (0.1)	1 FE(0.9)	0.0
(B)	12 AL	35 O (0.1)	4 FE(0.9)	0.0
(S)	49 O	12 AL(1.0)		0.1

125 701.9296 (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

126 704.8068 (B1U)

(S)	25 O	5 AL(0.7)	26 O (0.3)	0.0
(S)	26 O	5 AL(0.7)	25 O (0.3)	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(0.7)	24 O (0.3)	0.0
(S)	24 O	6 AL(0.7)	23 O (0.3)	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(0.7)	30 O (0.3)	0.0
(S)	30 O	7 AL(0.7)	29 O (0.3)	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(0.7)	28 O (0.3)	0.0
	(S)	28 O	8 AL(0.7)	27 O (0.3)	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
127	708.4184	(B2U)			
	(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)	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)	17 SI	53 O (0.0)	11 AL(1.0)	0.0
	(B)	18 SI	54 O (0.0)	12 AL(1.0)	0.0
	(B)	19 SI	42 O (0.0)	6 AL(1.0)	-0.1
	(B)	19 SI	45 O (0.0)	8 AL(1.0)	0.0
	(S)	55 O	19 SI(0.9)		0.0
	(B)	20 SI	41 O (0.0)	6 AL(1.0)	0.0
	(B)	20 SI	46 O (0.0)	8 AL(1.0)	0.0
	(S)	56 O	20 SI(0.9)		0.0
	(B)	21 SI	40 O (0.0)	5 AL(1.0)	0.0
	(B)	21 SI	43 O (0.0)	7 AL(1.0)	0.0
	(S)	57 O	21 SI(0.9)		0.0
	(B)	22 SI	39 O (0.0)	5 AL(1.0)	0.0
	(B)	22 SI	44 O (0.0)	7 AL(1.0)	0.0
	(S)	58 O	22 SI(0.9)		0.0
128	714.8734	(AG)			
	(S)	48 O	9 AL(1.0)		0.0
	(S)	47 O	10 AL(1.0)		0.1
	(S)	50 O	11 AL(1.0)		-0.1
	(S)	49 O	12 AL(1.0)		0.1
129	732.6340	(B1G)			
	(B)	25 O	15 SI(0.1)	51 O (0.9)	0.0
	(B)	30 O	15 SI(0.1)	51 O (0.9)	0.0
	(B)	26 O	16 SI(0.1)	52 O (0.9)	0.0
	(B)	29 O	16 SI(0.1)	52 O (0.9)	0.0
	(B)	23 O	17 SI(0.1)	53 O (0.9)	0.0
	(B)	28 O	17 SI(0.1)	53 O (0.9)	0.0
	(B)	24 O	18 SI(0.1)	54 O (0.9)	0.0
	(B)	27 O	18 SI(0.1)	54 O (0.9)	0.0
130	743.9264	(B3G)			
	(S)	5 AL	39 O (0.5)	22 SI(0.5)	0.0
	(S)	5 AL	40 O (0.5)	21 SI(0.5)	0.0
	(S)	6 AL	41 O (0.5)	20 SI(0.5)	0.0
	(S)	6 AL	42 O (0.5)	19 SI(0.5)	-0.1
	(S)	7 AL	43 O (0.5)	21 SI(0.5)	0.1
	(S)	7 AL	44 O (0.5)	22 SI(0.5)	-0.1
	(S)	8 AL	45 O (0.5)	19 SI(0.5)	0.0
	(S)	8 AL	46 O (0.5)	20 SI(0.5)	-0.1
131	744.1759	(AG)			

	(B)	15 SI	25 O (0.1)	5 AL(0.9)	0.0
	(B)	15 SI	30 O (0.1)	7 AL(0.9)	0.0
	(B)	16 SI	26 O (0.1)	5 AL(0.9)	0.0
	(B)	16 SI	29 O (0.1)	7 AL(0.9)	0.0
	(B)	17 SI	23 O (0.1)	6 AL(0.9)	0.0
	(B)	17 SI	28 O (0.1)	8 AL(0.9)	0.0
	(B)	18 SI	24 O (0.1)	6 AL(0.9)	0.0
	(B)	18 SI	27 O (0.1)	8 AL(0.9)	0.0
132	751.1454	(B2G)			
	(B)	13 SI	31 O (0.1)	2 FE(0.9)	0.0
	(B)	13 SI	32 O (0.1)	1 FE(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)	14 SI	35 O (0.1)	4 FE(0.9)	0.0
	(B)	14 SI	36 O (0.1)	3 FE(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 FE(0.9)	0.0
133	755.4451	(B3U)			
	(B)	15 SI	25 O (0.1)	1 FE(0.9)	0.0
	(B)	15 SI	30 O (0.1)	4 FE(0.9)	0.0
	(B)	16 SI	26 O (0.1)	2 FE(0.9)	0.0
	(B)	16 SI	29 O (0.1)	3 FE(0.9)	0.0
	(B)	17 SI	23 O (0.1)	1 FE(0.9)	0.0
	(B)	17 SI	28 O (0.1)	4 FE(0.9)	0.0
	(B)	18 SI	24 O (0.1)	2 FE(0.9)	0.0
	(B)	18 SI	27 O (0.1)	3 FE(0.9)	0.0
134	756.3146	(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)	-0.1
	(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
135	764.0901	(B2U)			
	(B)	13 SI	31 O (0.1)	2 FE(0.9)	0.0
	(B)	13 SI	32 O (0.1)	1 FE(0.9)	0.0
	(B)	13 SI	33 O (0.1)	2 FE(0.9)	0.0
	(B)	34 O	13 SI(0.1)	32 O (0.9)	0.0
	(B)	14 SI	35 O (0.1)	4 FE(0.9)	0.0
	(B)	14 SI	36 O (0.1)	3 FE(0.9)	0.0
	(B)	14 SI	37 O (0.1)	4 FE(0.9)	0.0
	(B)	14 SI	38 O (0.1)	3 FE(0.9)	0.0
136	768.5541	(B3U)			
	(B)	5 AL	39 O (0.3)	1 FE(0.7)	0.0
	(B)	5 AL	40 O (0.3)	2 FE(0.7)	0.0
	(B)	41 O	6 AL(0.3)	1 FE(0.7)	0.0
	(B)	6 AL	42 O (0.3)	2 FE(0.7)	-0.1
	(B)	43 O	7 AL(0.3)	3 FE(0.7)	0.1
	(B)	44 O	7 AL(0.3)	4 FE(0.7)	-0.1
	(B)	8 AL	45 O (0.3)	3 FE(0.7)	0.0
	(B)	46 O	8 AL(0.3)	4 FE(0.7)	-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)	0.0
	(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
137	812.2119	(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 (0.5)	22 SI(0.5)	0.0
	(S)	5 AL	40 O (0.5)	21 SI(0.5)	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 (0.5)	20 SI(0.5)	0.0
	(S)	6 AL	42 O (0.5)	19 SI(0.5)	-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 (0.5)	21 SI(0.5)	0.0
	(S)	7 AL	44 O (0.5)	22 SI(0.5)	-0.1
	(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 (0.5)	19 SI(0.5)	0.0
	(S)	8 AL	46 O (0.5)	20 SI(0.5)	-0.1
138	853.7652	(B2U)			
	(B)	25 O	5 AL(0.3)	2 FE(0.7)	0.0
	(B)	26 O	5 AL(0.3)	1 FE(0.7)	0.0
	(B)	39 O	5 AL(0.3)	2 FE(0.7)	0.0
	(B)	40 O	5 AL(0.3)	1 FE(0.7)	0.0
	(B)	23 O	6 AL(0.3)	2 FE(0.7)	0.0
	(B)	24 O	6 AL(0.3)	1 FE(0.7)	0.0
	(B)	41 O	6 AL(0.3)	2 FE(0.7)	0.0
	(B)	42 O	6 AL(0.3)	1 FE(0.7)	0.0
	(B)	29 O	7 AL(0.3)	4 FE(0.7)	0.0
	(B)	30 O	7 AL(0.3)	3 FE(0.7)	0.0
	(B)	43 O	7 AL(0.3)	4 FE(0.7)	0.0
	(B)	44 O	7 AL(0.3)	3 FE(0.7)	0.0
	(B)	27 O	8 AL(0.3)	4 FE(0.7)	0.0
	(B)	28 O	8 AL(0.3)	3 FE(0.7)	0.0
	(B)	45 O	8 AL(0.3)	4 FE(0.7)	0.0
	(B)	46 O	8 AL(0.3)	3 FE(0.7)	0.0
139	903.1641	(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
140	908.1529	(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
141	911.2973	(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
142	912.1763	(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
143	930.9990	(B3U)		
	(S)	25 O	5 AL(0.6) 39 O (0.4)	0.0
	(S)	26 O	5 AL(0.6) 40 O (0.4)	0.0
	(S)	23 O	6 AL(0.6) 41 O (0.4)	0.0
	(S)	24 O	6 AL(0.6) 42 O (0.4)	0.0
	(S)	29 O	7 AL(0.6) 43 O (0.4)	0.0
	(S)	30 O	7 AL(0.6) 44 O (0.4)	0.0
	(S)	27 O	8 AL(0.6) 45 O (0.4)	0.0
	(S)	28 O	8 AL(0.6) 46 O (0.4)	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
144	934.5829	(B3G)		
	(S)	31 O	13 SI(0.7) 34 O (0.3)	0.1
	(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
145	938.1959	(AG)		
	(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)	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	960.5788 (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	972.7567 (B3G)				
	(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
148	973.4032 (B2U)				
	(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
149	977.6823 (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
150	982.9113 (B3U)				
	(S)	31 O	13 SI(0.7)	34 O (0.3)	0.1
	(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
151	983.3954 (B2G)				
	(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
152	985.9941 (B1G)				
	(S)	25 O	15 SI(0.8)	55 O (0.1)	0.0
	(S)	30 O	15 SI(0.8)	55 O (0.1)	0.0
	(S)	26 O	16 SI(0.8)	56 O (0.1)	0.0
	(S)	29 O	16 SI(0.8)	56 O (0.1)	0.0
	(S)	23 O	17 SI(0.8)	57 O (0.1)	0.0
	(S)	28 O	17 SI(0.8)	57 O (0.1)	0.0
	(S)	24 O	18 SI(0.8)	58 O (0.1)	0.0
	(S)	27 O	18 SI(0.8)	58 O (0.1)	0.0
153	990.9444 (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)		-0.1
	(S)	44 O	7 AL(0.9)		0.0
	(S)	45 O	8 AL(0.9)		-0.1
	(S)	46 O	8 AL(0.9)		0.0
	(S)	42 O	19 SI(0.9)		-0.1
	(S)	45 O	19 SI(0.9)		-0.2
	(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)		-0.1
154	993.7037 (AG)				
	(S)	33 O	9 AL(0.7)	51 O (0.3)	0.0
	(S)	38 O	9 AL(0.7)	51 O (0.3)	0.0
	(S)	34 O	10 AL(0.7)	52 O (0.3)	0.0
	(S)	37 O	10 AL(0.7)	52 O (0.3)	0.0
	(S)	31 O	11 AL(0.7)	53 O (0.3)	0.1
	(S)	36 O	11 AL(0.7)	53 O (0.3)	0.0
	(S)	32 O	12 AL(0.7)	54 O (0.3)	0.0
	(S)	35 O	12 AL(0.7)	54 O (0.3)	0.1
155	995.1686 (AU)				
	(S)	33 O	9 AL(0.8)	48 O (0.2)	0.0
	(S)	38 O	9 AL(0.8)	48 O (0.2)	0.0
	(S)	34 O	10 AL(0.8)	47 O (0.2)	0.0
	(S)	37 O	10 AL(0.8)	47 O (0.2)	0.0
	(S)	31 O	11 AL(0.8)	50 O (0.2)	0.1
	(S)	36 O	11 AL(0.8)	50 O (0.2)	0.0

	(S)	32 O	12 AL(0.8)	49 O (0.2)	0.0
	(S)	35 O	12 AL(0.8)	49 O (0.2)	0.1
156	1011.1509 (B1U)				
	(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
157	1016.3645 (B3U)				
	(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)		0.1
	(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)		-0.1
158	1021.2647 (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)		0.1
	(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
159	1041.4230 (B1G)				
	(S)	31 O	13 SI(0.6)	32 O (0.4)	0.1
	(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
160	1051.5309 (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)		0.1
	(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
161	1062.1635 (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
162	1062.6691	(AG)		
	(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
163	1121.7156	(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
164	1123.2211	(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
165	1143.2858	(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	1152.9195	(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	1165.7302	(B3U)		
	(S)	48 O	9 AL(1.0)	0.0
	(S)	47 O	10 AL(1.0)	0.1
	(S)	50 O	11 AL(1.0)	-0.2
	(S)	49 O	12 AL(1.0)	0.1
	(S)	47 O	19 SI(1.0)	0.1
	(S)	48 O	20 SI(1.0)	-0.1
	(S)	49 O	21 SI(1.0)	0.1
	(S)	50 O	22 SI(1.0)	0.0
168	1168.8129	(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	1170.7659	(B1G)		
	(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	1177.4864	(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	1181.4463	(B3U)		
	(S)	55 O	15 SI(0.9)	0.0
	(S)	56 O	16 SI(0.9)	0.0
	(S)	57 O	17 SI(0.9)	0.0
	(S)	58 O	18 SI(0.9)	0.0
	(S)	55 O	19 SI(0.9)	0.0
	(S)	56 O	20 SI(0.9)	0.0
	(S)	57 O	21 SI(0.9)	0.0
	(S)	58 O	22 SI(0.9)	0.0
172	1186.3871	(B2U)		
	(S)	47 O	19 SI(1.0)	0.1
	(S)	48 O	20 SI(1.0)	-0.1
	(S)	49 O	21 SI(1.0)	0.1
	(S)	50 O	22 SI(1.0)	0.0
173	1197.6631	(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	1203.0469	(B1G)		
	(S)	47 O	19 SI(1.0)	0.1
	(S)	48 O	20 SI(1.0)	-0.1
	(S)	49 O	21 SI(1.0)	0.1
	(S)	50 O	22 SI(1.0)	0.0

NORMAL MODES NORMALIZED TO CLASSICAL AMPLITUDES

FREQ(CM**-1) -7.26 -5.58 -5.49 70.49 103.64 105.34

AT.	1 FE X	0.0000	0.1272	0.0000	0.0125	0.0000	-0.0174
	Y	0.1104	0.0000	0.0005	0.0000	0.0205	0.0000
	Z	-0.0010	0.0000	0.1282	0.0000	-0.0269	0.0000
AT.	2 FE X	0.0000	0.1272	0.0000	-0.0125	0.0000	-0.0174

	Y	0.1104	0.0000	-0.0005	0.0000	0.0205	0.0000
	Z	0.0010	0.0000	0.1282	0.0000	0.0269	0.0000
AT. 3	FE X	0.0000	0.1272	0.0000	-0.0125	0.0000	0.0174
	Y	0.1104	0.0000	0.0005	0.0000	-0.0205	0.0000
	Z	-0.0010	0.0000	0.1282	0.0000	0.0269	0.0000
AT. 4	FE X	0.0000	0.1272	0.0000	0.0125	0.0000	0.0174
	Y	0.1104	0.0000	-0.0005	0.0000	-0.0205	0.0000
	Z	0.0010	0.0000	0.1282	0.0000	-0.0269	0.0000
AT. 5	AL X	-0.0017	0.1295	0.0000	0.0000	-0.0249	0.0262
	Y	0.1124	-0.0009	0.0000	0.0000	0.0089	0.0288
	Z	0.0000	0.0000	0.1302	0.0105	0.0000	0.0000
AT. 6	AL X	0.0017	0.1295	0.0000	0.0000	0.0249	0.0262
	Y	0.1124	0.0009	0.0000	0.0000	0.0089	-0.0288
	Z	0.0000	0.0000	0.1302	-0.0105	0.0000	0.0000
AT. 7	AL X	-0.0017	0.1295	0.0000	0.0000	0.0249	-0.0262
	Y	0.1124	-0.0009	0.0000	0.0000	-0.0089	-0.0288
	Z	0.0000	0.0000	0.1302	-0.0105	0.0000	0.0000
AT. 8	AL X	0.0017	0.1295	0.0000	0.0000	-0.0249	-0.0262
	Y	0.1124	0.0009	0.0000	0.0000	-0.0089	0.0288
	Z	0.0000	0.0000	0.1302	0.0105	0.0000	0.0000
AT. 9	AL X	-0.0011	0.1261	0.0000	0.0113	0.0000	0.0000
	Y	0.1127	0.0001	0.0000	-0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.1302	0.0000	-0.0231	-0.0011
AT. 10	AL X	-0.0011	0.1261	0.0000	-0.0113	0.0000	0.0000
	Y	0.1127	0.0001	0.0000	0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.1302	0.0000	0.0231	0.0011
AT. 11	AL X	0.0011	0.1261	0.0000	0.0113	0.0000	0.0000
	Y	0.1127	-0.0001	0.0000	0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.1302	0.0000	-0.0231	0.0011
AT. 12	AL X	0.0011	0.1261	0.0000	-0.0113	0.0000	0.0000
	Y	0.1127	-0.0001	0.0000	-0.0099	0.0000	0.0000
	Z	0.0000	0.0000	0.1302	0.0000	0.0231	-0.0011
AT. 13	SI X	0.0000	0.1289	0.0000	0.0000	0.0000	-0.0221
	Y	0.1135	0.0000	0.0000	0.0000	-0.0402	0.0000
	Z	0.0000	0.0000	0.1307	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.1289	0.0000	0.0000	0.0000	0.0221
	Y	0.1135	0.0000	0.0000	0.0000	0.0402	0.0000
	Z	0.0000	0.0000	0.1307	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.1296	0.0000	0.0344	0.0000	0.0000
	Y	0.1138	0.0000	0.0000	0.0136	0.0000	0.0000
	Z	0.0000	0.0000	0.1318	0.0000	-0.0201	0.0263
AT. 16	SI X	0.0000	0.1296	0.0000	-0.0344	0.0000	0.0000
	Y	0.1138	0.0000	0.0000	-0.0136	0.0000	0.0000
	Z	0.0000	0.0000	0.1318	0.0000	0.0201	-0.0263
AT. 17	SI X	0.0000	0.1296	0.0000	0.0344	0.0000	0.0000
	Y	0.1138	0.0000	0.0000	-0.0136	0.0000	0.0000
	Z	0.0000	0.0000	0.1318	0.0000	-0.0201	-0.0263
AT. 18	SI X	0.0000	0.1296	0.0000	-0.0344	0.0000	0.0000
	Y	0.1138	0.0000	0.0000	0.0136	0.0000	0.0000
	Z	0.0000	0.0000	0.1318	0.0000	0.0201	0.0263
AT. 19	SI X	-0.0009	0.1296	0.0000	-0.0254	0.0000	0.0000
	Y	0.1125	-0.0009	0.0000	0.0452	0.0000	0.0000
	Z	0.0000	0.0000	0.1315	0.0000	0.0180	0.0295
AT. 20	SI X	-0.0009	0.1296	0.0000	0.0254	0.0000	0.0000

	Y	0.1125	-0.0009	0.0000	-0.0452	0.0000	0.0000
	Z	0.0000	0.0000	0.1315	0.0000	-0.0180	-0.0295
AT. 21	SI X	0.0009	0.1296	0.0000	-0.0254	0.0000	0.0000
	Y	0.1125	0.0009	0.0000	-0.0452	0.0000	0.0000
	Z	0.0000	0.0000	0.1315	0.0000	0.0180	-0.0295
AT. 22	SI X	0.0009	0.1296	0.0000	0.0254	0.0000	0.0000
	Y	0.1125	0.0009	0.0000	0.0452	0.0000	0.0000
	Z	0.0000	0.0000	0.1315	0.0000	-0.0180	0.0295
AT. 23	O X	-0.0017	0.1293	0.0022	0.0381	0.0250	0.0124
	Y	0.1150	0.0001	-0.0010	0.0046	0.0115	-0.0199
	Z	-0.0014	-0.0006	0.1337	-0.0036	-0.0042	-0.0136
AT. 24	O X	-0.0017	0.1293	-0.0022	-0.0381	0.0250	0.0124
	Y	0.1150	0.0001	0.0010	-0.0046	0.0115	-0.0199
	Z	0.0014	0.0006	0.1337	-0.0036	0.0042	0.0136
AT. 25	O X	0.0017	0.1293	-0.0022	0.0381	-0.0250	0.0124
	Y	0.1150	-0.0001	-0.0010	-0.0046	0.0115	0.0199
	Z	-0.0014	0.0006	0.1337	0.0036	-0.0042	0.0136
AT. 26	O X	0.0017	0.1293	0.0022	-0.0381	-0.0250	0.0124
	Y	0.1150	-0.0001	0.0010	0.0046	0.0115	0.0199
	Z	0.0014	-0.0006	0.1337	0.0036	0.0042	-0.0136
AT. 27	O X	-0.0017	0.1293	0.0022	-0.0381	-0.0250	-0.0124
	Y	0.1150	0.0001	-0.0010	-0.0046	-0.0115	0.0199
	Z	-0.0014	-0.0006	0.1337	0.0036	0.0042	0.0136
AT. 28	O X	-0.0017	0.1293	-0.0022	0.0381	-0.0250	-0.0124
	Y	0.1150	0.0001	0.0010	0.0046	-0.0115	0.0199
	Z	0.0014	0.0006	0.1337	0.0036	-0.0042	-0.0136
AT. 29	O X	0.0017	0.1293	-0.0022	-0.0381	0.0250	-0.0124
	Y	0.1150	-0.0001	-0.0010	0.0046	-0.0115	-0.0199
	Z	-0.0014	0.0006	0.1337	-0.0036	0.0042	-0.0136
AT. 30	O X	0.0017	0.1293	0.0022	0.0381	0.0250	-0.0124
	Y	0.1150	-0.0001	0.0010	-0.0046	-0.0115	-0.0199
	Z	0.0014	-0.0006	0.1337	-0.0036	-0.0042	0.0136
AT. 31	O X	0.0012	0.1287	0.0009	-0.0013	-0.0037	-0.0217
	Y	0.1122	0.0010	0.0005	0.0016	-0.0311	0.0058
	Z	0.0001	-0.0005	0.1279	0.0012	-0.0002	-0.0058
AT. 32	O X	0.0012	0.1287	-0.0009	0.0013	-0.0037	-0.0217
	Y	0.1122	0.0010	-0.0005	-0.0016	-0.0311	0.0058
	Z	-0.0001	0.0005	0.1279	0.0012	0.0002	0.0058
AT. 33	O X	-0.0012	0.1287	-0.0009	-0.0013	0.0037	-0.0217
	Y	0.1122	-0.0010	0.0005	-0.0016	-0.0311	-0.0058
	Z	0.0001	0.0005	0.1279	-0.0012	-0.0002	0.0058
AT. 34	O X	-0.0012	0.1287	0.0009	0.0013	0.0037	-0.0217
	Y	0.1122	-0.0010	-0.0005	0.0016	-0.0311	-0.0058
	Z	-0.0001	-0.0005	0.1279	-0.0012	0.0002	-0.0058
AT. 35	O X	0.0012	0.1287	0.0009	0.0013	0.0037	0.0217
	Y	0.1122	0.0010	0.0005	-0.0016	0.0311	-0.0058
	Z	0.0001	-0.0005	0.1279	-0.0012	0.0002	0.0058
AT. 36	O X	0.0012	0.1287	-0.0009	-0.0013	0.0037	0.0217
	Y	0.1122	0.0010	-0.0005	0.0016	0.0311	-0.0058
	Z	-0.0001	0.0005	0.1279	-0.0012	-0.0002	-0.0058
AT. 37	O X	-0.0012	0.1287	-0.0009	0.0013	-0.0037	0.0217
	Y	0.1122	-0.0010	0.0005	0.0016	0.0311	0.0058
	Z	0.0001	0.0005	0.1279	0.0012	0.0002	-0.0058
AT. 38	O X	-0.0012	0.1287	0.0009	-0.0013	-0.0037	0.0217

	Y	0.1122	-0.0010	-0.0005	-0.0016	0.0311	0.0058
	Z	-0.0001	-0.0005	0.1279	0.0012	-0.0002	0.0058
AT. 39	O X	0.0008	0.1310	-0.0002	0.0334	-0.0086	0.0178
	Y	0.1151	0.0004	-0.0016	0.0313	0.0136	0.0250
	Z	-0.0006	-0.0002	0.1319	-0.0048	-0.0199	0.0076
AT. 40	O X	0.0008	0.1310	0.0002	-0.0334	-0.0086	0.0178
	Y	0.1151	0.0004	0.0016	-0.0313	0.0136	0.0250
	Z	0.0006	0.0002	0.1319	-0.0048	0.0199	-0.0076
AT. 41	O X	-0.0008	0.1310	0.0002	0.0334	0.0086	0.0178
	Y	0.1151	-0.0004	-0.0016	-0.0313	0.0136	-0.0250
	Z	-0.0006	0.0002	0.1319	0.0048	-0.0199	-0.0076
AT. 42	O X	-0.0008	0.1310	-0.0002	-0.0334	0.0086	0.0178
	Y	0.1151	-0.0004	0.0016	0.0313	0.0136	-0.0250
	Z	0.0006	-0.0002	0.1319	0.0048	0.0199	0.0076
AT. 43	O X	0.0008	0.1310	-0.0002	-0.0334	0.0086	-0.0178
	Y	0.1151	0.0004	-0.0016	-0.0313	-0.0136	-0.0250
	Z	-0.0006	-0.0002	0.1319	0.0048	0.0199	-0.0076
AT. 44	O X	0.0008	0.1310	0.0002	0.0334	0.0086	-0.0178
	Y	0.1151	0.0004	0.0016	0.0313	-0.0136	-0.0250
	Z	0.0006	0.0002	0.1319	0.0048	-0.0199	0.0076
AT. 45	O X	-0.0008	0.1310	0.0002	-0.0334	-0.0086	-0.0178
	Y	0.1151	-0.0004	-0.0016	0.0313	-0.0136	0.0250
	Z	-0.0006	0.0002	0.1319	-0.0048	0.0199	0.0076
AT. 46	O X	-0.0008	0.1310	-0.0002	0.0334	-0.0086	-0.0178
	Y	0.1151	-0.0004	0.0016	-0.0313	-0.0136	0.0250
	Z	0.0006	-0.0002	0.1319	-0.0048	-0.0199	-0.0076
AT. 47	O X	-0.0006	0.1290	0.0000	-0.0290	0.0000	0.0000
	Y	0.1117	-0.0031	0.0000	0.0672	0.0000	0.0000
	Z	0.0000	0.0000	0.1269	0.0000	0.0359	0.0474
AT. 48	O X	-0.0006	0.1290	0.0000	0.0290	0.0000	0.0000
	Y	0.1117	-0.0031	0.0000	-0.0672	0.0000	0.0000
	Z	0.0000	0.0000	0.1269	0.0000	-0.0359	-0.0474
AT. 49	O X	0.0006	0.1290	0.0000	-0.0290	0.0000	0.0000
	Y	0.1117	0.0031	0.0000	-0.0672	0.0000	0.0000
	Z	0.0000	0.0000	0.1269	0.0000	0.0359	-0.0474
AT. 50	O X	0.0006	0.1290	0.0000	0.0290	0.0000	0.0000
	Y	0.1117	0.0031	0.0000	0.0672	0.0000	0.0000
	Z	0.0000	0.0000	0.1269	0.0000	-0.0359	0.0474
AT. 51	O X	0.0024	0.1322	0.0000	0.0600	0.0000	0.0000
	Y	0.1174	0.0034	0.0000	0.0385	0.0000	0.0000
	Z	0.0000	0.0000	0.1297	0.0000	-0.0562	0.0207
AT. 52	O X	0.0024	0.1322	0.0000	-0.0600	0.0000	0.0000
	Y	0.1174	0.0034	0.0000	-0.0385	0.0000	0.0000
	Z	0.0000	0.0000	0.1297	0.0000	0.0562	-0.0207
AT. 53	O X	-0.0024	0.1322	0.0000	0.0600	0.0000	0.0000
	Y	0.1174	-0.0034	0.0000	-0.0385	0.0000	0.0000
	Z	0.0000	0.0000	0.1297	0.0000	-0.0562	-0.0207
AT. 54	O X	-0.0024	0.1322	0.0000	-0.0600	0.0000	0.0000
	Y	0.1174	-0.0034	0.0000	0.0385	0.0000	0.0000
	Z	0.0000	0.0000	0.1297	0.0000	0.0562	0.0207
AT. 55	O X	-0.0034	0.1315	0.0000	0.0098	0.0000	0.0000
	Y	0.1163	-0.0008	0.0000	0.0270	0.0000	0.0000
	Z	0.0000	0.0000	0.1285	0.0000	-0.0119	0.0623
AT. 56	O X	-0.0034	0.1315	0.0000	-0.0098	0.0000	0.0000

	Y	0.1163	-0.0008	0.0000	-0.0270	0.0000	0.0000
	Z	0.0000	0.0000	0.1285	0.0000	0.0119	-0.0623
AT. 57 O	X	0.0034	0.1315	0.0000	0.0098	0.0000	0.0000
	Y	0.1163	0.0008	0.0000	-0.0270	0.0000	0.0000
	Z	0.0000	0.0000	0.1285	0.0000	-0.0119	-0.0623
AT. 58 O	X	0.0034	0.1315	0.0000	-0.0098	0.0000	0.0000
	Y	0.1163	0.0008	0.0000	0.0270	0.0000	0.0000
	Z	0.0000	0.0000	0.1285	0.0000	0.0119	0.0623

FREQ(CM**-1) 118.16 118.60 122.74 133.09 133.85 135.55

AT. 1 FE	X	0.0000	0.0000	0.0001	0.0000	0.0000	0.0399
	Y	0.0107	-0.0018	0.0000	-0.0148	-0.0311	0.0000
	Z	0.0456	-0.0026	0.0000	0.0062	0.0065	0.0000
AT. 2 FE	X	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0399
	Y	0.0107	0.0018	0.0000	0.0148	-0.0311	0.0000
	Z	-0.0456	-0.0026	0.0000	0.0062	-0.0065	0.0000
AT. 3 FE	X	0.0000	0.0000	0.0001	0.0000	0.0000	-0.0399
	Y	-0.0107	-0.0018	0.0000	0.0148	0.0311	0.0000
	Z	-0.0456	-0.0026	0.0000	-0.0062	-0.0065	0.0000
AT. 4 FE	X	0.0000	0.0000	-0.0001	0.0000	0.0000	-0.0399
	Y	-0.0107	0.0018	0.0000	-0.0148	0.0311	0.0000
	Z	0.0456	-0.0026	0.0000	-0.0062	0.0065	0.0000
AT. 5 AL	X	-0.0233	0.0000	0.0000	0.0000	0.0044	0.0171
	Y	-0.0013	0.0000	0.0000	0.0000	-0.0184	-0.0081
	Z	0.0000	0.0269	-0.0455	-0.0072	0.0000	0.0000
AT. 6 AL	X	0.0233	0.0000	0.0000	0.0000	-0.0044	0.0171
	Y	-0.0013	0.0000	0.0000	0.0000	-0.0184	0.0081
	Z	0.0000	0.0269	0.0455	-0.0072	0.0000	0.0000
AT. 7 AL	X	0.0233	0.0000	0.0000	0.0000	-0.0044	-0.0171
	Y	0.0013	0.0000	0.0000	0.0000	0.0184	0.0081
	Z	0.0000	0.0269	-0.0455	0.0072	0.0000	0.0000
AT. 8 AL	X	-0.0233	0.0000	0.0000	0.0000	0.0044	-0.0171
	Y	0.0013	0.0000	0.0000	0.0000	0.0184	-0.0081
	Z	0.0000	0.0269	0.0455	0.0072	0.0000	0.0000
AT. 9 AL	X	0.0000	0.0000	0.0000	0.0148	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0341	0.0000	0.0000
	Z	-0.0195	-0.0350	0.0024	0.0000	-0.0219	-0.0022
AT. 10 AL	X	0.0000	0.0000	0.0000	-0.0148	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0341	0.0000	0.0000
	Z	0.0195	-0.0350	0.0024	0.0000	0.0219	0.0022
AT. 11 AL	X	0.0000	0.0000	0.0000	-0.0148	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0341	0.0000	0.0000
	Z	-0.0195	-0.0350	-0.0024	0.0000	-0.0219	0.0022
AT. 12 AL	X	0.0000	0.0000	0.0000	0.0148	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0341	0.0000	0.0000
	Z	0.0195	-0.0350	-0.0024	0.0000	0.0219	-0.0022
AT. 13 SI	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0298
	Y	-0.0006	0.0000	0.0000	0.0000	-0.0220	0.0000
	Z	0.0000	-0.0528	0.0000	0.0133	0.0000	0.0000
AT. 14 SI	X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0298
	Y	0.0006	0.0000	0.0000	0.0000	0.0220	0.0000
	Z	0.0000	-0.0528	0.0000	-0.0133	0.0000	0.0000
AT. 15 SI	X	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000

	Y	0.0000	0.0000	0.0000	0.0082	0.0000	0.0000
	Z	0.0049	0.0141	-0.0289	0.0000	-0.0129	0.0117
AT. 16	SI X	0.0000	0.0000	0.0000	0.0122	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0082	0.0000	0.0000
	Z	-0.0049	0.0141	-0.0289	0.0000	0.0129	-0.0117
AT. 17	SI X	0.0000	0.0000	0.0000	0.0122	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0082	0.0000	0.0000
	Z	0.0049	0.0141	0.0289	0.0000	-0.0129	-0.0117
AT. 18	SI X	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0082	0.0000	0.0000
	Z	-0.0049	0.0141	0.0289	0.0000	0.0129	0.0117
AT. 19	SI X	0.0000	0.0000	0.0000	-0.0212	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0086	0.0000	0.0000
	Z	-0.0032	0.0183	0.0276	0.0000	0.0031	0.0142
AT. 20	SI X	0.0000	0.0000	0.0000	0.0212	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0086	0.0000	0.0000
	Z	0.0032	0.0183	0.0276	0.0000	-0.0031	-0.0142
AT. 21	SI X	0.0000	0.0000	0.0000	0.0212	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0086	0.0000	0.0000
	Z	-0.0032	0.0183	-0.0276	0.0000	0.0031	-0.0142
AT. 22	SI X	0.0000	0.0000	0.0000	-0.0212	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0086	0.0000	0.0000
	Z	0.0032	0.0183	-0.0276	0.0000	-0.0031	0.0142
AT. 23	O X	0.0190	0.0183	0.0133	0.0098	-0.0207	0.0284
	Y	-0.0145	0.0016	0.0072	-0.0081	0.0033	0.0030
	Z	0.0204	0.0269	0.0356	0.0013	-0.0290	0.0074
AT. 24	O X	0.0190	-0.0183	-0.0133	-0.0098	-0.0207	0.0284
	Y	-0.0145	-0.0016	-0.0072	0.0081	0.0033	0.0030
	Z	-0.0204	0.0269	0.0356	0.0013	0.0290	-0.0074
AT. 25	O X	-0.0190	-0.0183	0.0133	-0.0098	0.0207	0.0284
	Y	-0.0145	0.0016	-0.0072	-0.0081	0.0033	-0.0030
	Z	0.0204	0.0269	-0.0356	0.0013	-0.0290	-0.0074
AT. 26	O X	-0.0190	0.0183	-0.0133	0.0098	0.0207	0.0284
	Y	-0.0145	-0.0016	0.0072	0.0081	0.0033	-0.0030
	Z	-0.0204	0.0269	-0.0356	0.0013	0.0290	0.0074
AT. 27	O X	-0.0190	0.0183	0.0133	-0.0098	0.0207	-0.0284
	Y	0.0145	0.0016	0.0072	0.0081	-0.0033	-0.0030
	Z	-0.0204	0.0269	0.0356	-0.0013	0.0290	-0.0074
AT. 28	O X	-0.0190	-0.0183	-0.0133	0.0098	0.0207	-0.0284
	Y	0.0145	-0.0016	-0.0072	-0.0081	-0.0033	-0.0030
	Z	0.0204	0.0269	0.0356	-0.0013	-0.0290	0.0074
AT. 29	O X	0.0190	-0.0183	0.0133	0.0098	-0.0207	-0.0284
	Y	0.0145	0.0016	-0.0072	0.0081	-0.0033	0.0030
	Z	-0.0204	0.0269	-0.0356	-0.0013	0.0290	0.0074
AT. 30	O X	0.0190	0.0183	-0.0133	-0.0098	-0.0207	-0.0284
	Y	0.0145	-0.0016	0.0072	-0.0081	-0.0033	0.0030
	Z	0.0204	0.0269	-0.0356	-0.0013	-0.0290	-0.0074
AT. 31	O X	0.0129	-0.0161	0.0021	-0.0134	0.0047	0.0245
	Y	0.0048	0.0154	-0.0051	0.0234	-0.0197	-0.0185
	Z	-0.0201	-0.0472	0.0026	0.0064	-0.0064	0.0198
AT. 32	O X	0.0129	0.0161	-0.0021	0.0134	0.0047	0.0245
	Y	0.0048	-0.0154	0.0051	-0.0234	-0.0197	-0.0185
	Z	0.0201	-0.0472	0.0026	0.0064	0.0064	-0.0198
AT. 33	O X	-0.0129	0.0161	0.0021	0.0134	-0.0047	0.0245

	Y	0.0048	0.0154	0.0051	0.0234	-0.0197	0.0185
	Z	-0.0201	-0.0472	-0.0026	0.0064	-0.0064	-0.0198
AT. 34	O X	-0.0129	-0.0161	-0.0021	-0.0134	-0.0047	0.0245
	Y	0.0048	-0.0154	-0.0051	-0.0234	-0.0197	0.0185
	Z	0.0201	-0.0472	-0.0026	0.0064	0.0064	0.0198
AT. 35	O X	-0.0129	-0.0161	0.0021	0.0134	-0.0047	-0.0245
	Y	-0.0048	0.0154	-0.0051	-0.0234	0.0197	0.0185
	Z	0.0201	-0.0472	0.0026	-0.0064	0.0064	-0.0198
AT. 36	O X	-0.0129	0.0161	-0.0021	-0.0134	-0.0047	-0.0245
	Y	-0.0048	-0.0154	0.0051	0.0234	0.0197	0.0185
	Z	-0.0201	-0.0472	0.0026	-0.0064	-0.0064	0.0198
AT. 37	O X	0.0129	0.0161	0.0021	-0.0134	0.0047	-0.0245
	Y	-0.0048	0.0154	0.0051	-0.0234	0.0197	-0.0185
	Z	0.0201	-0.0472	-0.0026	-0.0064	0.0064	0.0198
AT. 38	O X	0.0129	-0.0161	-0.0021	0.0134	0.0047	-0.0245
	Y	-0.0048	-0.0154	-0.0051	0.0234	0.0197	-0.0185
	Z	-0.0201	-0.0472	-0.0026	-0.0064	-0.0064	-0.0198
AT. 39	O X	-0.0254	0.0027	0.0053	-0.0068	-0.0174	0.0076
	Y	0.0095	-0.0064	0.0237	-0.0167	-0.0293	-0.0043
	Z	0.0107	0.0194	-0.0418	-0.0023	0.0208	0.0126
AT. 40	O X	-0.0254	-0.0027	-0.0053	0.0068	-0.0174	0.0076
	Y	0.0095	0.0064	-0.0237	0.0167	-0.0293	-0.0043
	Z	-0.0107	0.0194	-0.0418	-0.0023	-0.0208	-0.0126
AT. 41	O X	0.0254	-0.0027	0.0053	0.0068	0.0174	0.0076
	Y	0.0095	-0.0064	-0.0237	-0.0167	-0.0293	0.0043
	Z	0.0107	0.0194	0.0418	-0.0023	0.0208	-0.0126
AT. 42	O X	0.0254	0.0027	-0.0053	-0.0068	0.0174	0.0076
	Y	0.0095	0.0064	0.0237	0.0167	-0.0293	0.0043
	Z	-0.0107	0.0194	0.0418	-0.0023	-0.0208	0.0126
AT. 43	O X	0.0254	0.0027	0.0053	0.0068	0.0174	-0.0076
	Y	-0.0095	-0.0064	0.0237	0.0167	0.0293	0.0043
	Z	-0.0107	0.0194	-0.0418	0.0023	-0.0208	-0.0126
AT. 44	O X	0.0254	-0.0027	-0.0053	-0.0068	0.0174	-0.0076
	Y	-0.0095	0.0064	-0.0237	-0.0167	0.0293	0.0043
	Z	0.0107	0.0194	-0.0418	0.0023	0.0208	0.0126
AT. 45	O X	-0.0254	-0.0027	0.0053	-0.0068	-0.0174	-0.0076
	Y	-0.0095	-0.0064	-0.0237	0.0167	0.0293	-0.0043
	Z	-0.0107	0.0194	0.0418	0.0023	-0.0208	0.0126
AT. 46	O X	-0.0254	0.0027	-0.0053	0.0068	-0.0174	-0.0076
	Y	-0.0095	0.0064	0.0237	-0.0167	0.0293	-0.0043
	Z	0.0107	0.0194	0.0418	0.0023	0.0208	-0.0126
AT. 47	O X	0.0000	0.0000	0.0000	-0.0172	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0281	0.0000	0.0000
	Z	0.0341	0.0137	0.0268	0.0000	0.0329	0.0084
AT. 48	O X	0.0000	0.0000	0.0000	0.0172	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0281	0.0000	0.0000
	Z	-0.0341	0.0137	0.0268	0.0000	-0.0329	-0.0084
AT. 49	O X	0.0000	0.0000	0.0000	0.0172	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0281	0.0000	0.0000
	Z	0.0341	0.0137	-0.0268	0.0000	0.0329	-0.0084
AT. 50	O X	0.0000	0.0000	0.0000	-0.0172	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0281	0.0000	0.0000
	Z	-0.0341	0.0137	-0.0268	0.0000	-0.0329	0.0084
AT. 51	O X	0.0000	0.0000	0.0000	0.0170	0.0000	0.0000

	Y	0.0000	0.0000	0.0000	0.0398	0.0000	0.0000
	Z	-0.0038	-0.0189	-0.0114	0.0000	-0.0177	0.0318
AT. 52 O	X	0.0000	0.0000	0.0000	-0.0170	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0398	0.0000	0.0000
	Z	0.0038	-0.0189	-0.0114	0.0000	0.0177	-0.0318
AT. 53 O	X	0.0000	0.0000	0.0000	-0.0170	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0398	0.0000	0.0000
	Z	-0.0038	-0.0189	0.0114	0.0000	-0.0177	-0.0318
AT. 54 O	X	0.0000	0.0000	0.0000	0.0170	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0398	0.0000	0.0000
	Z	0.0038	-0.0189	0.0114	0.0000	0.0177	0.0318
AT. 55 O	X	0.0000	0.0000	0.0000	-0.0586	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0213	0.0000	0.0000
	Z	-0.0242	0.0147	-0.0208	0.0000	0.0180	0.0190
AT. 56 O	X	0.0000	0.0000	0.0000	0.0586	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0213	0.0000	0.0000
	Z	0.0242	0.0147	-0.0208	0.0000	-0.0180	-0.0190
AT. 57 O	X	0.0000	0.0000	0.0000	0.0586	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0213	0.0000	0.0000
	Z	-0.0242	0.0147	0.0208	0.0000	0.0180	-0.0190
AT. 58 O	X	0.0000	0.0000	0.0000	-0.0586	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	-0.0213	0.0000	0.0000
	Z	0.0242	0.0147	0.0208	0.0000	-0.0180	0.0190

FREQ(CM**-1) 136.02 144.01 144.38 153.06 153.73 158.18

AT. 1 FE	X	0.0000	0.0000	0.0000	0.0000	0.0181	0.0000
	Y	0.0115	0.0104	-0.0010	-0.0040	0.0000	0.0268
	Z	0.0141	-0.0528	0.0552	0.0512	0.0000	-0.0101
AT. 2 FE	X	0.0000	0.0000	0.0000	0.0000	0.0181	0.0000
	Y	0.0115	0.0104	0.0010	0.0040	0.0000	0.0268
	Z	-0.0141	0.0528	0.0552	0.0512	0.0000	0.0101
AT. 3 FE	X	0.0000	0.0000	0.0000	0.0000	-0.0181	0.0000
	Y	0.0115	0.0104	0.0010	-0.0040	0.0000	-0.0268
	Z	0.0141	-0.0528	-0.0552	0.0512	0.0000	0.0101
AT. 4 FE	X	0.0000	0.0000	0.0000	0.0000	-0.0181	0.0000
	Y	0.0115	0.0104	-0.0010	0.0040	0.0000	-0.0268
	Z	-0.0141	0.0528	-0.0552	0.0512	0.0000	-0.0101
AT. 5 AL	X	-0.0382	-0.0117	0.0000	0.0000	0.0115	-0.0110
	Y	-0.0107	0.0008	0.0000	0.0000	-0.0037	0.0104
	Z	0.0000	0.0000	-0.0125	-0.0134	0.0000	0.0000
AT. 6 AL	X	0.0382	0.0117	0.0000	0.0000	0.0115	0.0110
	Y	-0.0107	0.0008	0.0000	0.0000	0.0037	0.0104
	Z	0.0000	0.0000	-0.0125	-0.0134	0.0000	0.0000
AT. 7 AL	X	-0.0382	-0.0117	0.0000	0.0000	-0.0115	0.0110
	Y	-0.0107	0.0008	0.0000	0.0000	0.0037	-0.0104
	Z	0.0000	0.0000	0.0125	-0.0134	0.0000	0.0000
AT. 8 AL	X	0.0382	0.0117	0.0000	0.0000	-0.0115	-0.0110
	Y	-0.0107	0.0008	0.0000	0.0000	-0.0037	-0.0104
	Z	0.0000	0.0000	0.0125	-0.0134	0.0000	0.0000
AT. 9 AL	X	0.0008	0.0063	0.0127	0.0000	0.0000	0.0000
	Y	0.0080	0.0097	-0.0038	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0105	0.0081	0.0056
AT. 10 AL	X	0.0008	0.0063	-0.0127	0.0000	0.0000	0.0000

	Y	0.0080	0.0097	0.0038	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0105	-0.0081	-0.0056
AT. 11	AL X	-0.0008	-0.0063	-0.0127	0.0000	0.0000	0.0000
	Y	0.0080	0.0097	-0.0038	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0105	-0.0081	0.0056
AT. 12	AL X	-0.0008	-0.0063	0.0127	0.0000	0.0000	0.0000
	Y	0.0080	0.0097	0.0038	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0105	0.0081	-0.0056
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0137	0.0000
	Y	0.0221	0.0002	0.0000	0.0000	0.0000	0.0251
	Z	0.0000	0.0000	-0.0082	-0.0163	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	-0.0137	0.0000
	Y	0.0221	0.0002	0.0000	0.0000	0.0000	-0.0251
	Z	0.0000	0.0000	0.0082	-0.0163	0.0000	0.0000
AT. 15	SI X	-0.0117	-0.0133	0.0106	0.0000	0.0000	0.0000
	Y	-0.0062	-0.0055	-0.0126	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0071	-0.0006	-0.0068
AT. 16	SI X	-0.0117	-0.0133	-0.0106	0.0000	0.0000	0.0000
	Y	-0.0062	-0.0055	0.0126	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0071	0.0006	0.0068
AT. 17	SI X	0.0117	0.0133	-0.0106	0.0000	0.0000	0.0000
	Y	-0.0062	-0.0055	-0.0126	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0071	0.0006	-0.0068
AT. 18	SI X	0.0117	0.0133	0.0106	0.0000	0.0000	0.0000
	Y	-0.0062	-0.0055	0.0126	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0071	-0.0006	0.0068
AT. 19	SI X	0.0195	0.0113	-0.0057	0.0000	0.0000	0.0000
	Y	-0.0122	-0.0109	-0.0105	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0101	-0.0065	-0.0003
AT. 20	SI X	0.0195	0.0113	0.0057	0.0000	0.0000	0.0000
	Y	-0.0122	-0.0109	0.0105	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0101	0.0065	0.0003
AT. 21	SI X	-0.0195	-0.0113	0.0057	0.0000	0.0000	0.0000
	Y	-0.0122	-0.0109	-0.0105	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0101	0.0065	-0.0003
AT. 22	SI X	-0.0195	-0.0113	-0.0057	0.0000	0.0000	0.0000
	Y	-0.0122	-0.0109	0.0105	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0101	-0.0065	0.0003
AT. 23	O X	0.0157	0.0123	-0.0076	0.0060	-0.0045	-0.0201
	Y	-0.0147	0.0017	-0.0083	-0.0054	0.0050	0.0235
	Z	0.0036	-0.0027	0.0021	-0.0027	-0.0035	-0.0253
AT. 24	O X	0.0157	0.0123	0.0076	-0.0060	-0.0045	-0.0201
	Y	-0.0147	0.0017	0.0083	0.0054	0.0050	0.0235
	Z	-0.0036	0.0027	0.0021	-0.0027	0.0035	0.0253
AT. 25	O X	-0.0157	-0.0123	0.0076	-0.0060	-0.0045	0.0201
	Y	-0.0147	0.0017	-0.0083	-0.0054	-0.0050	0.0235
	Z	0.0036	-0.0027	0.0021	-0.0027	0.0035	-0.0253
AT. 26	O X	-0.0157	-0.0123	-0.0076	0.0060	-0.0045	0.0201
	Y	-0.0147	0.0017	0.0083	0.0054	-0.0050	0.0235
	Z	-0.0036	0.0027	0.0021	-0.0027	-0.0035	0.0253
AT. 27	O X	0.0157	0.0123	0.0076	0.0060	0.0045	0.0201
	Y	-0.0147	0.0017	0.0083	-0.0054	-0.0050	-0.0235
	Z	0.0036	-0.0027	-0.0021	-0.0027	0.0035	0.0253
AT. 28	O X	0.0157	0.0123	-0.0076	-0.0060	0.0045	0.0201

	Y	-0.0147	0.0017	-0.0083	0.0054	-0.0050	-0.0235
	Z	-0.0036	0.0027	-0.0021	-0.0027	-0.0035	-0.0253
AT. 29	O X	-0.0157	-0.0123	-0.0076	-0.0060	0.0045	-0.0201
	Y	-0.0147	0.0017	0.0083	-0.0054	0.0050	-0.0235
	Z	0.0036	-0.0027	-0.0021	-0.0027	-0.0035	0.0253
AT. 30	O X	-0.0157	-0.0123	0.0076	0.0060	0.0045	-0.0201
	Y	-0.0147	0.0017	-0.0083	0.0054	0.0050	-0.0235
	Z	-0.0036	0.0027	-0.0021	-0.0027	0.0035	-0.0253
AT. 31	O X	0.0092	-0.0050	-0.0037	-0.0008	0.0122	0.0095
	Y	0.0190	0.0036	-0.0052	-0.0053	0.0388	0.0263
	Z	-0.0072	0.0049	0.0041	-0.0071	-0.0349	-0.0125
AT. 32	O X	0.0092	-0.0050	0.0037	0.0008	0.0122	0.0095
	Y	0.0190	0.0036	0.0052	0.0053	0.0388	0.0263
	Z	0.0072	-0.0049	0.0041	-0.0071	0.0349	0.0125
AT. 33	O X	-0.0092	0.0050	0.0037	0.0008	0.0122	-0.0095
	Y	0.0190	0.0036	-0.0052	-0.0053	-0.0388	0.0263
	Z	-0.0072	0.0049	0.0041	-0.0071	0.0349	-0.0125
AT. 34	O X	-0.0092	0.0050	-0.0037	-0.0008	0.0122	-0.0095
	Y	0.0190	0.0036	0.0052	0.0053	-0.0388	0.0263
	Z	0.0072	-0.0049	0.0041	-0.0071	-0.0349	0.0125
AT. 35	O X	0.0092	-0.0050	0.0037	-0.0008	-0.0122	-0.0095
	Y	0.0190	0.0036	0.0052	-0.0053	-0.0388	-0.0263
	Z	-0.0072	0.0049	-0.0041	-0.0071	0.0349	0.0125
AT. 36	O X	0.0092	-0.0050	-0.0037	0.0008	-0.0122	-0.0095
	Y	0.0190	0.0036	-0.0052	0.0053	-0.0388	-0.0263
	Z	0.0072	-0.0049	-0.0041	-0.0071	-0.0349	-0.0125
AT. 37	O X	-0.0092	0.0050	-0.0037	0.0008	-0.0122	0.0095
	Y	0.0190	0.0036	0.0052	-0.0053	0.0388	-0.0263
	Z	-0.0072	0.0049	-0.0041	-0.0071	-0.0349	0.0125
AT. 38	O X	-0.0092	0.0050	0.0037	-0.0008	-0.0122	0.0095
	Y	0.0190	0.0036	-0.0052	0.0053	0.0388	-0.0263
	Z	0.0072	-0.0049	-0.0041	-0.0071	0.0349	-0.0125
AT. 39	O X	-0.0357	-0.0096	-0.0060	-0.0081	0.0339	-0.0268
	Y	-0.0005	-0.0041	0.0078	-0.0073	0.0043	-0.0035
	Z	0.0029	-0.0044	0.0025	-0.0029	-0.0264	0.0159
AT. 40	O X	-0.0357	-0.0096	0.0060	0.0081	0.0339	-0.0268
	Y	-0.0005	-0.0041	-0.0078	0.0073	0.0043	-0.0035
	Z	-0.0029	0.0044	0.0025	-0.0029	0.0264	-0.0159
AT. 41	O X	0.0357	0.0096	0.0060	0.0081	0.0339	0.0268
	Y	-0.0005	-0.0041	0.0078	-0.0073	-0.0043	-0.0035
	Z	0.0029	-0.0044	0.0025	-0.0029	0.0264	0.0159
AT. 42	O X	0.0357	0.0096	-0.0060	-0.0081	0.0339	0.0268
	Y	-0.0005	-0.0041	-0.0078	0.0073	-0.0043	-0.0035
	Z	-0.0029	0.0044	0.0025	-0.0029	-0.0264	-0.0159
AT. 43	O X	-0.0357	-0.0096	0.0060	-0.0081	-0.0339	0.0268
	Y	-0.0005	-0.0041	-0.0078	-0.0073	-0.0043	0.0035
	Z	0.0029	-0.0044	-0.0025	-0.0029	0.0264	-0.0159
AT. 44	O X	-0.0357	-0.0096	-0.0060	0.0081	-0.0339	0.0268
	Y	-0.0005	-0.0041	0.0078	0.0073	-0.0043	0.0035
	Z	-0.0029	0.0044	-0.0025	-0.0029	-0.0264	0.0159
AT. 45	O X	0.0357	0.0096	-0.0060	0.0081	-0.0339	-0.0268
	Y	-0.0005	-0.0041	-0.0078	-0.0073	0.0043	0.0035
	Z	0.0029	-0.0044	-0.0025	-0.0029	-0.0264	-0.0159
AT. 46	O X	0.0357	0.0096	0.0060	-0.0081	-0.0339	-0.0268

	Y	-0.0005	-0.0041	0.0078	0.0073	0.0043	0.0035
	Z	-0.0029	0.0044	-0.0025	-0.0029	0.0264	0.0159
AT. 47	O X	0.0222	0.0087	-0.0074	0.0000	0.0000	0.0000
	Y	-0.0467	0.0008	-0.0009	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0253	0.0253	0.0205
AT. 48	O X	0.0222	0.0087	0.0074	0.0000	0.0000	0.0000
	Y	-0.0467	0.0008	0.0009	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0253	-0.0253	-0.0205
AT. 49	O X	-0.0222	-0.0087	0.0074	0.0000	0.0000	0.0000
	Y	-0.0467	0.0008	-0.0009	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0253	-0.0253	0.0205
AT. 50	O X	-0.0222	-0.0087	-0.0074	0.0000	0.0000	0.0000
	Y	-0.0467	0.0008	0.0009	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0253	0.0253	-0.0205
AT. 51	O X	0.0089	-0.0192	0.0103	0.0000	0.0000	0.0000
	Y	0.0166	-0.0159	-0.0096	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0177	-0.0126	0.0172
AT. 52	O X	0.0089	-0.0192	-0.0103	0.0000	0.0000	0.0000
	Y	0.0166	-0.0159	0.0096	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0177	0.0126	-0.0172
AT. 53	O X	-0.0089	0.0192	-0.0103	0.0000	0.0000	0.0000
	Y	0.0166	-0.0159	-0.0096	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0177	0.0126	0.0172
AT. 54	O X	-0.0089	0.0192	0.0103	0.0000	0.0000	0.0000
	Y	0.0166	-0.0159	0.0096	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0177	-0.0126	-0.0172
AT. 55	O X	-0.0263	0.0125	0.0075	0.0000	0.0000	0.0000
	Y	-0.0001	-0.0115	-0.0124	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	-0.0105	0.0139
AT. 56	O X	-0.0263	0.0125	-0.0075	0.0000	0.0000	0.0000
	Y	-0.0001	-0.0115	0.0124	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	0.0105	-0.0139
AT. 57	O X	0.0263	-0.0125	-0.0075	0.0000	0.0000	0.0000
	Y	-0.0001	-0.0115	-0.0124	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	0.0105	0.0139
AT. 58	O X	0.0263	-0.0125	0.0075	0.0000	0.0000	0.0000
	Y	-0.0001	-0.0115	0.0124	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0242	-0.0105	-0.0139

FREQ(CM**-1) 162.52 165.30 165.70 166.65 171.43 172.12

AT. 1	FE X	0.0000	0.0298	0.0000	0.0112	-0.0160	0.0000
	Y	-0.0163	0.0000	0.0180	0.0000	0.0000	-0.0272
	Z	-0.0282	0.0000	0.0065	0.0000	0.0000	-0.0072
AT. 2	FE X	0.0000	0.0298	0.0000	-0.0112	-0.0160	0.0000
	Y	-0.0163	0.0000	0.0180	0.0000	0.0000	-0.0272
	Z	0.0282	0.0000	-0.0065	0.0000	0.0000	0.0072
AT. 3	FE X	0.0000	0.0298	0.0000	-0.0112	-0.0160	0.0000
	Y	0.0163	0.0000	0.0180	0.0000	0.0000	-0.0272
	Z	0.0282	0.0000	0.0065	0.0000	0.0000	-0.0072
AT. 4	FE X	0.0000	0.0298	0.0000	0.0112	-0.0160	0.0000
	Y	0.0163	0.0000	0.0180	0.0000	0.0000	-0.0272
	Z	-0.0282	0.0000	-0.0065	0.0000	0.0000	0.0072
AT. 5	AL X	-0.0198	-0.0221	-0.0105	0.0000	0.0081	0.0056

	Y	-0.0226	-0.0212	0.0117	0.0000	0.0093	-0.0129
	Z	0.0000	0.0000	0.0000	0.0065	0.0000	0.0000
AT. 6	AL X	0.0198	-0.0221	0.0105	0.0000	0.0081	-0.0056
	Y	-0.0226	0.0212	0.0117	0.0000	-0.0093	-0.0129
	Z	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000
AT. 7	AL X	0.0198	-0.0221	-0.0105	0.0000	0.0081	0.0056
	Y	0.0226	-0.0212	0.0117	0.0000	0.0093	-0.0129
	Z	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000
AT. 8	AL X	-0.0198	-0.0221	0.0105	0.0000	0.0081	-0.0056
	Y	0.0226	0.0212	0.0117	0.0000	-0.0093	-0.0129
	Z	0.0000	0.0000	0.0000	0.0065	0.0000	0.0000
AT. 9	AL X	0.0000	-0.0023	0.0237	-0.0070	0.0017	0.0157
	Y	0.0000	-0.0108	-0.0113	-0.0253	-0.0158	0.0228
	Z	0.0065	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0000	-0.0023	0.0237	0.0070	0.0017	0.0157
	Y	0.0000	-0.0108	-0.0113	0.0253	-0.0158	0.0228
	Z	-0.0065	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0000	-0.0023	-0.0237	-0.0070	0.0017	-0.0157
	Y	0.0000	0.0108	-0.0113	0.0253	0.0158	0.0228
	Z	0.0065	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0000	-0.0023	-0.0237	0.0070	0.0017	-0.0157
	Y	0.0000	0.0108	-0.0113	-0.0253	0.0158	0.0228
	Z	-0.0065	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0272	0.0000	0.0000	-0.0091	0.0000
	Y	0.0189	0.0000	-0.0253	0.0000	0.0000	0.0314
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0272	0.0000	0.0000	-0.0091	0.0000
	Y	-0.0189	0.0000	-0.0253	0.0000	0.0000	0.0314
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	-0.0088	0.0287	0.0138	0.0004	0.0132
	Y	0.0000	-0.0206	-0.0030	-0.0088	-0.0168	0.0016
	Z	-0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0000	-0.0088	0.0287	-0.0138	0.0004	0.0132
	Y	0.0000	-0.0206	-0.0030	0.0088	-0.0168	0.0016
	Z	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	0.0000	-0.0088	-0.0287	0.0138	0.0004	-0.0132
	Y	0.0000	0.0206	-0.0030	0.0088	0.0168	0.0016
	Z	-0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0000	-0.0088	-0.0287	-0.0138	0.0004	-0.0132
	Y	0.0000	0.0206	-0.0030	-0.0088	0.0168	0.0016
	Z	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	0.0000	-0.0134	0.0221	0.0101	0.0140	0.0129
	Y	0.0000	-0.0111	-0.0005	-0.0053	-0.0264	-0.0010
	Z	0.0056	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0000	-0.0134	0.0221	-0.0101	0.0140	0.0129
	Y	0.0000	-0.0111	-0.0005	0.0053	-0.0264	-0.0010
	Z	-0.0056	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0000	-0.0134	-0.0221	0.0101	0.0140	-0.0129
	Y	0.0000	0.0111	-0.0005	0.0053	0.0264	-0.0010
	Z	0.0056	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	0.0000	-0.0134	-0.0221	-0.0101	0.0140	-0.0129
	Y	0.0000	0.0111	-0.0005	-0.0053	0.0264	-0.0010
	Z	-0.0056	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0098	-0.0091	-0.0192	0.0080	-0.0067	-0.0151

	Y	-0.0303	0.0202	0.0086	-0.0050	-0.0019	-0.0106
	Z	0.0105	-0.0008	0.0004	-0.0004	-0.0048	-0.0013
AT. 24	O X	0.0098	-0.0091	-0.0192	-0.0080	-0.0067	-0.0151
	Y	-0.0303	0.0202	0.0086	0.0050	-0.0019	-0.0106
	Z	-0.0105	0.0008	-0.0004	-0.0004	0.0048	0.0013
AT. 25	O X	-0.0098	-0.0091	0.0192	0.0080	-0.0067	0.0151
	Y	-0.0303	-0.0202	0.0086	0.0050	0.0019	-0.0106
	Z	0.0105	0.0008	0.0004	0.0004	0.0048	-0.0013
AT. 26	O X	-0.0098	-0.0091	0.0192	-0.0080	-0.0067	0.0151
	Y	-0.0303	-0.0202	0.0086	-0.0050	0.0019	-0.0106
	Z	-0.0105	-0.0008	-0.0004	0.0004	-0.0048	0.0013
AT. 27	O X	-0.0098	-0.0091	-0.0192	-0.0080	-0.0067	-0.0151
	Y	0.0303	0.0202	0.0086	0.0050	-0.0019	-0.0106
	Z	-0.0105	-0.0008	0.0004	0.0004	-0.0048	-0.0013
AT. 28	O X	-0.0098	-0.0091	-0.0192	0.0080	-0.0067	-0.0151
	Y	0.0303	0.0202	0.0086	-0.0050	-0.0019	-0.0106
	Z	0.0105	0.0008	-0.0004	0.0004	0.0048	0.0013
AT. 29	O X	0.0098	-0.0091	0.0192	-0.0080	-0.0067	0.0151
	Y	0.0303	-0.0202	0.0086	-0.0050	0.0019	-0.0106
	Z	-0.0105	0.0008	0.0004	-0.0004	0.0048	-0.0013
AT. 30	O X	0.0098	-0.0091	0.0192	0.0080	-0.0067	0.0151
	Y	0.0303	-0.0202	0.0086	0.0050	0.0019	-0.0106
	Z	0.0105	-0.0008	-0.0004	-0.0004	-0.0048	0.0013
AT. 31	O X	0.0075	0.0187	-0.0124	-0.0084	-0.0112	-0.0010
	Y	0.0131	0.0060	-0.0147	0.0118	0.0109	0.0239
	Z	-0.0028	0.0022	0.0037	0.0011	-0.0039	0.0024
AT. 32	O X	0.0075	0.0187	-0.0124	0.0084	-0.0112	-0.0010
	Y	0.0131	0.0060	-0.0147	-0.0118	0.0109	0.0239
	Z	0.0028	-0.0022	-0.0037	0.0011	0.0039	-0.0024
AT. 33	O X	-0.0075	0.0187	0.0124	-0.0084	-0.0112	0.0010
	Y	0.0131	-0.0060	-0.0147	-0.0118	-0.0109	0.0239
	Z	-0.0028	-0.0022	0.0037	-0.0011	0.0039	0.0024
AT. 34	O X	-0.0075	0.0187	0.0124	0.0084	-0.0112	0.0010
	Y	0.0131	-0.0060	-0.0147	0.0118	-0.0109	0.0239
	Z	0.0028	0.0022	-0.0037	-0.0011	-0.0039	-0.0024
AT. 35	O X	-0.0075	0.0187	-0.0124	0.0084	-0.0112	-0.0010
	Y	-0.0131	0.0060	-0.0147	-0.0118	0.0109	0.0239
	Z	0.0028	0.0022	0.0037	-0.0011	-0.0039	0.0024
AT. 36	O X	-0.0075	0.0187	-0.0124	-0.0084	-0.0112	-0.0010
	Y	-0.0131	0.0060	-0.0147	0.0118	0.0109	0.0239
	Z	-0.0028	-0.0022	-0.0037	-0.0011	0.0039	-0.0024
AT. 37	O X	0.0075	0.0187	0.0124	0.0084	-0.0112	0.0010
	Y	-0.0131	-0.0060	-0.0147	0.0118	-0.0109	0.0239
	Z	0.0028	-0.0022	0.0037	0.0011	0.0039	0.0024
AT. 38	O X	0.0075	0.0187	0.0124	-0.0084	-0.0112	0.0010
	Y	-0.0131	-0.0060	-0.0147	-0.0118	-0.0109	0.0239
	Z	-0.0028	0.0022	-0.0037	0.0011	-0.0039	-0.0024
AT. 39	O X	-0.0159	-0.0136	-0.0171	0.0033	0.0127	-0.0045
	Y	-0.0004	0.0055	-0.0021	-0.0134	0.0235	-0.0148
	Z	0.0039	0.0015	0.0018	-0.0020	-0.0004	0.0053
AT. 40	O X	-0.0159	-0.0136	-0.0171	-0.0033	0.0127	-0.0045
	Y	-0.0004	0.0055	-0.0021	0.0134	0.0235	-0.0148
	Z	-0.0039	-0.0015	-0.0018	-0.0020	0.0004	-0.0053
AT. 41	O X	0.0159	-0.0136	0.0171	0.0033	0.0127	0.0045

	Y	-0.0004	-0.0055	-0.0021	0.0134	-0.0235	-0.0148
	Z	0.0039	-0.0015	0.0018	0.0020	0.0004	0.0053
AT. 42 O	X	0.0159	-0.0136	0.0171	-0.0033	0.0127	0.0045
	Y	-0.0004	-0.0055	-0.0021	-0.0134	-0.0235	-0.0148
	Z	-0.0039	0.0015	-0.0018	0.0020	-0.0004	-0.0053
AT. 43 O	X	0.0159	-0.0136	-0.0171	-0.0033	0.0127	-0.0045
	Y	0.0004	0.0055	-0.0021	0.0134	0.0235	-0.0148
	Z	-0.0039	0.0015	0.0018	0.0020	-0.0004	0.0053
AT. 44 O	X	0.0159	-0.0136	-0.0171	0.0033	0.0127	-0.0045
	Y	0.0004	0.0055	-0.0021	-0.0134	0.0235	-0.0148
	Z	0.0039	-0.0015	-0.0018	0.0020	0.0004	-0.0053
AT. 45 O	X	-0.0159	-0.0136	0.0171	-0.0033	0.0127	0.0045
	Y	0.0004	-0.0055	-0.0021	-0.0134	-0.0235	-0.0148
	Z	-0.0039	-0.0015	0.0018	-0.0020	0.0004	0.0053
AT. 46 O	X	-0.0159	-0.0136	0.0171	0.0033	0.0127	0.0045
	Y	0.0004	-0.0055	-0.0021	0.0134	-0.0235	-0.0148
	Z	0.0039	0.0015	-0.0018	-0.0020	-0.0004	-0.0053
AT. 47 O	X	0.0000	-0.0130	0.0217	0.0060	0.0123	0.0119
	Y	0.0000	0.0078	0.0001	0.0328	-0.0317	0.0239
	Z	0.0249	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48 O	X	0.0000	-0.0130	0.0217	-0.0060	0.0123	0.0119
	Y	0.0000	0.0078	0.0001	-0.0328	-0.0317	0.0239
	Z	-0.0249	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49 O	X	0.0000	-0.0130	-0.0217	0.0060	0.0123	-0.0119
	Y	0.0000	-0.0078	0.0001	-0.0328	0.0317	0.0239
	Z	0.0249	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50 O	X	0.0000	-0.0130	-0.0217	-0.0060	0.0123	-0.0119
	Y	0.0000	-0.0078	0.0001	0.0328	0.0317	0.0239
	Z	-0.0249	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51 O	X	0.0000	-0.0220	0.0247	-0.0181	-0.0181	0.0303
	Y	0.0000	-0.0341	-0.0080	-0.0416	-0.0379	0.0276
	Z	0.0284	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52 O	X	0.0000	-0.0220	0.0247	0.0181	-0.0181	0.0303
	Y	0.0000	-0.0341	-0.0080	0.0416	-0.0379	0.0276
	Z	-0.0284	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53 O	X	0.0000	-0.0220	-0.0247	-0.0181	-0.0181	-0.0303
	Y	0.0000	0.0341	-0.0080	0.0416	0.0379	0.0276
	Z	0.0284	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54 O	X	0.0000	-0.0220	-0.0247	0.0181	-0.0181	-0.0303
	Y	0.0000	0.0341	-0.0080	-0.0416	0.0379	0.0276
	Z	-0.0284	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55 O	X	0.0000	-0.0019	0.0465	0.0646	0.0362	0.0176
	Y	0.0000	-0.0190	-0.0081	-0.0244	-0.0308	-0.0004
	Z	-0.0347	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56 O	X	0.0000	-0.0019	0.0465	-0.0646	0.0362	0.0176
	Y	0.0000	-0.0190	-0.0081	0.0244	-0.0308	-0.0004
	Z	0.0347	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57 O	X	0.0000	-0.0019	-0.0465	0.0646	0.0362	-0.0176
	Y	0.0000	0.0190	-0.0081	0.0244	0.0308	-0.0004
	Z	-0.0347	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	0.0000	-0.0019	-0.0465	-0.0646	0.0362	-0.0176
	Y	0.0000	0.0190	-0.0081	-0.0244	0.0308	-0.0004
	Z	0.0347	0.0000	0.0000	0.0000	0.0000	0.0000

FREQ(CM**-1) 172.35 186.53 188.76 194.80 195.67 201.61

AT. 1 FE X	0.0000	-0.0071	0.0000	0.0291	0.0000	0.0002
Y	0.0092	0.0000	0.0338	0.0000	-0.0211	0.0000
Z	0.0007	0.0000	0.0096	0.0000	0.0088	0.0000
AT. 2 FE X	0.0000	-0.0071	0.0000	-0.0291	0.0000	0.0002
Y	-0.0092	0.0000	-0.0338	0.0000	0.0211	0.0000
Z	0.0007	0.0000	0.0096	0.0000	0.0088	0.0000
AT. 3 FE X	0.0000	-0.0071	0.0000	0.0291	0.0000	-0.0002
Y	-0.0092	0.0000	0.0338	0.0000	-0.0211	0.0000
Z	-0.0007	0.0000	0.0096	0.0000	0.0088	0.0000
AT. 4 FE X	0.0000	-0.0071	0.0000	-0.0291	0.0000	-0.0002
Y	0.0092	0.0000	-0.0338	0.0000	0.0211	0.0000
Z	-0.0007	0.0000	0.0096	0.0000	0.0088	0.0000
AT. 5 AL X	0.0000	-0.0065	0.0000	0.0000	0.0000	-0.0072
Y	0.0000	0.0171	0.0000	0.0000	0.0000	0.0100
Z	0.0011	0.0000	-0.0065	-0.0026	-0.0134	0.0000
AT. 6 AL X	0.0000	-0.0065	0.0000	0.0000	0.0000	-0.0072
Y	0.0000	-0.0171	0.0000	0.0000	0.0000	-0.0100
Z	0.0011	0.0000	-0.0065	0.0026	-0.0134	0.0000
AT. 7 AL X	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0072
Y	0.0000	0.0171	0.0000	0.0000	0.0000	-0.0100
Z	-0.0011	0.0000	-0.0065	-0.0026	-0.0134	0.0000
AT. 8 AL X	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0072
Y	0.0000	-0.0171	0.0000	0.0000	0.0000	0.0100
Z	-0.0011	0.0000	-0.0065	0.0026	-0.0134	0.0000
AT. 9 AL X	0.0003	0.0078	0.0000	0.0000	0.0000	0.0000
Y	0.0117	0.0133	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0106	-0.0044	0.0071	-0.0114
AT. 10 AL X	-0.0003	0.0078	0.0000	0.0000	0.0000	0.0000
Y	-0.0117	0.0133	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0106	-0.0044	0.0071	0.0114
AT. 11 AL X	-0.0003	0.0078	0.0000	0.0000	0.0000	0.0000
Y	0.0117	-0.0133	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0106	0.0044	0.0071	0.0114
AT. 12 AL X	0.0003	0.0078	0.0000	0.0000	0.0000	0.0000
Y	-0.0117	-0.0133	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0106	0.0044	0.0071	-0.0114
AT. 13 SI X	0.0000	0.0070	0.0000	0.0000	0.0000	0.0079
Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Z	0.0004	0.0000	-0.0091	0.0000	-0.0131	0.0000
AT. 14 SI X	0.0000	0.0070	0.0000	0.0000	0.0000	-0.0079
Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Z	-0.0004	0.0000	-0.0091	0.0000	-0.0131	0.0000
AT. 15 SI X	-0.0224	0.0022	0.0000	0.0000	0.0000	0.0000
Y	-0.0112	0.0074	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0025	0.0145	0.0055	0.0113
AT. 16 SI X	0.0224	0.0022	0.0000	0.0000	0.0000	0.0000
Y	0.0112	0.0074	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0025	0.0145	0.0055	-0.0113
AT. 17 SI X	0.0224	0.0022	0.0000	0.0000	0.0000	0.0000
Y	-0.0112	-0.0074	0.0000	0.0000	0.0000	0.0000
Z	0.0000	0.0000	-0.0025	-0.0145	0.0055	-0.0113
AT. 18 SI X	-0.0224	0.0022	0.0000	0.0000	0.0000	0.0000

	Y	0.0112	-0.0074	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0025	-0.0145	0.0055	0.0113
AT. 19	SI X	0.0078	0.0008	0.0000	0.0000	0.0000	0.0000
	Y	-0.0257	0.0106	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0128	-0.0044	-0.0024	-0.0170
AT. 20	SI X	-0.0078	0.0008	0.0000	0.0000	0.0000	0.0000
	Y	0.0257	0.0106	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0128	-0.0044	-0.0024	0.0170
AT. 21	SI X	-0.0078	0.0008	0.0000	0.0000	0.0000	0.0000
	Y	-0.0257	-0.0106	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0128	0.0044	-0.0024	0.0170
AT. 22	SI X	0.0078	0.0008	0.0000	0.0000	0.0000	0.0000
	Y	0.0257	-0.0106	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0128	0.0044	-0.0024	-0.0170
AT. 23	O X	0.0195	-0.0041	-0.0159	0.0237	-0.0252	-0.0188
	Y	0.0014	-0.0181	0.0123	0.0059	-0.0019	0.0038
	Z	-0.0004	-0.0014	-0.0162	0.0020	-0.0138	-0.0227
AT. 24	O X	-0.0195	-0.0041	0.0159	-0.0237	0.0252	-0.0188
	Y	-0.0014	-0.0181	-0.0123	-0.0059	0.0019	0.0038
	Z	-0.0004	0.0014	-0.0162	0.0020	-0.0138	0.0227
AT. 25	O X	-0.0195	-0.0041	0.0159	0.0237	0.0252	-0.0188
	Y	0.0014	0.0181	0.0123	-0.0059	-0.0019	-0.0038
	Z	-0.0004	0.0014	-0.0162	-0.0020	-0.0138	0.0227
AT. 26	O X	0.0195	-0.0041	-0.0159	-0.0237	-0.0252	-0.0188
	Y	-0.0014	0.0181	-0.0123	0.0059	0.0019	-0.0038
	Z	-0.0004	-0.0014	-0.0162	-0.0020	-0.0138	-0.0227
AT. 27	O X	-0.0195	-0.0041	-0.0159	0.0237	-0.0252	0.0188
	Y	-0.0014	-0.0181	0.0123	0.0059	-0.0019	-0.0038
	Z	0.0004	-0.0014	-0.0162	0.0020	-0.0138	0.0227
AT. 28	O X	0.0195	-0.0041	0.0159	-0.0237	0.0252	0.0188
	Y	0.0014	-0.0181	-0.0123	-0.0059	0.0019	-0.0038
	Z	0.0004	0.0014	-0.0162	0.0020	-0.0138	-0.0227
AT. 29	O X	0.0195	-0.0041	0.0159	0.0237	0.0252	0.0188
	Y	-0.0014	0.0181	0.0123	-0.0059	-0.0019	0.0038
	Z	0.0004	0.0014	-0.0162	-0.0020	-0.0138	-0.0227
AT. 30	O X	-0.0195	-0.0041	-0.0159	-0.0237	-0.0252	0.0188
	Y	0.0014	0.0181	-0.0123	0.0059	0.0019	0.0038
	Z	0.0004	-0.0014	-0.0162	-0.0020	-0.0138	0.0227
AT. 31	O X	-0.0099	0.0128	0.0028	-0.0083	-0.0147	0.0065
	Y	0.0085	-0.0112	-0.0070	0.0002	0.0251	-0.0239
	Z	0.0011	0.0044	-0.0047	0.0035	-0.0160	0.0256
AT. 32	O X	0.0099	0.0128	-0.0028	0.0083	0.0147	0.0065
	Y	-0.0085	-0.0112	0.0070	-0.0002	-0.0251	-0.0239
	Z	0.0011	-0.0044	-0.0047	0.0035	-0.0160	-0.0256
AT. 33	O X	0.0099	0.0128	-0.0028	-0.0083	0.0147	0.0065
	Y	0.0085	0.0112	-0.0070	-0.0002	0.0251	0.0239
	Z	0.0011	-0.0044	-0.0047	-0.0035	-0.0160	-0.0256
AT. 34	O X	-0.0099	0.0128	0.0028	0.0083	-0.0147	0.0065
	Y	-0.0085	0.0112	0.0070	0.0002	-0.0251	0.0239
	Z	0.0011	0.0044	-0.0047	-0.0035	-0.0160	0.0256
AT. 35	O X	0.0099	0.0128	0.0028	-0.0083	-0.0147	-0.0065
	Y	-0.0085	-0.0112	-0.0070	0.0002	0.0251	0.0239
	Z	-0.0011	0.0044	-0.0047	0.0035	-0.0160	-0.0256
AT. 36	O X	-0.0099	0.0128	-0.0028	0.0083	0.0147	-0.0065

	Y	0.0085	-0.0112	0.0070	-0.0002	-0.0251	0.0239
	Z	-0.0011	-0.0044	-0.0047	0.0035	-0.0160	0.0256
AT. 37	O X	-0.0099	0.0128	-0.0028	-0.0083	0.0147	-0.0065
	Y	-0.0085	0.0112	-0.0070	-0.0002	0.0251	-0.0239
	Z	-0.0011	-0.0044	-0.0047	-0.0035	-0.0160	0.0256
AT. 38	O X	0.0099	0.0128	0.0028	0.0083	-0.0147	-0.0065
	Y	0.0085	0.0112	0.0070	0.0002	-0.0251	-0.0239
	Z	-0.0011	0.0044	-0.0047	-0.0035	-0.0160	-0.0256
AT. 39	O X	0.0108	-0.0119	0.0051	0.0124	0.0109	0.0194
	Y	0.0173	0.0063	0.0246	0.0126	0.0133	0.0192
	Z	-0.0005	-0.0010	-0.0042	-0.0079	-0.0147	-0.0336
AT. 40	O X	-0.0108	-0.0119	-0.0051	-0.0124	-0.0109	0.0194
	Y	-0.0173	0.0063	-0.0246	-0.0126	-0.0133	0.0192
	Z	-0.0005	0.0010	-0.0042	-0.0079	-0.0147	0.0336
AT. 41	O X	-0.0108	-0.0119	-0.0051	0.0124	-0.0109	0.0194
	Y	0.0173	-0.0063	0.0246	-0.0126	0.0133	-0.0192
	Z	-0.0005	0.0010	-0.0042	0.0079	-0.0147	0.0336
AT. 42	O X	0.0108	-0.0119	0.0051	-0.0124	0.0109	0.0194
	Y	-0.0173	-0.0063	-0.0246	0.0126	-0.0133	-0.0192
	Z	-0.0005	-0.0010	-0.0042	0.0079	-0.0147	-0.0336
AT. 43	O X	-0.0108	-0.0119	0.0051	0.0124	0.0109	-0.0194
	Y	-0.0173	0.0063	0.0246	0.0126	0.0133	-0.0192
	Z	0.0005	-0.0010	-0.0042	-0.0079	-0.0147	0.0336
AT. 44	O X	0.0108	-0.0119	-0.0051	-0.0124	-0.0109	-0.0194
	Y	0.0173	0.0063	-0.0246	-0.0126	-0.0133	-0.0192
	Z	0.0005	0.0010	-0.0042	-0.0079	-0.0147	-0.0336
AT. 45	O X	0.0108	-0.0119	-0.0051	0.0124	-0.0109	-0.0194
	Y	-0.0173	-0.0063	0.0246	-0.0126	0.0133	0.0192
	Z	0.0005	0.0010	-0.0042	0.0079	-0.0147	-0.0336
AT. 46	O X	-0.0108	-0.0119	0.0051	-0.0124	0.0109	-0.0194
	Y	0.0173	-0.0063	-0.0246	0.0126	-0.0133	0.0192
	Z	0.0005	-0.0010	-0.0042	0.0079	-0.0147	0.0336
AT. 47	O X	0.0128	-0.0064	0.0000	0.0000	0.0000	0.0000
	Y	-0.0562	0.0615	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	-0.0353	0.0279	-0.0006
AT. 48	O X	-0.0128	-0.0064	0.0000	0.0000	0.0000	0.0000
	Y	0.0562	0.0615	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	-0.0353	0.0279	0.0006
AT. 49	O X	-0.0128	-0.0064	0.0000	0.0000	0.0000	0.0000
	Y	-0.0562	-0.0615	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	0.0353	0.0279	0.0006
AT. 50	O X	0.0128	-0.0064	0.0000	0.0000	0.0000	0.0000
	Y	0.0562	-0.0615	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0029	0.0353	0.0279	-0.0006
AT. 51	O X	-0.0389	-0.0212	0.0000	0.0000	0.0000	0.0000
	Y	-0.0288	-0.0176	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0108	0.0535	0.0363	0.0047
AT. 52	O X	0.0389	-0.0212	0.0000	0.0000	0.0000	0.0000
	Y	0.0288	-0.0176	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0108	0.0535	0.0363	-0.0047
AT. 53	O X	0.0389	-0.0212	0.0000	0.0000	0.0000	0.0000
	Y	-0.0288	0.0176	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0108	-0.0535	0.0363	-0.0047
AT. 54	O X	-0.0389	-0.0212	0.0000	0.0000	0.0000	0.0000

	Y	0.0288	0.0176	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0108	-0.0535	0.0363	0.0047
AT. 55	O X	-0.0113	0.0480	0.0000	0.0000	0.0000	0.0000
	Y	-0.0175	-0.0057	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0460	-0.0039	0.0143	-0.0002
AT. 56	O X	0.0113	0.0480	0.0000	0.0000	0.0000	0.0000
	Y	0.0175	-0.0057	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0460	-0.0039	0.0143	0.0002
AT. 57	O X	0.0113	0.0480	0.0000	0.0000	0.0000	0.0000
	Y	-0.0175	0.0057	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0460	0.0039	0.0143	0.0002
AT. 58	O X	-0.0113	0.0480	0.0000	0.0000	0.0000	0.0000
	Y	0.0175	0.0057	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0460	0.0039	0.0143	-0.0002

FREQ(CM**-1) 202.42 206.44 208.59 211.99 213.55 213.95

AT. 1	FE X	0.0000	0.0000	-0.0039	0.0000	0.0062	0.0061
	Y	-0.0025	0.0014	0.0000	0.0362	0.0000	0.0000
	Z	-0.0187	0.0000	0.0000	0.0102	0.0000	0.0000
AT. 2	FE X	0.0000	0.0000	-0.0039	0.0000	-0.0062	0.0061
	Y	-0.0025	0.0014	0.0000	-0.0362	0.0000	0.0000
	Z	0.0187	0.0000	0.0000	0.0102	0.0000	0.0000
AT. 3	FE X	0.0000	0.0000	0.0039	0.0000	0.0062	-0.0061
	Y	-0.0025	-0.0014	0.0000	-0.0362	0.0000	0.0000
	Z	-0.0187	0.0000	0.0000	-0.0102	0.0000	0.0000
AT. 4	FE X	0.0000	0.0000	0.0039	0.0000	-0.0062	-0.0061
	Y	-0.0025	-0.0014	0.0000	0.0362	0.0000	0.0000
	Z	0.0187	0.0000	0.0000	-0.0102	0.0000	0.0000
AT. 5	AL X	0.0007	0.0050	0.0192	0.0000	0.0000	0.0027
	Y	0.0016	-0.0094	-0.0110	0.0000	0.0000	0.0138
	Z	0.0000	0.0000	0.0000	0.0011	-0.0024	0.0000
AT. 6	AL X	-0.0007	-0.0050	0.0192	0.0000	0.0000	0.0027
	Y	0.0016	-0.0094	0.0110	0.0000	0.0000	-0.0138
	Z	0.0000	0.0000	0.0000	0.0011	0.0024	0.0000
AT. 7	AL X	0.0007	-0.0050	-0.0192	0.0000	0.0000	-0.0027
	Y	0.0016	0.0094	0.0110	0.0000	0.0000	-0.0138
	Z	0.0000	0.0000	0.0000	-0.0011	-0.0024	0.0000
AT. 8	AL X	-0.0007	0.0050	-0.0192	0.0000	0.0000	-0.0027
	Y	0.0016	0.0094	-0.0110	0.0000	0.0000	0.0138
	Z	0.0000	0.0000	0.0000	-0.0011	0.0024	0.0000
AT. 9	AL X	-0.0013	0.0000	0.0000	-0.0173	0.0000	0.0000
	Y	-0.0100	0.0000	0.0000	0.0054	0.0000	0.0000
	Z	0.0000	0.0040	-0.0174	0.0000	0.0103	-0.0138
AT. 10	AL X	-0.0013	0.0000	0.0000	0.0173	0.0000	0.0000
	Y	-0.0100	0.0000	0.0000	-0.0054	0.0000	0.0000
	Z	0.0000	-0.0040	0.0174	0.0000	0.0103	0.0138
AT. 11	AL X	0.0013	0.0000	0.0000	0.0173	0.0000	0.0000
	Y	-0.0100	0.0000	0.0000	0.0054	0.0000	0.0000
	Z	0.0000	0.0040	0.0174	0.0000	-0.0103	0.0138
AT. 12	AL X	0.0013	0.0000	0.0000	-0.0173	0.0000	0.0000
	Y	-0.0100	0.0000	0.0000	-0.0054	0.0000	0.0000
	Z	0.0000	-0.0040	-0.0174	0.0000	-0.0103	-0.0138
AT. 13	SI X	0.0000	0.0000	-0.0079	0.0000	0.0000	0.0208

	Y	-0.0181	0.0038	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0178	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0079	0.0000	0.0000	-0.0208
	Y	-0.0181	-0.0038	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0178	0.0000	0.0000
AT. 15	SI X	0.0100	0.0000	0.0000	-0.0112	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	0.0112	0.0000	0.0000
	Z	0.0000	-0.0234	-0.0136	0.0000	0.0098	-0.0082
AT. 16	SI X	0.0100	0.0000	0.0000	0.0112	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	-0.0112	0.0000	0.0000
	Z	0.0000	0.0234	0.0136	0.0000	0.0098	0.0082
AT. 17	SI X	-0.0100	0.0000	0.0000	0.0112	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	0.0112	0.0000	0.0000
	Z	0.0000	-0.0234	0.0136	0.0000	-0.0098	0.0082
AT. 18	SI X	-0.0100	0.0000	0.0000	-0.0112	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	-0.0112	0.0000	0.0000
	Z	0.0000	0.0234	-0.0136	0.0000	-0.0098	-0.0082
AT. 19	SI X	-0.0040	0.0000	0.0000	0.0068	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	0.0043	0.0000	0.0000
	Z	0.0000	-0.0270	0.0098	0.0000	0.0181	0.0077
AT. 20	SI X	-0.0040	0.0000	0.0000	-0.0068	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	-0.0043	0.0000	0.0000
	Z	0.0000	0.0270	-0.0098	0.0000	0.0181	-0.0077
AT. 21	SI X	0.0040	0.0000	0.0000	-0.0068	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	0.0043	0.0000	0.0000
	Z	0.0000	-0.0270	-0.0098	0.0000	-0.0181	-0.0077
AT. 22	SI X	0.0040	0.0000	0.0000	0.0068	0.0000	0.0000
	Y	0.0057	0.0000	0.0000	-0.0043	0.0000	0.0000
	Z	0.0000	0.0270	0.0098	0.0000	-0.0181	0.0077
AT. 23	O X	-0.0150	0.0039	-0.0049	0.0107	0.0205	-0.0085
	Y	-0.0019	0.0001	0.0067	0.0038	-0.0074	-0.0185
	Z	-0.0022	-0.0160	0.0064	0.0023	0.0104	0.0042
AT. 24	O X	-0.0150	0.0039	-0.0049	-0.0107	-0.0205	-0.0085
	Y	-0.0019	0.0001	0.0067	-0.0038	0.0074	-0.0185
	Z	0.0022	0.0160	-0.0064	0.0023	0.0104	-0.0042
AT. 25	O X	0.0150	-0.0039	-0.0049	-0.0107	0.0205	-0.0085
	Y	-0.0019	0.0001	-0.0067	0.0038	0.0074	0.0185
	Z	-0.0022	-0.0160	-0.0064	0.0023	-0.0104	-0.0042
AT. 26	O X	0.0150	-0.0039	-0.0049	0.0107	-0.0205	-0.0085
	Y	-0.0019	0.0001	-0.0067	-0.0038	-0.0074	0.0185
	Z	0.0022	0.0160	0.0064	0.0023	-0.0104	0.0042
AT. 27	O X	-0.0150	-0.0039	0.0049	-0.0107	0.0205	0.0085
	Y	-0.0019	-0.0001	-0.0067	-0.0038	-0.0074	0.0185
	Z	-0.0022	0.0160	-0.0064	-0.0023	0.0104	-0.0042
AT. 28	O X	-0.0150	-0.0039	0.0049	0.0107	-0.0205	0.0085
	Y	-0.0019	-0.0001	-0.0067	0.0038	0.0074	0.0185
	Z	0.0022	-0.0160	0.0064	-0.0023	0.0104	0.0042
AT. 29	O X	0.0150	0.0039	0.0049	0.0107	0.0205	0.0085
	Y	-0.0019	-0.0001	0.0067	-0.0038	0.0074	-0.0185
	Z	-0.0022	0.0160	0.0064	-0.0023	-0.0104	0.0042
AT. 30	O X	0.0150	0.0039	0.0049	-0.0107	-0.0205	0.0085
	Y	-0.0019	-0.0001	0.0067	0.0038	-0.0074	-0.0185
	Z	0.0022	-0.0160	-0.0064	-0.0023	-0.0104	-0.0042
AT. 31	O X	0.0013	-0.0027	-0.0115	0.0140	0.0021	0.0142

	Y	-0.0184	0.0067	-0.0117	-0.0114	-0.0050	0.0022
	Z	0.0036	-0.0010	0.0175	0.0122	-0.0002	0.0077
AT. 32	O X	0.0013	-0.0027	-0.0115	-0.0140	-0.0021	0.0142
	Y	-0.0184	0.0067	-0.0117	0.0114	0.0050	0.0022
	Z	-0.0036	0.0010	-0.0175	0.0122	-0.0002	-0.0077
AT. 33	O X	-0.0013	0.0027	-0.0115	-0.0140	0.0021	0.0142
	Y	-0.0184	0.0067	0.0117	-0.0114	0.0050	-0.0022
	Z	0.0036	-0.0010	-0.0175	0.0122	0.0002	-0.0077
AT. 34	O X	-0.0013	0.0027	-0.0115	0.0140	-0.0021	0.0142
	Y	-0.0184	0.0067	0.0117	0.0114	-0.0050	-0.0022
	Z	-0.0036	0.0010	0.0175	0.0122	0.0002	0.0077
AT. 35	O X	0.0013	0.0027	0.0115	-0.0140	0.0021	-0.0142
	Y	-0.0184	-0.0067	0.0117	0.0114	-0.0050	-0.0022
	Z	0.0036	0.0010	-0.0175	-0.0122	-0.0002	-0.0077
AT. 36	O X	0.0013	0.0027	0.0115	0.0140	-0.0021	-0.0142
	Y	-0.0184	-0.0067	0.0117	-0.0114	0.0050	-0.0022
	Z	-0.0036	-0.0010	0.0175	-0.0122	-0.0002	0.0077
AT. 37	O X	-0.0013	-0.0027	0.0115	0.0140	0.0021	-0.0142
	Y	-0.0184	-0.0067	-0.0117	0.0114	0.0050	0.0022
	Z	0.0036	0.0010	0.0175	-0.0122	0.0002	0.0077
AT. 38	O X	-0.0013	-0.0027	0.0115	-0.0140	-0.0021	-0.0142
	Y	-0.0184	-0.0067	-0.0117	-0.0114	-0.0050	0.0022
	Z	-0.0036	-0.0010	-0.0175	-0.0122	0.0002	-0.0077
AT. 39	O X	0.0014	-0.0029	0.0153	0.0018	-0.0145	-0.0052
	Y	0.0124	0.0056	-0.0146	0.0002	-0.0221	0.0060
	Z	-0.0014	0.0208	0.0067	-0.0001	0.0042	0.0056
AT. 40	O X	0.0014	-0.0029	0.0153	-0.0018	0.0145	-0.0052
	Y	0.0124	0.0056	-0.0146	-0.0002	0.0221	0.0060
	Z	0.0014	-0.0208	-0.0067	-0.0001	0.0042	-0.0056
AT. 41	O X	-0.0014	0.0029	0.0153	-0.0018	-0.0145	-0.0052
	Y	0.0124	0.0056	0.0146	0.0002	0.0221	-0.0060
	Z	-0.0014	0.0208	-0.0067	-0.0001	-0.0042	-0.0056
AT. 42	O X	-0.0014	0.0029	0.0153	0.0018	0.0145	-0.0052
	Y	0.0124	0.0056	0.0146	-0.0002	-0.0221	-0.0060
	Z	0.0014	-0.0208	0.0067	-0.0001	-0.0042	0.0056
AT. 43	O X	0.0014	0.0029	-0.0153	-0.0018	-0.0145	0.0052
	Y	0.0124	-0.0056	0.0146	-0.0002	-0.0221	-0.0060
	Z	-0.0014	-0.0208	-0.0067	0.0001	0.0042	-0.0056
AT. 44	O X	0.0014	0.0029	-0.0153	0.0018	0.0145	0.0052
	Y	0.0124	-0.0056	0.0146	0.0002	0.0221	-0.0060
	Z	0.0014	0.0208	0.0067	0.0001	0.0042	0.0056
AT. 45	O X	-0.0014	-0.0029	-0.0153	0.0018	-0.0145	0.0052
	Y	0.0124	-0.0056	-0.0146	-0.0002	0.0221	0.0060
	Z	-0.0014	-0.0208	0.0067	0.0001	-0.0042	0.0056
AT. 46	O X	-0.0014	-0.0029	-0.0153	-0.0018	0.0145	0.0052
	Y	0.0124	-0.0056	-0.0146	0.0002	-0.0221	0.0060
	Z	0.0014	0.0208	-0.0067	0.0001	-0.0042	-0.0056
AT. 47	O X	0.0014	0.0000	0.0000	0.0066	0.0000	0.0000
	Y	-0.0292	0.0000	0.0000	0.0095	0.0000	0.0000
	Z	0.0000	-0.0367	0.0543	0.0000	0.0408	-0.0065
AT. 48	O X	0.0014	0.0000	0.0000	-0.0066	0.0000	0.0000
	Y	-0.0292	0.0000	0.0000	-0.0095	0.0000	0.0000
	Z	0.0000	0.0367	-0.0543	0.0000	0.0408	0.0065
AT. 49	O X	-0.0014	0.0000	0.0000	-0.0066	0.0000	0.0000

	Y	-0.0292	0.0000	0.0000	0.0095	0.0000	0.0000
	Z	0.0000	-0.0367	-0.0543	0.0000	-0.0408	0.0065
AT. 50	O X	-0.0014	0.0000	0.0000	0.0066	0.0000	0.0000
	Y	-0.0292	0.0000	0.0000	-0.0095	0.0000	0.0000
	Z	0.0000	0.0367	0.0543	0.0000	-0.0408	-0.0065
AT. 51	O X	0.0403	0.0000	0.0000	0.0040	0.0000	0.0000
	Y	0.0366	0.0000	0.0000	0.0271	0.0000	0.0000
	Z	0.0000	-0.0354	-0.0217	0.0000	0.0200	-0.0705
AT. 52	O X	0.0403	0.0000	0.0000	-0.0040	0.0000	0.0000
	Y	0.0366	0.0000	0.0000	-0.0271	0.0000	0.0000
	Z	0.0000	0.0354	0.0217	0.0000	0.0200	0.0705
AT. 53	O X	-0.0403	0.0000	0.0000	-0.0040	0.0000	0.0000
	Y	0.0366	0.0000	0.0000	0.0271	0.0000	0.0000
	Z	0.0000	-0.0354	0.0217	0.0000	-0.0200	0.0705
AT. 54	O X	-0.0403	0.0000	0.0000	0.0040	0.0000	0.0000
	Y	0.0366	0.0000	0.0000	-0.0271	0.0000	0.0000
	Z	0.0000	0.0354	-0.0217	0.0000	-0.0200	-0.0705
AT. 55	O X	-0.0393	0.0000	0.0000	-0.0162	0.0000	0.0000
	Y	0.0206	0.0000	0.0000	0.0132	0.0000	0.0000
	Z	0.0000	-0.0495	-0.0362	0.0000	0.0550	0.0286
AT. 56	O X	-0.0393	0.0000	0.0000	0.0162	0.0000	0.0000
	Y	0.0206	0.0000	0.0000	-0.0132	0.0000	0.0000
	Z	0.0000	0.0495	0.0362	0.0000	0.0550	-0.0286
AT. 57	O X	0.0393	0.0000	0.0000	0.0162	0.0000	0.0000
	Y	0.0206	0.0000	0.0000	0.0132	0.0000	0.0000
	Z	0.0000	-0.0495	0.0362	0.0000	-0.0550	-0.0286
AT. 58	O X	0.0393	0.0000	0.0000	-0.0162	0.0000	0.0000
	Y	0.0206	0.0000	0.0000	-0.0132	0.0000	0.0000
	Z	0.0000	0.0495	-0.0362	0.0000	-0.0550	0.0286

FREQ(CM**-1) 216.23 226.34 229.29 232.65 234.90 239.24

AT. 1	FE X	0.0000	0.0000	0.0364	0.0167	0.0000	0.0000
	Y	-0.0004	0.0204	0.0000	0.0000	0.0255	-0.0058
	Z	0.0038	-0.0153	0.0000	0.0000	0.0010	-0.0111
AT. 2	FE X	0.0000	0.0000	-0.0364	-0.0167	0.0000	0.0000
	Y	0.0004	-0.0204	0.0000	0.0000	-0.0255	-0.0058
	Z	0.0038	-0.0153	0.0000	0.0000	0.0010	0.0111
AT. 3	FE X	0.0000	0.0000	-0.0364	0.0167	0.0000	0.0000
	Y	-0.0004	-0.0204	0.0000	0.0000	0.0255	0.0058
	Z	0.0038	0.0153	0.0000	0.0000	0.0010	0.0111
AT. 4	FE X	0.0000	0.0000	0.0364	-0.0167	0.0000	0.0000
	Y	0.0004	0.0204	0.0000	0.0000	-0.0255	0.0058
	Z	0.0038	0.0153	0.0000	0.0000	0.0010	-0.0111
AT. 5	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0133
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0095
	Z	-0.0005	-0.0168	-0.0131	0.0033	-0.0045	0.0000
AT. 6	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0133
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0095
	Z	-0.0005	-0.0168	0.0131	-0.0033	-0.0045	0.0000
AT. 7	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0133
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0095
	Z	-0.0005	0.0168	0.0131	0.0033	-0.0045	0.0000
AT. 8	AL X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0133

	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0095
	Z	-0.0005	0.0168	-0.0131	-0.0033	-0.0045	0.0000
AT. 9	AL X	0.0000	0.0205	0.0090	0.0000	0.0000	0.0000
	Y	0.0000	-0.0036	-0.0067	0.0000	0.0000	0.0000
	Z	0.0114	0.0000	0.0000	-0.0179	0.0023	-0.0084
AT. 10	AL X	0.0000	-0.0205	-0.0090	0.0000	0.0000	0.0000
	Y	0.0000	0.0036	0.0067	0.0000	0.0000	0.0000
	Z	0.0114	0.0000	0.0000	-0.0179	0.0023	0.0084
AT. 11	AL X	0.0000	-0.0205	0.0090	0.0000	0.0000	0.0000
	Y	0.0000	-0.0036	0.0067	0.0000	0.0000	0.0000
	Z	0.0114	0.0000	0.0000	0.0179	0.0023	-0.0084
AT. 12	AL X	0.0000	0.0205	-0.0090	0.0000	0.0000	0.0000
	Y	0.0000	0.0036	-0.0067	0.0000	0.0000	0.0000
	Z	0.0114	0.0000	0.0000	0.0179	0.0023	0.0084
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	0.0000	0.0124
	Z	0.0075	-0.0026	0.0000	0.0000	-0.0018	0.0000
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	0.0000	-0.0124
	Z	0.0075	0.0026	0.0000	0.0000	-0.0018	0.0000
AT. 15	SI X	0.0000	0.0085	0.0105	0.0000	0.0000	0.0000
	Y	0.0000	-0.0207	-0.0122	0.0000	0.0000	0.0000
	Z	-0.0116	0.0000	0.0000	-0.0026	0.0085	0.0092
AT. 16	SI X	0.0000	-0.0085	-0.0105	0.0000	0.0000	0.0000
	Y	0.0000	0.0207	0.0122	0.0000	0.0000	0.0000
	Z	-0.0116	0.0000	0.0000	-0.0026	0.0085	-0.0092
AT. 17	SI X	0.0000	-0.0085	0.0105	0.0000	0.0000	0.0000
	Y	0.0000	-0.0207	0.0122	0.0000	0.0000	0.0000
	Z	-0.0116	0.0000	0.0000	0.0026	0.0085	0.0092
AT. 18	SI X	0.0000	0.0085	-0.0105	0.0000	0.0000	0.0000
	Y	0.0000	0.0207	-0.0122	0.0000	0.0000	0.0000
	Z	-0.0116	0.0000	0.0000	0.0026	0.0085	-0.0092
AT. 19	SI X	0.0000	-0.0165	0.0028	0.0000	0.0000	0.0000
	Y	0.0000	-0.0167	-0.0104	0.0000	0.0000	0.0000
	Z	0.0018	0.0000	0.0000	0.0066	-0.0109	-0.0040
AT. 20	SI X	0.0000	0.0165	-0.0028	0.0000	0.0000	0.0000
	Y	0.0000	0.0167	0.0104	0.0000	0.0000	0.0000
	Z	0.0018	0.0000	0.0000	0.0066	-0.0109	0.0040
AT. 21	SI X	0.0000	0.0165	0.0028	0.0000	0.0000	0.0000
	Y	0.0000	-0.0167	0.0104	0.0000	0.0000	0.0000
	Z	0.0018	0.0000	0.0000	-0.0066	-0.0109	-0.0040
AT. 22	SI X	0.0000	-0.0165	-0.0028	0.0000	0.0000	0.0000
	Y	0.0000	0.0167	-0.0104	0.0000	0.0000	0.0000
	Z	0.0018	0.0000	0.0000	-0.0066	-0.0109	0.0040
AT. 23	O X	0.0188	-0.0119	0.0142	-0.0024	0.0129	0.0186
	Y	0.0007	-0.0113	0.0091	-0.0078	-0.0154	-0.0005
	Z	0.0021	-0.0054	0.0039	0.0035	0.0205	0.0208
AT. 24	O X	-0.0188	0.0119	-0.0142	0.0024	-0.0129	0.0186
	Y	-0.0007	0.0113	-0.0091	0.0078	0.0154	-0.0005
	Z	0.0021	-0.0054	0.0039	0.0035	0.0205	-0.0208
AT. 25	O X	-0.0188	0.0119	0.0142	-0.0024	-0.0129	-0.0186
	Y	0.0007	-0.0113	-0.0091	0.0078	-0.0154	-0.0005
	Z	0.0021	-0.0054	-0.0039	-0.0035	0.0205	0.0208
AT. 26	O X	0.0188	-0.0119	-0.0142	0.0024	0.0129	-0.0186

	Y	-0.0007	0.0113	0.0091	-0.0078	0.0154	-0.0005
	Z	0.0021	-0.0054	-0.0039	-0.0035	0.0205	-0.0208
AT. 27	O X	0.0188	0.0119	-0.0142	-0.0024	0.0129	-0.0186
	Y	0.0007	0.0113	-0.0091	-0.0078	-0.0154	0.0005
	Z	0.0021	0.0054	-0.0039	0.0035	0.0205	-0.0208
AT. 28	O X	-0.0188	-0.0119	0.0142	0.0024	-0.0129	-0.0186
	Y	-0.0007	-0.0113	0.0091	0.0078	0.0154	0.0005
	Z	0.0021	0.0054	-0.0039	0.0035	0.0205	0.0208
AT. 29	O X	-0.0188	-0.0119	-0.0142	-0.0024	-0.0129	0.0186
	Y	0.0007	0.0113	0.0091	0.0078	-0.0154	0.0005
	Z	0.0021	0.0054	0.0039	-0.0035	0.0205	-0.0208
AT. 30	O X	0.0188	0.0119	0.0142	0.0024	0.0129	0.0186
	Y	-0.0007	-0.0113	-0.0091	-0.0078	0.0154	0.0005
	Z	0.0021	0.0054	0.0039	-0.0035	0.0205	0.0208
AT. 31	O X	-0.0074	-0.0041	-0.0037	-0.0076	-0.0022	0.0102
	Y	0.0051	0.0017	0.0052	0.0095	0.0090	0.0182
	Z	0.0078	-0.0031	-0.0020	0.0017	-0.0062	-0.0185
AT. 32	O X	0.0074	0.0041	0.0037	0.0076	0.0022	0.0102
	Y	-0.0051	-0.0017	-0.0052	-0.0095	-0.0090	0.0182
	Z	0.0078	-0.0031	-0.0020	0.0017	-0.0062	0.0185
AT. 33	O X	0.0074	0.0041	-0.0037	-0.0076	0.0022	-0.0102
	Y	0.0051	0.0017	-0.0052	-0.0095	0.0090	0.0182
	Z	0.0078	-0.0031	0.0020	-0.0017	-0.0062	-0.0185
AT. 34	O X	-0.0074	-0.0041	0.0037	0.0076	-0.0022	-0.0102
	Y	-0.0051	-0.0017	0.0052	0.0095	-0.0090	0.0182
	Z	0.0078	-0.0031	0.0020	-0.0017	-0.0062	0.0185
AT. 35	O X	-0.0074	0.0041	0.0037	-0.0076	-0.0022	-0.0102
	Y	0.0051	-0.0017	-0.0052	0.0095	0.0090	-0.0182
	Z	0.0078	0.0031	0.0020	0.0017	-0.0062	0.0185
AT. 36	O X	0.0074	-0.0041	-0.0037	0.0076	0.0022	-0.0102
	Y	-0.0051	0.0017	0.0052	-0.0095	-0.0090	-0.0182
	Z	0.0078	0.0031	0.0020	0.0017	-0.0062	-0.0185
AT. 37	O X	0.0074	-0.0041	0.0037	-0.0076	0.0022	0.0102
	Y	0.0051	-0.0017	0.0052	-0.0095	0.0090	-0.0182
	Z	0.0078	0.0031	-0.0020	-0.0017	-0.0062	0.0185
AT. 38	O X	-0.0074	0.0041	-0.0037	0.0076	-0.0022	0.0102
	Y	-0.0051	0.0017	-0.0052	0.0095	-0.0090	-0.0182
	Z	0.0078	0.0031	-0.0020	-0.0017	-0.0062	-0.0185
AT. 39	O X	0.0185	-0.0047	-0.0044	0.0122	0.0109	-0.0054
	Y	0.0111	0.0170	-0.0002	-0.0043	0.0053	-0.0107
	Z	-0.0155	-0.0071	-0.0042	-0.0120	-0.0185	0.0128
AT. 40	O X	-0.0185	0.0047	0.0044	-0.0122	-0.0109	-0.0054
	Y	-0.0111	-0.0170	0.0002	0.0043	-0.0053	-0.0107
	Z	-0.0155	-0.0071	-0.0042	-0.0120	-0.0185	-0.0128
AT. 41	O X	-0.0185	0.0047	-0.0044	0.0122	-0.0109	0.0054
	Y	0.0111	0.0170	0.0002	0.0043	0.0053	-0.0107
	Z	-0.0155	-0.0071	0.0042	0.0120	-0.0185	0.0128
AT. 42	O X	0.0185	-0.0047	0.0044	-0.0122	0.0109	0.0054
	Y	-0.0111	-0.0170	-0.0002	-0.0043	-0.0053	-0.0107
	Z	-0.0155	-0.0071	0.0042	0.0120	-0.0185	-0.0128
AT. 43	O X	0.0185	0.0047	0.0044	0.0122	0.0109	0.0054
	Y	0.0111	-0.0170	0.0002	-0.0043	0.0053	0.0107
	Z	-0.0155	0.0071	0.0042	-0.0120	-0.0185	-0.0128
AT. 44	O X	-0.0185	-0.0047	-0.0044	-0.0122	-0.0109	0.0054

	Y	-0.0111	0.0170	-0.0002	0.0043	-0.0053	0.0107
	Z	-0.0155	0.0071	0.0042	-0.0120	-0.0185	0.0128
AT. 45	O X	-0.0185	-0.0047	0.0044	0.0122	-0.0109	-0.0054
	Y	0.0111	-0.0170	-0.0002	0.0043	0.0053	0.0107
	Z	-0.0155	0.0071	-0.0042	0.0120	-0.0185	-0.0128
AT. 46	O X	0.0185	0.0047	-0.0044	-0.0122	0.0109	-0.0054
	Y	-0.0111	0.0170	0.0002	-0.0043	-0.0053	0.0107
	Z	-0.0155	0.0071	-0.0042	0.0120	-0.0185	0.0128
AT. 47	O X	0.0000	-0.0181	0.0043	0.0000	0.0000	0.0000
	Y	0.0000	0.0003	-0.0324	0.0000	0.0000	0.0000
	Z	0.0553	0.0000	0.0000	-0.0280	0.0018	-0.0091
AT. 48	O X	0.0000	0.0181	-0.0043	0.0000	0.0000	0.0000
	Y	0.0000	-0.0003	0.0324	0.0000	0.0000	0.0000
	Z	0.0553	0.0000	0.0000	-0.0280	0.0018	0.0091
AT. 49	O X	0.0000	0.0181	0.0043	0.0000	0.0000	0.0000
	Y	0.0000	0.0003	0.0324	0.0000	0.0000	0.0000
	Z	0.0553	0.0000	0.0000	0.0280	0.0018	-0.0091
AT. 50	O X	0.0000	-0.0181	-0.0043	0.0000	0.0000	0.0000
	Y	0.0000	-0.0003	-0.0324	0.0000	0.0000	0.0000
	Z	0.0553	0.0000	0.0000	0.0280	0.0018	0.0091
AT. 51	O X	0.0000	0.0306	0.0130	0.0000	0.0000	0.0000
	Y	0.0000	0.0057	-0.0037	0.0000	0.0000	0.0000
	Z	-0.0496	0.0000	0.0000	-0.0534	0.0402	-0.0396
AT. 52	O X	0.0000	-0.0306	-0.0130	0.0000	0.0000	0.0000
	Y	0.0000	-0.0057	0.0037	0.0000	0.0000	0.0000
	Z	-0.0496	0.0000	0.0000	-0.0534	0.0402	0.0396
AT. 53	O X	0.0000	-0.0306	0.0130	0.0000	0.0000	0.0000
	Y	0.0000	0.0057	0.0037	0.0000	0.0000	0.0000
	Z	-0.0496	0.0000	0.0000	0.0534	0.0402	-0.0396
AT. 54	O X	0.0000	0.0306	-0.0130	0.0000	0.0000	0.0000
	Y	0.0000	-0.0057	-0.0037	0.0000	0.0000	0.0000
	Z	-0.0496	0.0000	0.0000	0.0534	0.0402	0.0396
AT. 55	O X	0.0000	-0.0113	-0.0202	0.0000	0.0000	0.0000
	Y	0.0000	-0.0139	-0.0028	0.0000	0.0000	0.0000
	Z	-0.0140	0.0000	0.0000	0.0420	-0.0293	0.0325
AT. 56	O X	0.0000	0.0113	0.0202	0.0000	0.0000	0.0000
	Y	0.0000	0.0139	0.0028	0.0000	0.0000	0.0000
	Z	-0.0140	0.0000	0.0000	0.0420	-0.0293	-0.0325
AT. 57	O X	0.0000	0.0113	-0.0202	0.0000	0.0000	0.0000
	Y	0.0000	-0.0139	0.0028	0.0000	0.0000	0.0000
	Z	-0.0140	0.0000	0.0000	-0.0420	-0.0293	0.0325
AT. 58	O X	0.0000	-0.0113	0.0202	0.0000	0.0000	0.0000
	Y	0.0000	0.0139	-0.0028	0.0000	0.0000	0.0000
	Z	-0.0140	0.0000	0.0000	-0.0420	-0.0293	-0.0325

FREQ(CM**-1) 246.77 248.32 255.86 258.18 258.32 259.19

AT. 1	FE X	0.0325	0.0000	0.0000	0.0105	0.0000	-0.0060
	Y	0.0000	0.0121	0.0143	0.0000	0.0026	0.0000
	Z	0.0000	-0.0054	0.0004	0.0000	0.0005	0.0000
AT. 2	FE X	-0.0325	0.0000	0.0000	0.0105	0.0000	-0.0060
	Y	0.0000	0.0121	-0.0143	0.0000	-0.0026	0.0000
	Z	0.0000	0.0054	0.0004	0.0000	0.0005	0.0000
AT. 3	FE X	0.0325	0.0000	0.0000	-0.0105	0.0000	-0.0060

	Y	0.0000	-0.0121	0.0143	0.0000	-0.0026	0.0000
	Z	0.0000	0.0054	0.0004	0.0000	-0.0005	0.0000
AT. 4	FE X	-0.0325	0.0000	0.0000	-0.0105	0.0000	-0.0060
	Y	0.0000	-0.0121	-0.0143	0.0000	0.0026	0.0000
	Z	0.0000	-0.0054	0.0004	0.0000	-0.0005	0.0000
AT. 5	AL X	0.0000	0.0023	0.0000	-0.0028	0.0000	-0.0194
	Y	0.0000	0.0026	0.0000	-0.0012	0.0000	-0.0031
	Z	-0.0002	0.0000	0.0020	0.0000	-0.0172	0.0000
AT. 6	AL X	0.0000	-0.0023	0.0000	-0.0028	0.0000	-0.0194
	Y	0.0000	0.0026	0.0000	0.0012	0.0000	0.0031
	Z	0.0002	0.0000	0.0020	0.0000	-0.0172	0.0000
AT. 7	AL X	0.0000	-0.0023	0.0000	0.0028	0.0000	-0.0194
	Y	0.0000	-0.0026	0.0000	0.0012	0.0000	-0.0031
	Z	-0.0002	0.0000	0.0020	0.0000	0.0172	0.0000
AT. 8	AL X	0.0000	0.0023	0.0000	0.0028	0.0000	-0.0194
	Y	0.0000	-0.0026	0.0000	-0.0012	0.0000	0.0031
	Z	0.0002	0.0000	0.0020	0.0000	0.0172	0.0000
AT. 9	AL X	0.0000	0.0000	0.0000	0.0000	-0.0019	0.0043
	Y	0.0000	0.0000	0.0000	0.0000	-0.0023	-0.0106
	Z	-0.0038	0.0112	0.0044	0.0023	0.0000	0.0000
AT. 10	AL X	0.0000	0.0000	0.0000	0.0000	0.0019	0.0043
	Y	0.0000	0.0000	0.0000	0.0000	0.0023	-0.0106
	Z	-0.0038	-0.0112	0.0044	-0.0023	0.0000	0.0000
AT. 11	AL X	0.0000	0.0000	0.0000	0.0000	0.0019	0.0043
	Y	0.0000	0.0000	0.0000	0.0000	-0.0023	0.0106
	Z	0.0038	0.0112	0.0044	-0.0023	0.0000	0.0000
AT. 12	AL X	0.0000	0.0000	0.0000	0.0000	-0.0019	0.0043
	Y	0.0000	0.0000	0.0000	0.0000	0.0023	0.0106
	Z	0.0038	-0.0112	0.0044	0.0023	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0016	0.0000	-0.0055
	Y	0.0000	-0.0199	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0019	0.0000	-0.0029	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	-0.0016	0.0000	-0.0055
	Y	0.0000	0.0199	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0019	0.0000	0.0029	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	0.0000	-0.0218	0.0217
	Y	0.0000	0.0000	0.0000	0.0000	-0.0059	-0.0107
	Z	-0.0042	0.0125	-0.0144	0.0190	0.0000	0.0000
AT. 16	SI X	0.0000	0.0000	0.0000	0.0000	0.0218	0.0217
	Y	0.0000	0.0000	0.0000	0.0000	0.0059	-0.0107
	Z	-0.0042	-0.0125	-0.0144	-0.0190	0.0000	0.0000
AT. 17	SI X	0.0000	0.0000	0.0000	0.0000	0.0218	0.0217
	Y	0.0000	0.0000	0.0000	0.0000	-0.0059	0.0107
	Z	0.0042	0.0125	-0.0144	-0.0190	0.0000	0.0000
AT. 18	SI X	0.0000	0.0000	0.0000	0.0000	-0.0218	0.0217
	Y	0.0000	0.0000	0.0000	0.0000	0.0059	0.0107
	Z	0.0042	-0.0125	-0.0144	0.0190	0.0000	0.0000
AT. 19	SI X	0.0000	0.0000	0.0000	0.0000	-0.0194	-0.0074
	Y	0.0000	0.0000	0.0000	0.0000	0.0066	-0.0072
	Z	-0.0043	-0.0165	0.0110	0.0134	0.0000	0.0000
AT. 20	SI X	0.0000	0.0000	0.0000	0.0000	0.0194	-0.0074
	Y	0.0000	0.0000	0.0000	0.0000	-0.0066	-0.0072
	Z	-0.0043	0.0165	0.0110	-0.0134	0.0000	0.0000
AT. 21	SI X	0.0000	0.0000	0.0000	0.0000	0.0194	-0.0074

	Y	0.0000	0.0000	0.0000	0.0000	0.0066	0.0072
	Z	0.0043	-0.0165	0.0110	-0.0134	0.0000	0.0000
AT. 22	SI X	0.0000	0.0000	0.0000	0.0000	-0.0194	-0.0074
	Y	0.0000	0.0000	0.0000	0.0000	-0.0066	0.0072
	Z	0.0043	0.0165	0.0110	0.0134	0.0000	0.0000
AT. 23	O X	-0.0086	0.0011	-0.0110	-0.0238	0.0180	0.0126
	Y	0.0036	-0.0090	0.0087	0.0185	-0.0023	0.0100
	Z	-0.0031	0.0156	-0.0205	-0.0351	-0.0046	-0.0029
AT. 24	O X	0.0086	0.0011	0.0110	-0.0238	-0.0180	0.0126
	Y	-0.0036	-0.0090	-0.0087	0.0185	0.0023	0.0100
	Z	-0.0031	-0.0156	-0.0205	0.0351	-0.0046	0.0029
AT. 25	O X	-0.0086	-0.0011	0.0110	-0.0238	-0.0180	0.0126
	Y	-0.0036	-0.0090	0.0087	-0.0185	-0.0023	-0.0100
	Z	0.0031	0.0156	-0.0205	0.0351	-0.0046	0.0029
AT. 26	O X	0.0086	-0.0011	-0.0110	-0.0238	0.0180	0.0126
	Y	0.0036	-0.0090	-0.0087	-0.0185	0.0023	-0.0100
	Z	0.0031	-0.0156	-0.0205	-0.0351	-0.0046	-0.0029
AT. 27	O X	-0.0086	-0.0011	-0.0110	0.0238	-0.0180	0.0126
	Y	0.0036	0.0090	0.0087	-0.0185	0.0023	0.0100
	Z	-0.0031	-0.0156	-0.0205	0.0351	0.0046	-0.0029
AT. 28	O X	0.0086	-0.0011	0.0110	0.0238	0.0180	0.0126
	Y	-0.0036	0.0090	-0.0087	-0.0185	-0.0023	0.0100
	Z	-0.0031	0.0156	-0.0205	-0.0351	0.0046	0.0029
AT. 29	O X	-0.0086	0.0011	0.0110	0.0238	0.0180	0.0126
	Y	-0.0036	0.0090	0.0087	0.0185	0.0023	-0.0100
	Z	0.0031	-0.0156	-0.0205	-0.0351	0.0046	0.0029
AT. 30	O X	0.0086	0.0011	-0.0110	0.0238	-0.0180	0.0126
	Y	0.0036	0.0090	-0.0087	0.0185	-0.0023	-0.0100
	Z	0.0031	0.0156	-0.0205	0.0351	0.0046	-0.0029
AT. 31	O X	-0.0007	-0.0126	-0.0089	-0.0013	-0.0016	-0.0067
	Y	0.0029	-0.0218	0.0113	0.0052	0.0043	0.0051
	Z	-0.0022	0.0209	-0.0040	-0.0042	-0.0065	-0.0017
AT. 32	O X	0.0007	-0.0126	0.0089	-0.0013	0.0016	-0.0067
	Y	-0.0029	-0.0218	-0.0113	0.0052	-0.0043	0.0051
	Z	-0.0022	-0.0209	-0.0040	0.0042	-0.0065	0.0017
AT. 33	O X	-0.0007	0.0126	0.0089	-0.0013	0.0016	-0.0067
	Y	-0.0029	-0.0218	0.0113	-0.0052	0.0043	-0.0051
	Z	0.0022	0.0209	-0.0040	0.0042	-0.0065	0.0017
AT. 34	O X	0.0007	0.0126	-0.0089	-0.0013	-0.0016	-0.0067
	Y	0.0029	-0.0218	-0.0113	-0.0052	-0.0043	-0.0051
	Z	0.0022	-0.0209	-0.0040	-0.0042	-0.0065	-0.0017
AT. 35	O X	-0.0007	0.0126	-0.0089	0.0013	0.0016	-0.0067
	Y	0.0029	0.0218	0.0113	-0.0052	-0.0043	0.0051
	Z	-0.0022	-0.0209	-0.0040	0.0042	0.0065	-0.0017
AT. 36	O X	0.0007	0.0126	0.0089	0.0013	-0.0016	-0.0067
	Y	-0.0029	0.0218	-0.0113	-0.0052	0.0043	0.0051
	Z	-0.0022	0.0209	-0.0040	-0.0042	0.0065	0.0017
AT. 37	O X	-0.0007	-0.0126	0.0089	0.0013	-0.0016	-0.0067
	Y	-0.0029	0.0218	0.0113	0.0052	-0.0043	-0.0051
	Z	0.0022	-0.0209	-0.0040	-0.0042	0.0065	0.0017
AT. 38	O X	0.0007	-0.0126	-0.0089	0.0013	0.0016	-0.0067
	Y	0.0029	0.0218	-0.0113	0.0052	0.0043	-0.0051
	Z	0.0022	0.0209	-0.0040	0.0042	0.0065	-0.0017
AT. 39	O X	-0.0130	-0.0199	-0.0142	-0.0158	-0.0160	-0.0232

	Y	-0.0048	-0.0104	-0.0179	-0.0015	-0.0056	0.0085
	Z	0.0134	0.0287	0.0225	0.0209	-0.0023	0.0077
AT. 40	O X	0.0130	-0.0199	0.0142	-0.0158	0.0160	-0.0232
	Y	0.0048	-0.0104	0.0179	-0.0015	0.0056	0.0085
	Z	0.0134	-0.0287	0.0225	-0.0209	-0.0023	-0.0077
AT. 41	O X	-0.0130	0.0199	0.0142	-0.0158	0.0160	-0.0232
	Y	0.0048	-0.0104	-0.0179	0.0015	-0.0056	-0.0085
	Z	-0.0134	0.0287	0.0225	-0.0209	-0.0023	-0.0077
AT. 42	O X	0.0130	0.0199	-0.0142	-0.0158	-0.0160	-0.0232
	Y	-0.0048	-0.0104	0.0179	0.0015	0.0056	-0.0085
	Z	-0.0134	-0.0287	0.0225	0.0209	-0.0023	0.0077
AT. 43	O X	-0.0130	0.0199	-0.0142	0.0158	0.0160	-0.0232
	Y	-0.0048	0.0104	-0.0179	0.0015	0.0056	0.0085
	Z	0.0134	-0.0287	0.0225	-0.0209	0.0023	0.0077
AT. 44	O X	0.0130	0.0199	0.0142	0.0158	-0.0160	-0.0232
	Y	0.0048	0.0104	0.0179	0.0015	-0.0056	0.0085
	Z	0.0134	0.0287	0.0225	0.0209	0.0023	-0.0077
AT. 45	O X	-0.0130	-0.0199	0.0142	0.0158	-0.0160	-0.0232
	Y	0.0048	0.0104	-0.0179	-0.0015	0.0056	-0.0085
	Z	-0.0134	-0.0287	0.0225	0.0209	0.0023	-0.0077
AT. 46	O X	0.0130	-0.0199	-0.0142	0.0158	0.0160	-0.0232
	Y	-0.0048	0.0104	0.0179	-0.0015	-0.0056	-0.0085
	Z	-0.0134	0.0287	0.0225	-0.0209	0.0023	0.0077
AT. 47	O X	0.0000	0.0000	0.0000	0.0000	-0.0194	-0.0052
	Y	0.0000	0.0000	0.0000	0.0000	0.0426	0.0073
	Z	0.0379	-0.0017	0.0275	0.0087	0.0000	0.0000
AT. 48	O X	0.0000	0.0000	0.0000	0.0000	0.0194	-0.0052
	Y	0.0000	0.0000	0.0000	0.0000	-0.0426	0.0073
	Z	0.0379	0.0017	0.0275	-0.0087	0.0000	0.0000
AT. 49	O X	0.0000	0.0000	0.0000	0.0000	0.0194	-0.0052
	Y	0.0000	0.0000	0.0000	0.0000	0.0426	-0.0073
	Z	-0.0379	-0.0017	0.0275	-0.0087	0.0000	0.0000
AT. 50	O X	0.0000	0.0000	0.0000	0.0000	-0.0194	-0.0052
	Y	0.0000	0.0000	0.0000	0.0000	-0.0426	-0.0073
	Z	-0.0379	0.0017	0.0275	0.0087	0.0000	0.0000
AT. 51	O X	0.0000	0.0000	0.0000	0.0000	-0.0307	0.0439
	Y	0.0000	0.0000	0.0000	0.0000	-0.0226	0.0205
	Z	-0.0192	0.0094	0.0104	-0.0067	0.0000	0.0000
AT. 52	O X	0.0000	0.0000	0.0000	0.0000	0.0307	0.0439
	Y	0.0000	0.0000	0.0000	0.0000	0.0226	0.0205
	Z	-0.0192	-0.0094	0.0104	0.0067	0.0000	0.0000
AT. 53	O X	0.0000	0.0000	0.0000	0.0000	0.0307	0.0439
	Y	0.0000	0.0000	0.0000	0.0000	-0.0226	-0.0205
	Z	0.0192	0.0094	0.0104	0.0067	0.0000	0.0000
AT. 54	O X	0.0000	0.0000	0.0000	0.0000	-0.0307	0.0439
	Y	0.0000	0.0000	0.0000	0.0000	0.0226	-0.0205
	Z	0.0192	-0.0094	0.0104	-0.0067	0.0000	0.0000
AT. 55	O X	0.0000	0.0000	0.0000	0.0000	-0.0058	0.0206
	Y	0.0000	0.0000	0.0000	0.0000	-0.0040	-0.0122
	Z	-0.0327	0.0096	-0.0378	-0.0072	0.0000	0.0000
AT. 56	O X	0.0000	0.0000	0.0000	0.0000	0.0058	0.0206
	Y	0.0000	0.0000	0.0000	0.0000	0.0040	-0.0122
	Z	-0.0327	-0.0096	-0.0378	0.0072	0.0000	0.0000
AT. 57	O X	0.0000	0.0000	0.0000	0.0000	0.0058	0.0206

	Y	0.0000	0.0000	0.0000	0.0000	-0.0040	0.0122
	Z	0.0327	0.0096	-0.0378	0.0072	0.0000	0.0000
AT. 58 O	X	0.0000	0.0000	0.0000	0.0000	-0.0058	0.0206
	Y	0.0000	0.0000	0.0000	0.0000	0.0040	0.0122
	Z	0.0327	-0.0096	-0.0378	-0.0072	0.0000	0.0000

FREQ(CM**-1) 265.92 270.57 270.84 274.81 277.78 291.26

AT. 1 FE	X	0.0151	-0.0028	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0081	0.0000	0.0033	-0.0251
	Z	0.0000	0.0000	0.0032	0.0000	-0.0095	0.0025
AT. 2 FE	X	-0.0151	0.0028	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0081	0.0000	0.0033	-0.0251
	Z	0.0000	0.0000	-0.0032	0.0000	0.0095	-0.0025
AT. 3 FE	X	-0.0151	-0.0028	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0081	0.0000	-0.0033	-0.0251
	Z	0.0000	0.0000	0.0032	0.0000	0.0095	0.0025
AT. 4 FE	X	0.0151	0.0028	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0081	0.0000	-0.0033	-0.0251
	Z	0.0000	0.0000	-0.0032	0.0000	-0.0095	-0.0025
AT. 5 AL	X	0.0000	0.0000	-0.0132	0.0005	0.0169	-0.0127
	Y	0.0000	0.0000	-0.0156	0.0103	0.0078	0.0093
	Z	-0.0065	-0.0050	0.0000	0.0000	0.0000	0.0000
AT. 6 AL	X	0.0000	0.0000	0.0132	0.0005	-0.0169	0.0127
	Y	0.0000	0.0000	-0.0156	-0.0103	0.0078	0.0093
	Z	0.0065	0.0050	0.0000	0.0000	0.0000	0.0000
AT. 7 AL	X	0.0000	0.0000	-0.0132	0.0005	-0.0169	-0.0127
	Y	0.0000	0.0000	-0.0156	0.0103	-0.0078	0.0093
	Z	0.0065	-0.0050	0.0000	0.0000	0.0000	0.0000
AT. 8 AL	X	0.0000	0.0000	0.0132	0.0005	0.0169	0.0127
	Y	0.0000	0.0000	-0.0156	-0.0103	-0.0078	0.0093
	Z	-0.0065	0.0050	0.0000	0.0000	0.0000	0.0000
AT. 9 AL	X	-0.0319	0.0000	0.0128	-0.0053	0.0000	0.0035
	Y	-0.0057	0.0000	0.0082	-0.0130	0.0000	0.0046
	Z	0.0000	0.0017	0.0000	0.0000	-0.0298	0.0000
AT. 10 AL	X	0.0319	0.0000	0.0128	-0.0053	0.0000	0.0035
	Y	0.0057	0.0000	0.0082	-0.0130	0.0000	0.0046
	Z	0.0000	0.0017	0.0000	0.0000	0.0298	0.0000
AT. 11 AL	X	-0.0319	0.0000	-0.0128	-0.0053	0.0000	-0.0035
	Y	0.0057	0.0000	0.0082	0.0130	0.0000	0.0046
	Z	0.0000	-0.0017	0.0000	0.0000	-0.0298	0.0000
AT. 12 AL	X	0.0319	0.0000	-0.0128	-0.0053	0.0000	-0.0035
	Y	-0.0057	0.0000	0.0082	0.0130	0.0000	0.0046
	Z	0.0000	-0.0017	0.0000	0.0000	0.0298	0.0000
AT. 13 SI	X	0.0000	0.0000	0.0000	0.0106	0.0000	0.0000
	Y	0.0000	0.0000	-0.0171	0.0000	-0.0295	-0.0115
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14 SI	X	0.0000	0.0000	0.0000	0.0106	0.0000	0.0000
	Y	0.0000	0.0000	-0.0171	0.0000	0.0295	-0.0115
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15 SI	X	-0.0137	0.0000	-0.0050	0.0047	0.0000	-0.0060
	Y	0.0186	0.0000	-0.0069	0.0070	0.0000	0.0136
	Z	0.0000	-0.0178	0.0000	0.0000	0.0099	0.0000
AT. 16 SI	X	0.0137	0.0000	-0.0050	0.0047	0.0000	-0.0060

	Y	-0.0186	0.0000	-0.0069	0.0070	0.0000	0.0136
	Z	0.0000	-0.0178	0.0000	0.0000	-0.0099	0.0000
AT. 17 SI	X	-0.0137	0.0000	0.0050	0.0047	0.0000	0.0060
	Y	-0.0186	0.0000	-0.0069	-0.0070	0.0000	0.0136
	Z	0.0000	0.0178	0.0000	0.0000	0.0099	0.0000
AT. 18 SI	X	0.0137	0.0000	0.0050	0.0047	0.0000	0.0060
	Y	0.0186	0.0000	-0.0069	-0.0070	0.0000	0.0136
	Z	0.0000	0.0178	0.0000	0.0000	-0.0099	0.0000
AT. 19 SI	X	0.0183	0.0000	-0.0018	-0.0067	0.0000	0.0127
	Y	0.0162	0.0000	0.0075	0.0101	0.0000	0.0115
	Z	0.0000	-0.0151	0.0000	0.0000	-0.0137	0.0000
AT. 20 SI	X	-0.0183	0.0000	-0.0018	-0.0067	0.0000	0.0127
	Y	-0.0162	0.0000	0.0075	0.0101	0.0000	0.0115
	Z	0.0000	-0.0151	0.0000	0.0000	0.0137	0.0000
AT. 21 SI	X	0.0183	0.0000	0.0018	-0.0067	0.0000	-0.0127
	Y	-0.0162	0.0000	0.0075	-0.0101	0.0000	0.0115
	Z	0.0000	0.0151	0.0000	0.0000	-0.0137	0.0000
AT. 22 SI	X	-0.0183	0.0000	0.0018	-0.0067	0.0000	-0.0127
	Y	0.0162	0.0000	0.0075	-0.0101	0.0000	0.0115
	Z	0.0000	0.0151	0.0000	0.0000	0.0137	0.0000
AT. 23 O	X	-0.0088	0.0189	0.0124	0.0060	-0.0103	0.0120
	Y	-0.0035	-0.0089	-0.0224	-0.0130	0.0006	0.0130
	Z	0.0012	0.0277	0.0093	0.0032	0.0040	0.0022
AT. 24 O	X	0.0088	-0.0189	0.0124	0.0060	-0.0103	0.0120
	Y	0.0035	0.0089	-0.0224	-0.0130	0.0006	0.0130
	Z	0.0012	0.0277	-0.0093	-0.0032	-0.0040	-0.0022
AT. 25 O	X	-0.0088	0.0189	-0.0124	0.0060	0.0103	-0.0120
	Y	0.0035	0.0089	-0.0224	0.0130	0.0006	0.0130
	Z	-0.0012	-0.0277	0.0093	-0.0032	0.0040	0.0022
AT. 26 O	X	0.0088	-0.0189	-0.0124	0.0060	0.0103	-0.0120
	Y	-0.0035	-0.0089	-0.0224	0.0130	0.0006	0.0130
	Z	-0.0012	-0.0277	-0.0093	0.0032	-0.0040	-0.0022
AT. 27 O	X	0.0088	0.0189	0.0124	0.0060	0.0103	0.0120
	Y	0.0035	-0.0089	-0.0224	-0.0130	-0.0006	0.0130
	Z	-0.0012	0.0277	0.0093	0.0032	-0.0040	0.0022
AT. 28 O	X	-0.0088	-0.0189	0.0124	0.0060	0.0103	0.0120
	Y	-0.0035	0.0089	-0.0224	-0.0130	-0.0006	0.0130
	Z	-0.0012	0.0277	-0.0093	-0.0032	0.0040	-0.0022
AT. 29 O	X	0.0088	0.0189	-0.0124	0.0060	-0.0103	-0.0120
	Y	-0.0035	0.0089	-0.0224	0.0130	-0.0006	0.0130
	Z	0.0012	-0.0277	0.0093	-0.0032	-0.0040	0.0022
AT. 30 O	X	-0.0088	-0.0189	-0.0124	0.0060	-0.0103	-0.0120
	Y	0.0035	-0.0089	-0.0224	0.0130	-0.0006	0.0130
	Z	0.0012	-0.0277	-0.0093	0.0032	0.0040	-0.0022
AT. 31 O	X	-0.0107	-0.0027	-0.0166	0.0054	0.0072	-0.0065
	Y	0.0059	0.0211	-0.0105	0.0416	-0.0047	-0.0149
	Z	0.0016	-0.0179	0.0115	-0.0284	-0.0244	0.0095
AT. 32 O	X	0.0107	0.0027	-0.0166	0.0054	0.0072	-0.0065
	Y	-0.0059	-0.0211	-0.0105	0.0416	-0.0047	-0.0149
	Z	0.0016	-0.0179	-0.0115	0.0284	0.0244	-0.0095
AT. 33 O	X	-0.0107	-0.0027	0.0166	0.0054	-0.0072	0.0065
	Y	-0.0059	-0.0211	-0.0105	-0.0416	-0.0047	-0.0149
	Z	-0.0016	0.0179	0.0115	0.0284	-0.0244	0.0095
AT. 34 O	X	0.0107	0.0027	0.0166	0.0054	-0.0072	0.0065

	Y	0.0059	0.0211	-0.0105	-0.0416	-0.0047	-0.0149
	Z	-0.0016	0.0179	-0.0115	-0.0284	0.0244	-0.0095
AT. 35	O X	0.0107	-0.0027	-0.0166	0.0054	-0.0072	-0.0065
	Y	-0.0059	0.0211	-0.0105	0.0416	0.0047	-0.0149
	Z	-0.0016	-0.0179	0.0115	-0.0284	0.0244	0.0095
AT. 36	O X	-0.0107	0.0027	-0.0166	0.0054	-0.0072	-0.0065
	Y	0.0059	-0.0211	-0.0105	0.0416	0.0047	-0.0149
	Z	-0.0016	-0.0179	-0.0115	0.0284	-0.0244	-0.0095
AT. 37	O X	0.0107	-0.0027	0.0166	0.0054	0.0072	0.0065
	Y	0.0059	-0.0211	-0.0105	-0.0416	0.0047	-0.0149
	Z	0.0016	0.0179	0.0115	0.0284	0.0244	0.0095
AT. 38	O X	-0.0107	0.0027	0.0166	0.0054	0.0072	0.0065
	Y	-0.0059	0.0211	-0.0105	-0.0416	0.0047	-0.0149
	Z	0.0016	0.0179	-0.0115	-0.0284	-0.0244	-0.0095
AT. 39	O X	-0.0083	-0.0155	0.0011	-0.0028	0.0088	-0.0149
	Y	0.0038	-0.0041	0.0044	-0.0047	0.0074	0.0131
	Z	0.0021	0.0215	-0.0012	-0.0030	0.0057	0.0002
AT. 40	O X	0.0083	0.0155	0.0011	-0.0028	0.0088	-0.0149
	Y	-0.0038	0.0041	0.0044	-0.0047	0.0074	0.0131
	Z	0.0021	0.0215	0.0012	0.0030	-0.0057	-0.0002
AT. 41	O X	-0.0083	-0.0155	-0.0011	-0.0028	-0.0088	0.0149
	Y	-0.0038	0.0041	0.0044	0.0047	0.0074	0.0131
	Z	-0.0021	-0.0215	-0.0012	0.0030	0.0057	0.0002
AT. 42	O X	0.0083	0.0155	-0.0011	-0.0028	-0.0088	0.0149
	Y	0.0038	-0.0041	0.0044	0.0047	0.0074	0.0131
	Z	-0.0021	-0.0215	0.0012	-0.0030	-0.0057	-0.0002
AT. 43	O X	0.0083	-0.0155	0.0011	-0.0028	-0.0088	-0.0149
	Y	-0.0038	-0.0041	0.0044	-0.0047	-0.0074	0.0131
	Z	-0.0021	0.0215	-0.0012	-0.0030	-0.0057	0.0002
AT. 44	O X	-0.0083	0.0155	0.0011	-0.0028	-0.0088	-0.0149
	Y	0.0038	0.0041	0.0044	-0.0047	-0.0074	0.0131
	Z	-0.0021	0.0215	0.0012	0.0030	0.0057	-0.0002
AT. 45	O X	0.0083	-0.0155	-0.0011	-0.0028	0.0088	0.0149
	Y	0.0038	0.0041	0.0044	0.0047	-0.0074	0.0131
	Z	0.0021	-0.0215	-0.0012	0.0030	-0.0057	0.0002
AT. 46	O X	-0.0083	0.0155	-0.0011	-0.0028	0.0088	0.0149
	Y	-0.0038	-0.0041	0.0044	0.0047	-0.0074	0.0131
	Z	0.0021	-0.0215	0.0012	-0.0030	0.0057	-0.0002
AT. 47	O X	0.0184	0.0000	-0.0042	-0.0080	0.0000	0.0102
	Y	0.0214	0.0000	0.0451	0.0038	0.0000	-0.0014
	Z	0.0000	-0.0220	0.0000	0.0000	-0.0030	0.0000
AT. 48	O X	-0.0184	0.0000	-0.0042	-0.0080	0.0000	0.0102
	Y	-0.0214	0.0000	0.0451	0.0038	0.0000	-0.0014
	Z	0.0000	-0.0220	0.0000	0.0000	0.0030	0.0000
AT. 49	O X	0.0184	0.0000	0.0042	-0.0080	0.0000	-0.0102
	Y	-0.0214	0.0000	0.0451	-0.0038	0.0000	-0.0014
	Z	0.0000	0.0220	0.0000	0.0000	-0.0030	0.0000
AT. 50	O X	-0.0184	0.0000	0.0042	-0.0080	0.0000	-0.0102
	Y	0.0214	0.0000	0.0451	-0.0038	0.0000	-0.0014
	Z	0.0000	0.0220	0.0000	0.0000	0.0030	0.0000
AT. 51	O X	-0.0161	0.0000	0.0082	-0.0045	0.0000	-0.0179
	Y	0.0135	0.0000	0.0065	-0.0066	0.0000	-0.0054
	Z	0.0000	-0.0036	0.0000	0.0000	0.0287	0.0000
AT. 52	O X	0.0161	0.0000	0.0082	-0.0045	0.0000	-0.0179

	Y	-0.0135	0.0000	0.0065	-0.0066	0.0000	-0.0054
	Z	0.0000	-0.0036	0.0000	0.0000	-0.0287	0.0000
AT. 53 O	X	-0.0161	0.0000	-0.0082	-0.0045	0.0000	0.0179
	Y	-0.0135	0.0000	0.0065	0.0066	0.0000	-0.0054
	Z	0.0000	0.0036	0.0000	0.0000	0.0287	0.0000
AT. 54 O	X	0.0161	0.0000	-0.0082	-0.0045	0.0000	0.0179
	Y	0.0135	0.0000	0.0065	0.0066	0.0000	-0.0054
	Z	0.0000	0.0036	0.0000	0.0000	-0.0287	0.0000
AT. 55 O	X	-0.0124	0.0000	-0.0187	-0.0023	0.0000	0.0019
	Y	0.0201	0.0000	0.0052	0.0087	0.0000	0.0126
	Z	0.0000	-0.0058	0.0000	0.0000	-0.0185	0.0000
AT. 56 O	X	0.0124	0.0000	-0.0187	-0.0023	0.0000	0.0019
	Y	-0.0201	0.0000	0.0052	0.0087	0.0000	0.0126
	Z	0.0000	-0.0058	0.0000	0.0000	0.0185	0.0000
AT. 57 O	X	-0.0124	0.0000	0.0187	-0.0023	0.0000	-0.0019
	Y	-0.0201	0.0000	0.0052	-0.0087	0.0000	0.0126
	Z	0.0000	0.0058	0.0000	0.0000	-0.0185	0.0000
AT. 58 O	X	0.0124	0.0000	0.0187	-0.0023	0.0000	-0.0019
	Y	0.0201	0.0000	0.0052	-0.0087	0.0000	0.0126
	Z	0.0000	0.0058	0.0000	0.0000	0.0185	0.0000

FREQ(CM**-1) 291.91 296.09 298.08 298.22 299.10 303.40

AT. 1 FE	X	0.0000	0.0125	-0.0099	0.0000	-0.0015	-0.0054
	Y	-0.0157	0.0000	0.0000	-0.0048	0.0000	0.0000
	Z	-0.0040	0.0000	0.0000	0.0007	0.0000	0.0000
AT. 2 FE	X	0.0000	-0.0125	-0.0099	0.0000	0.0015	-0.0054
	Y	0.0157	0.0000	0.0000	0.0048	0.0000	0.0000
	Z	-0.0040	0.0000	0.0000	0.0007	0.0000	0.0000
AT. 3 FE	X	0.0000	-0.0125	0.0099	0.0000	-0.0015	-0.0054
	Y	0.0157	0.0000	0.0000	0.0048	0.0000	0.0000
	Z	0.0040	0.0000	0.0000	-0.0007	0.0000	0.0000
AT. 4 FE	X	0.0000	0.0125	0.0099	0.0000	0.0015	-0.0054
	Y	-0.0157	0.0000	0.0000	-0.0048	0.0000	0.0000
	Z	0.0040	0.0000	0.0000	-0.0007	0.0000	0.0000
AT. 5 AL	X	0.0000	0.0000	0.0323	0.0000	0.0000	-0.0037
	Y	0.0000	0.0000	0.0197	0.0000	0.0000	-0.0138
	Z	-0.0120	0.0138	0.0000	0.0012	0.0006	0.0000
AT. 6 AL	X	0.0000	0.0000	0.0323	0.0000	0.0000	-0.0037
	Y	0.0000	0.0000	-0.0197	0.0000	0.0000	0.0138
	Z	-0.0120	-0.0138	0.0000	0.0012	-0.0006	0.0000
AT. 7 AL	X	0.0000	0.0000	-0.0323	0.0000	0.0000	-0.0037
	Y	0.0000	0.0000	-0.0197	0.0000	0.0000	-0.0138
	Z	0.0120	-0.0138	0.0000	-0.0012	0.0006	0.0000
AT. 8 AL	X	0.0000	0.0000	-0.0323	0.0000	0.0000	-0.0037
	Y	0.0000	0.0000	0.0197	0.0000	0.0000	0.0138
	Z	0.0120	0.0138	0.0000	-0.0012	-0.0006	0.0000
AT. 9 AL	X	-0.0029	0.0070	0.0000	-0.0031	0.0000	0.0111
	Y	0.0059	0.0075	0.0000	-0.0277	0.0000	0.0182
	Z	0.0000	0.0000	0.0074	0.0000	-0.0212	0.0000
AT. 10 AL	X	0.0029	-0.0070	0.0000	0.0031	0.0000	0.0111
	Y	-0.0059	-0.0075	0.0000	0.0277	0.0000	0.0182
	Z	0.0000	0.0000	-0.0074	0.0000	-0.0212	0.0000
AT. 11 AL	X	0.0029	0.0070	0.0000	0.0031	0.0000	0.0111

	Y	0.0059	-0.0075	0.0000	-0.0277	0.0000	-0.0182
	Z	0.0000	0.0000	-0.0074	0.0000	0.0212	0.0000
AT. 12	AL X	-0.0029	-0.0070	0.0000	-0.0031	0.0000	0.0111
	Y	-0.0059	0.0075	0.0000	0.0277	0.0000	-0.0182
	Z	0.0000	0.0000	0.0074	0.0000	0.0212	0.0000
AT. 13	SI X	0.0000	0.0000	0.0086	0.0000	0.0000	-0.0065
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0331	0.0000	0.0000	-0.0270	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	-0.0086	0.0000	0.0000	-0.0065
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	-0.0331	0.0000	0.0000	0.0270	0.0000	0.0000
AT. 15	SI X	-0.0067	-0.0095	0.0000	-0.0014	0.0000	-0.0106
	Y	-0.0056	0.0055	0.0000	-0.0059	0.0000	-0.0035
	Z	0.0000	0.0000	0.0113	0.0000	-0.0084	0.0000
AT. 16	SI X	0.0067	0.0095	0.0000	0.0014	0.0000	-0.0106
	Y	0.0056	-0.0055	0.0000	0.0059	0.0000	-0.0035
	Z	0.0000	0.0000	-0.0113	0.0000	-0.0084	0.0000
AT. 17	SI X	0.0067	-0.0095	0.0000	0.0014	0.0000	-0.0106
	Y	-0.0056	-0.0055	0.0000	-0.0059	0.0000	0.0035
	Z	0.0000	0.0000	-0.0113	0.0000	0.0084	0.0000
AT. 18	SI X	-0.0067	0.0095	0.0000	-0.0014	0.0000	-0.0106
	Y	0.0056	0.0055	0.0000	0.0059	0.0000	0.0035
	Z	0.0000	0.0000	0.0113	0.0000	0.0084	0.0000
AT. 19	SI X	-0.0053	-0.0165	0.0000	0.0021	0.0000	0.0097
	Y	-0.0061	0.0110	0.0000	0.0019	0.0000	-0.0031
	Z	0.0000	0.0000	0.0022	0.0000	-0.0095	0.0000
AT. 20	SI X	0.0053	0.0165	0.0000	-0.0021	0.0000	0.0097
	Y	0.0061	-0.0110	0.0000	-0.0019	0.0000	-0.0031
	Z	0.0000	0.0000	-0.0022	0.0000	-0.0095	0.0000
AT. 21	SI X	0.0053	-0.0165	0.0000	-0.0021	0.0000	0.0097
	Y	-0.0061	-0.0110	0.0000	0.0019	0.0000	0.0031
	Z	0.0000	0.0000	-0.0022	0.0000	0.0095	0.0000
AT. 22	SI X	-0.0053	0.0165	0.0000	0.0021	0.0000	0.0097
	Y	0.0061	0.0110	0.0000	-0.0019	0.0000	0.0031
	Z	0.0000	0.0000	0.0022	0.0000	0.0095	0.0000
AT. 23	O X	-0.0006	-0.0049	-0.0002	0.0020	0.0074	-0.0179
	Y	-0.0072	-0.0083	-0.0102	-0.0066	-0.0060	0.0196
	Z	-0.0046	0.0010	-0.0088	0.0016	0.0127	-0.0093
AT. 24	O X	0.0006	0.0049	-0.0002	-0.0020	-0.0074	-0.0179
	Y	0.0072	0.0083	-0.0102	0.0066	0.0060	0.0196
	Z	-0.0046	0.0010	0.0088	0.0016	0.0127	0.0093
AT. 25	O X	0.0006	-0.0049	-0.0002	-0.0020	0.0074	-0.0179
	Y	-0.0072	0.0083	0.0102	-0.0066	0.0060	-0.0196
	Z	-0.0046	-0.0010	0.0088	0.0016	-0.0127	0.0093
AT. 26	O X	-0.0006	0.0049	-0.0002	0.0020	-0.0074	-0.0179
	Y	0.0072	-0.0083	0.0102	0.0066	-0.0060	-0.0196
	Z	-0.0046	-0.0010	-0.0088	0.0016	-0.0127	-0.0093
AT. 27	O X	0.0006	0.0049	0.0002	-0.0020	0.0074	-0.0179
	Y	0.0072	0.0083	0.0102	0.0066	-0.0060	0.0196
	Z	0.0046	-0.0010	0.0088	-0.0016	0.0127	-0.0093
AT. 28	O X	-0.0006	-0.0049	0.0002	0.0020	-0.0074	-0.0179
	Y	-0.0072	-0.0083	0.0102	-0.0066	0.0060	0.0196
	Z	0.0046	-0.0010	-0.0088	-0.0016	0.0127	0.0093
AT. 29	O X	-0.0006	0.0049	0.0002	0.0020	0.0074	-0.0179

	Y	0.0072	-0.0083	-0.0102	0.0066	0.0060	-0.0196
	Z	0.0046	0.0010	-0.0088	-0.0016	-0.0127	0.0093
AT. 30	O X	0.0006	-0.0049	0.0002	-0.0020	-0.0074	-0.0179
	Y	-0.0072	0.0083	-0.0102	-0.0066	-0.0060	-0.0196
	Z	0.0046	0.0010	0.0088	-0.0016	-0.0127	-0.0093
AT. 31	O X	0.0213	0.0064	0.0142	0.0059	0.0000	0.0020
	Y	-0.0234	-0.0128	-0.0030	-0.0199	-0.0307	0.0124
	Z	0.0269	0.0061	-0.0015	-0.0084	0.0343	-0.0187
AT. 32	O X	-0.0213	-0.0064	0.0142	-0.0059	0.0000	0.0020
	Y	0.0234	0.0128	-0.0030	0.0199	0.0307	0.0124
	Z	0.0269	0.0061	0.0015	-0.0084	0.0343	0.0187
AT. 33	O X	-0.0213	0.0064	0.0142	-0.0059	0.0000	0.0020
	Y	-0.0234	0.0128	0.0030	-0.0199	0.0307	-0.0124
	Z	0.0269	-0.0061	0.0015	-0.0084	-0.0343	0.0187
AT. 34	O X	0.0213	-0.0064	0.0142	0.0059	0.0000	0.0020
	Y	0.0234	-0.0128	0.0030	0.0199	-0.0307	-0.0124
	Z	0.0269	-0.0061	-0.0015	-0.0084	-0.0343	-0.0187
AT. 35	O X	-0.0213	-0.0064	-0.0142	-0.0059	0.0000	0.0020
	Y	0.0234	0.0128	0.0030	0.0199	-0.0307	0.0124
	Z	-0.0269	-0.0061	0.0015	0.0084	0.0343	-0.0187
AT. 36	O X	0.0213	0.0064	-0.0142	0.0059	0.0000	0.0020
	Y	-0.0234	-0.0128	0.0030	-0.0199	0.0307	0.0124
	Z	-0.0269	-0.0061	-0.0015	0.0084	0.0343	0.0187
AT. 37	O X	0.0213	-0.0064	-0.0142	0.0059	0.0000	0.0020
	Y	0.0234	-0.0128	-0.0030	0.0199	0.0307	-0.0124
	Z	-0.0269	0.0061	-0.0015	0.0084	-0.0343	0.0187
AT. 38	O X	-0.0213	0.0064	-0.0142	-0.0059	0.0000	0.0020
	Y	-0.0234	0.0128	-0.0030	-0.0199	-0.0307	-0.0124
	Z	-0.0269	0.0061	0.0015	0.0084	-0.0343	-0.0187
AT. 39	O X	0.0001	0.0171	0.0098	0.0090	-0.0072	0.0154
	Y	0.0109	0.0138	-0.0166	-0.0016	-0.0034	0.0089
	Z	-0.0063	-0.0030	0.0054	-0.0059	0.0124	-0.0103
AT. 40	O X	-0.0001	-0.0171	0.0098	-0.0090	0.0072	0.0154
	Y	-0.0109	-0.0138	-0.0166	0.0016	0.0034	0.0089
	Z	-0.0063	-0.0030	-0.0054	-0.0059	0.0124	0.0103
AT. 41	O X	-0.0001	0.0171	0.0098	-0.0090	-0.0072	0.0154
	Y	0.0109	-0.0138	0.0166	-0.0016	0.0034	-0.0089
	Z	-0.0063	0.0030	-0.0054	-0.0059	-0.0124	0.0103
AT. 42	O X	0.0001	-0.0171	0.0098	0.0090	0.0072	0.0154
	Y	-0.0109	0.0138	0.0166	0.0016	-0.0034	-0.0089
	Z	-0.0063	0.0030	0.0054	-0.0059	-0.0124	-0.0103
AT. 43	O X	-0.0001	-0.0171	-0.0098	-0.0090	-0.0072	0.0154
	Y	-0.0109	-0.0138	0.0166	0.0016	-0.0034	0.0089
	Z	0.0063	0.0030	-0.0054	0.0059	0.0124	-0.0103
AT. 44	O X	0.0001	0.0171	-0.0098	0.0090	0.0072	0.0154
	Y	0.0109	0.0138	0.0166	-0.0016	0.0034	0.0089
	Z	0.0063	0.0030	0.0054	0.0059	0.0124	0.0103
AT. 45	O X	0.0001	-0.0171	-0.0098	0.0090	-0.0072	0.0154
	Y	-0.0109	0.0138	-0.0166	0.0016	0.0034	-0.0089
	Z	0.0063	-0.0030	0.0054	0.0059	-0.0124	0.0103
AT. 46	O X	-0.0001	0.0171	-0.0098	-0.0090	0.0072	0.0154
	Y	0.0109	-0.0138	-0.0166	-0.0016	-0.0034	-0.0089
	Z	0.0063	-0.0030	-0.0054	0.0059	-0.0124	-0.0103
AT. 47	O X	-0.0014	-0.0121	0.0000	0.0067	0.0000	0.0066

	Y	-0.0002	-0.0059	0.0000	-0.0045	0.0000	0.0264
	Z	0.0000	0.0000	-0.0289	0.0000	-0.0071	0.0000
AT. 48 O	X	0.0014	0.0121	0.0000	-0.0067	0.0000	0.0066
	Y	0.0002	0.0059	0.0000	0.0045	0.0000	0.0264
	Z	0.0000	0.0000	0.0289	0.0000	-0.0071	0.0000
AT. 49 O	X	0.0014	-0.0121	0.0000	-0.0067	0.0000	0.0066
	Y	-0.0002	0.0059	0.0000	-0.0045	0.0000	-0.0264
	Z	0.0000	0.0000	0.0289	0.0000	0.0071	0.0000
AT. 50 O	X	-0.0014	0.0121	0.0000	0.0067	0.0000	0.0066
	Y	0.0002	-0.0059	0.0000	0.0045	0.0000	-0.0264
	Z	0.0000	0.0000	-0.0289	0.0000	0.0071	0.0000
AT. 51 O	X	-0.0026	-0.0389	0.0000	0.0014	0.0000	0.0093
	Y	0.0002	-0.0312	0.0000	-0.0087	0.0000	0.0166
	Z	0.0000	0.0000	0.0011	0.0000	-0.0042	0.0000
AT. 52 O	X	0.0026	0.0389	0.0000	-0.0014	0.0000	0.0093
	Y	-0.0002	0.0312	0.0000	0.0087	0.0000	0.0166
	Z	0.0000	0.0000	-0.0011	0.0000	-0.0042	0.0000
AT. 53 O	X	0.0026	-0.0389	0.0000	-0.0014	0.0000	0.0093
	Y	0.0002	0.0312	0.0000	-0.0087	0.0000	-0.0166
	Z	0.0000	0.0000	-0.0011	0.0000	0.0042	0.0000
AT. 54 O	X	-0.0026	0.0389	0.0000	0.0014	0.0000	0.0093
	Y	-0.0002	-0.0312	0.0000	0.0087	0.0000	-0.0166
	Z	0.0000	0.0000	0.0011	0.0000	0.0042	0.0000
AT. 55 O	X	-0.0011	-0.0077	0.0000	-0.0503	0.0000	-0.0022
	Y	-0.0086	0.0056	0.0000	0.0134	0.0000	-0.0029
	Z	0.0000	0.0000	-0.0273	0.0000	-0.0034	0.0000
AT. 56 O	X	0.0011	0.0077	0.0000	0.0503	0.0000	-0.0022
	Y	0.0086	-0.0056	0.0000	-0.0134	0.0000	-0.0029
	Z	0.0000	0.0000	0.0273	0.0000	-0.0034	0.0000
AT. 57 O	X	0.0011	-0.0077	0.0000	0.0503	0.0000	-0.0022
	Y	-0.0086	-0.0056	0.0000	0.0134	0.0000	0.0029
	Z	0.0000	0.0000	0.0273	0.0000	0.0034	0.0000
AT. 58 O	X	-0.0011	0.0077	0.0000	-0.0503	0.0000	-0.0022
	Y	0.0086	0.0056	0.0000	-0.0134	0.0000	0.0029
	Z	0.0000	0.0000	-0.0273	0.0000	0.0034	0.0000

FREQ(CM**-1) 306.51 313.24 316.38 317.48 330.46 331.12

AT. 1 FE	X	-0.0129	0.0000	0.0245	0.0000	0.0163	0.0000
	Y	0.0000	-0.0088	0.0000	-0.0142	0.0000	0.0051
	Z	0.0000	0.0009	0.0000	-0.0004	0.0000	-0.0005
AT. 2 FE	X	0.0129	0.0000	0.0245	0.0000	0.0163	0.0000
	Y	0.0000	0.0088	0.0000	-0.0142	0.0000	-0.0051
	Z	0.0000	0.0009	0.0000	0.0004	0.0000	-0.0005
AT. 3 FE	X	0.0129	0.0000	0.0245	0.0000	-0.0163	0.0000
	Y	0.0000	0.0088	0.0000	0.0142	0.0000	0.0051
	Z	0.0000	-0.0009	0.0000	0.0004	0.0000	-0.0005
AT. 4 FE	X	-0.0129	0.0000	0.0245	0.0000	-0.0163	0.0000
	Y	0.0000	-0.0088	0.0000	0.0142	0.0000	-0.0051
	Z	0.0000	-0.0009	0.0000	-0.0004	0.0000	-0.0005
AT. 5 AL	X	0.0000	0.0000	-0.0058	0.0136	0.0126	0.0000
	Y	0.0000	0.0000	0.0104	0.0272	-0.0032	0.0000
	Z	-0.0181	-0.0021	0.0000	0.0000	0.0000	-0.0041
AT. 6 AL	X	0.0000	0.0000	-0.0058	-0.0136	0.0126	0.0000

	Y	0.0000	0.0000	-0.0104	0.0272	0.0032	0.0000
	Z	0.0181	-0.0021	0.0000	0.0000	0.0000	-0.0041
AT. 7	AL X	0.0000	0.0000	-0.0058	-0.0136	-0.0126	0.0000
	Y	0.0000	0.0000	0.0104	-0.0272	0.0032	0.0000
	Z	0.0181	0.0021	0.0000	0.0000	0.0000	-0.0041
AT. 8	AL X	0.0000	0.0000	-0.0058	0.0136	-0.0126	0.0000
	Y	0.0000	0.0000	-0.0104	-0.0272	-0.0032	0.0000
	Z	-0.0181	0.0021	0.0000	0.0000	0.0000	-0.0041
AT. 9	AL X	-0.0059	-0.0100	-0.0134	0.0000	0.0000	0.0000
	Y	0.0003	-0.0010	0.0118	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0097	0.0157	0.0218
AT. 10	AL X	0.0059	0.0100	-0.0134	0.0000	0.0000	0.0000
	Y	-0.0003	0.0010	0.0118	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0097	-0.0157	0.0218
AT. 11	AL X	-0.0059	0.0100	-0.0134	0.0000	0.0000	0.0000
	Y	-0.0003	-0.0010	-0.0118	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0097	-0.0157	0.0218
AT. 12	AL X	0.0059	-0.0100	-0.0134	0.0000	0.0000	0.0000
	Y	0.0003	0.0010	-0.0118	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0097	0.0157	0.0218
AT. 13	SI X	0.0000	0.0000	-0.0165	0.0000	-0.0357	0.0000
	Y	0.0000	0.0000	0.0000	0.0148	0.0000	0.0000
	Z	0.0000	-0.0066	0.0000	0.0000	0.0000	0.0173
AT. 14	SI X	0.0000	0.0000	-0.0165	0.0000	0.0357	0.0000
	Y	0.0000	0.0000	0.0000	-0.0148	0.0000	0.0000
	Z	0.0000	0.0066	0.0000	0.0000	0.0000	0.0173
AT. 15	SI X	0.0056	-0.0074	-0.0046	0.0000	0.0000	0.0000
	Y	0.0033	-0.0032	0.0114	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0082	0.0004	-0.0047
AT. 16	SI X	-0.0056	0.0074	-0.0046	0.0000	0.0000	0.0000
	Y	-0.0033	0.0032	0.0114	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0082	-0.0004	-0.0047
AT. 17	SI X	0.0056	0.0074	-0.0046	0.0000	0.0000	0.0000
	Y	-0.0033	-0.0032	-0.0114	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0082	-0.0004	-0.0047
AT. 18	SI X	-0.0056	-0.0074	-0.0046	0.0000	0.0000	0.0000
	Y	0.0033	0.0032	-0.0114	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0082	0.0004	-0.0047
AT. 19	SI X	0.0120	0.0093	-0.0005	0.0000	0.0000	0.0000
	Y	0.0105	-0.0095	-0.0043	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0068	-0.0019	-0.0020
AT. 20	SI X	-0.0120	-0.0093	-0.0005	0.0000	0.0000	0.0000
	Y	-0.0105	0.0095	-0.0043	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0068	0.0019	-0.0020
AT. 21	SI X	0.0120	-0.0093	-0.0005	0.0000	0.0000	0.0000
	Y	-0.0105	-0.0095	0.0043	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0068	0.0019	-0.0020
AT. 22	SI X	-0.0120	0.0093	-0.0005	0.0000	0.0000	0.0000
	Y	0.0105	0.0095	0.0043	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0068	-0.0019	-0.0020
AT. 23	O X	0.0252	0.0237	-0.0053	0.0022	-0.0020	0.0093
	Y	-0.0018	-0.0135	-0.0116	0.0208	0.0000	0.0019
	Z	0.0158	0.0154	-0.0018	0.0043	-0.0001	0.0009
AT. 24	O X	-0.0252	-0.0237	-0.0053	0.0022	-0.0020	-0.0093

	Y	0.0018	0.0135	-0.0116	0.0208	0.0000	-0.0019
	Z	0.0158	0.0154	0.0018	-0.0043	0.0001	0.0009
AT. 25	O X	0.0252	-0.0237	-0.0053	-0.0022	-0.0020	-0.0093
	Y	0.0018	-0.0135	0.0116	0.0208	0.0000	0.0019
	Z	-0.0158	0.0154	0.0018	0.0043	0.0001	0.0009
AT. 26	O X	-0.0252	0.0237	-0.0053	-0.0022	-0.0020	0.0093
	Y	-0.0018	0.0135	0.0116	0.0208	0.0000	-0.0019
	Z	-0.0158	0.0154	-0.0018	-0.0043	-0.0001	0.0009
AT. 27	O X	-0.0252	-0.0237	-0.0053	-0.0022	0.0020	0.0093
	Y	0.0018	0.0135	-0.0116	-0.0208	0.0000	0.0019
	Z	-0.0158	-0.0154	-0.0018	-0.0043	0.0001	0.0009
AT. 28	O X	0.0252	0.0237	-0.0053	-0.0022	0.0020	-0.0093
	Y	-0.0018	-0.0135	-0.0116	-0.0208	0.0000	-0.0019
	Z	-0.0158	-0.0154	0.0018	0.0043	-0.0001	0.0009
AT. 29	O X	-0.0252	0.0237	-0.0053	0.0022	0.0020	-0.0093
	Y	-0.0018	0.0135	0.0116	-0.0208	0.0000	0.0019
	Z	0.0158	-0.0154	0.0018	-0.0043	-0.0001	0.0009
AT. 30	O X	0.0252	-0.0237	-0.0053	0.0022	0.0020	0.0093
	Y	0.0018	-0.0135	0.0116	-0.0208	0.0000	-0.0019
	Z	0.0158	-0.0154	-0.0018	0.0043	0.0001	0.0009
AT. 31	O X	0.0033	-0.0008	-0.0189	0.0034	-0.0268	-0.0152
	Y	0.0030	0.0091	0.0015	-0.0034	-0.0117	0.0330
	Z	-0.0031	-0.0106	-0.0051	0.0111	-0.0011	-0.0041
AT. 32	O X	-0.0033	0.0008	-0.0189	0.0034	-0.0268	0.0152
	Y	-0.0030	-0.0091	0.0015	-0.0034	-0.0117	-0.0330
	Z	-0.0031	-0.0106	0.0051	-0.0111	0.0011	-0.0041
AT. 33	O X	0.0033	0.0008	-0.0189	-0.0034	-0.0268	0.0152
	Y	-0.0030	0.0091	-0.0015	-0.0034	0.0117	0.0330
	Z	0.0031	-0.0106	0.0051	0.0111	0.0011	-0.0041
AT. 34	O X	-0.0033	-0.0008	-0.0189	-0.0034	-0.0268	-0.0152
	Y	0.0030	-0.0091	-0.0015	-0.0034	0.0117	-0.0330
	Z	0.0031	-0.0106	-0.0051	-0.0111	-0.0011	-0.0041
AT. 35	O X	-0.0033	0.0008	-0.0189	-0.0034	0.0268	-0.0152
	Y	-0.0030	-0.0091	0.0015	0.0034	0.0117	0.0330
	Z	0.0031	0.0106	-0.0051	-0.0111	0.0011	-0.0041
AT. 36	O X	0.0033	-0.0008	-0.0189	-0.0034	0.0268	0.0152
	Y	0.0030	0.0091	0.0015	0.0034	0.0117	-0.0330
	Z	0.0031	0.0106	0.0051	0.0111	-0.0011	-0.0041
AT. 37	O X	-0.0033	-0.0008	-0.0189	0.0034	0.0268	0.0152
	Y	0.0030	-0.0091	-0.0015	0.0034	-0.0117	0.0330
	Z	-0.0031	0.0106	0.0051	-0.0111	-0.0011	-0.0041
AT. 38	O X	0.0033	0.0008	-0.0189	0.0034	0.0268	-0.0152
	Y	-0.0030	0.0091	-0.0015	0.0034	-0.0117	-0.0330
	Z	-0.0031	0.0106	-0.0051	0.0111	0.0011	-0.0041
AT. 39	O X	-0.0012	0.0126	0.0003	-0.0032	0.0096	-0.0073
	Y	0.0229	0.0177	0.0166	0.0123	-0.0022	-0.0010
	Z	-0.0115	-0.0080	-0.0056	0.0046	-0.0035	0.0021
AT. 40	O X	0.0012	-0.0126	0.0003	-0.0032	0.0096	0.0073
	Y	-0.0229	-0.0177	0.0166	0.0123	-0.0022	0.0010
	Z	-0.0115	-0.0080	0.0056	-0.0046	0.0035	0.0021
AT. 41	O X	-0.0012	-0.0126	0.0003	0.0032	0.0096	0.0073
	Y	-0.0229	0.0177	-0.0166	0.0123	0.0022	-0.0010
	Z	0.0115	-0.0080	0.0056	0.0046	0.0035	0.0021
AT. 42	O X	0.0012	0.0126	0.0003	0.0032	0.0096	-0.0073

	Y	0.0229	-0.0177	-0.0166	0.0123	0.0022	0.0010
	Z	0.0115	-0.0080	-0.0056	-0.0046	-0.0035	0.0021
AT. 43	O X	0.0012	-0.0126	0.0003	0.0032	-0.0096	-0.0073
	Y	-0.0229	-0.0177	0.0166	-0.0123	0.0022	-0.0010
	Z	0.0115	0.0080	-0.0056	-0.0046	0.0035	0.0021
AT. 44	O X	-0.0012	0.0126	0.0003	0.0032	-0.0096	0.0073
	Y	0.0229	0.0177	0.0166	-0.0123	0.0022	0.0010
	Z	0.0115	0.0080	0.0056	0.0046	-0.0035	0.0021
AT. 45	O X	0.0012	0.0126	0.0003	-0.0032	-0.0096	0.0073
	Y	0.0229	-0.0177	-0.0166	-0.0123	-0.0022	-0.0010
	Z	-0.0115	0.0080	0.0056	-0.0046	-0.0035	0.0021
AT. 46	O X	-0.0012	-0.0126	0.0003	-0.0032	-0.0096	-0.0073
	Y	-0.0229	0.0177	-0.0166	-0.0123	-0.0022	0.0010
	Z	-0.0115	0.0080	-0.0056	0.0046	0.0035	0.0021
AT. 47	O X	0.0152	0.0049	-0.0023	0.0000	0.0000	0.0000
	Y	-0.0229	0.0211	-0.0076	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0313	-0.0247	-0.0306
AT. 48	O X	-0.0152	-0.0049	-0.0023	0.0000	0.0000	0.0000
	Y	0.0229	-0.0211	-0.0076	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0313	0.0247	-0.0306
AT. 49	O X	0.0152	-0.0049	-0.0023	0.0000	0.0000	0.0000
	Y	0.0229	0.0211	0.0076	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0313	0.0247	-0.0306
AT. 50	O X	-0.0152	0.0049	-0.0023	0.0000	0.0000	0.0000
	Y	-0.0229	-0.0211	0.0076	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0313	-0.0247	-0.0306
AT. 51	O X	-0.0115	0.0180	0.0007	0.0000	0.0000	0.0000
	Y	-0.0154	0.0263	0.0199	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0035	-0.0189	-0.0164
AT. 52	O X	0.0115	-0.0180	0.0007	0.0000	0.0000	0.0000
	Y	0.0154	-0.0263	0.0199	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0035	0.0189	-0.0164
AT. 53	O X	-0.0115	-0.0180	0.0007	0.0000	0.0000	0.0000
	Y	0.0154	0.0263	-0.0199	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0035	0.0189	-0.0164
AT. 54	O X	0.0115	0.0180	0.0007	0.0000	0.0000	0.0000
	Y	-0.0154	-0.0263	-0.0199	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0035	-0.0189	-0.0164
AT. 55	O X	0.0094	0.0089	0.0184	0.0000	0.0000	0.0000
	Y	0.0076	-0.0099	-0.0042	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0235	0.0064	0.0165
AT. 56	O X	-0.0094	-0.0089	0.0184	0.0000	0.0000	0.0000
	Y	-0.0076	0.0099	-0.0042	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0235	-0.0064	0.0165
AT. 57	O X	0.0094	-0.0089	0.0184	0.0000	0.0000	0.0000
	Y	-0.0076	-0.0099	0.0042	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0235	-0.0064	0.0165
AT. 58	O X	-0.0094	0.0089	0.0184	0.0000	0.0000	0.0000
	Y	0.0076	0.0099	0.0042	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0235	0.0064	0.0165

FREQ(CM**-1) 335.88 338.71 341.63 343.91 345.20 345.89

AT. 1 FE X 0.0077 0.0000 0.0000 -0.0026 -0.0042 -0.0139

	Y	0.0000	-0.0147	0.0018	0.0000	0.0000	0.0000
	Z	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
AT. 2	FE X	-0.0077	0.0000	0.0000	0.0026	-0.0042	-0.0139
	Y	0.0000	-0.0147	0.0018	0.0000	0.0000	0.0000
	Z	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
AT. 3	FE X	-0.0077	0.0000	0.0000	0.0026	-0.0042	0.0139
	Y	0.0000	0.0147	0.0018	0.0000	0.0000	0.0000
	Z	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
AT. 4	FE X	0.0077	0.0000	0.0000	-0.0026	-0.0042	0.0139
	Y	0.0000	0.0147	0.0018	0.0000	0.0000	0.0000
	Z	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000
AT. 5	AL X	0.0000	-0.0259	-0.0015	0.0000	-0.0105	0.0095
	Y	0.0000	0.0125	-0.0065	0.0000	0.0228	-0.0277
	Z	0.0115	0.0000	0.0000	0.0253	0.0000	0.0000
AT. 6	AL X	0.0000	0.0259	0.0015	0.0000	-0.0105	0.0095
	Y	0.0000	0.0125	-0.0065	0.0000	-0.0228	0.0277
	Z	-0.0115	0.0000	0.0000	-0.0253	0.0000	0.0000
AT. 7	AL X	0.0000	0.0259	-0.0015	0.0000	-0.0105	-0.0095
	Y	0.0000	-0.0125	-0.0065	0.0000	0.0228	0.0277
	Z	-0.0115	0.0000	0.0000	-0.0253	0.0000	0.0000
AT. 8	AL X	0.0000	-0.0259	0.0015	0.0000	-0.0105	-0.0095
	Y	0.0000	-0.0125	-0.0065	0.0000	-0.0228	-0.0277
	Z	0.0115	0.0000	0.0000	0.0253	0.0000	0.0000
AT. 9	AL X	-0.0035	0.0000	-0.0007	0.0040	0.0020	0.0000
	Y	0.0191	0.0000	-0.0003	-0.0052	-0.0026	0.0000
	Z	0.0000	-0.0040	0.0000	0.0000	0.0000	-0.0004
AT. 10	AL X	0.0035	0.0000	-0.0007	-0.0040	0.0020	0.0000
	Y	-0.0191	0.0000	-0.0003	0.0052	-0.0026	0.0000
	Z	0.0000	0.0040	0.0000	0.0000	0.0000	0.0004
AT. 11	AL X	-0.0035	0.0000	0.0007	0.0040	0.0020	0.0000
	Y	-0.0191	0.0000	-0.0003	0.0052	0.0026	0.0000
	Z	0.0000	-0.0040	0.0000	0.0000	0.0000	0.0004
AT. 12	AL X	0.0035	0.0000	0.0007	-0.0040	0.0020	0.0000
	Y	0.0191	0.0000	-0.0003	-0.0052	0.0026	0.0000
	Z	0.0000	0.0040	0.0000	0.0000	0.0000	-0.0004
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0264	0.0050
	Y	0.0000	-0.0125	-0.0051	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0264	-0.0050
	Y	0.0000	0.0125	-0.0051	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0061	0.0000	-0.0015	0.0122	-0.0030	0.0000
	Y	0.0162	0.0000	0.0006	0.0124	0.0008	0.0000
	Z	0.0000	0.0044	0.0000	0.0000	0.0000	-0.0031
AT. 16	SI X	-0.0061	0.0000	-0.0015	-0.0122	-0.0030	0.0000
	Y	-0.0162	0.0000	0.0006	-0.0124	0.0008	0.0000
	Z	0.0000	-0.0044	0.0000	0.0000	0.0000	0.0031
AT. 17	SI X	0.0061	0.0000	0.0015	0.0122	-0.0030	0.0000
	Y	-0.0162	0.0000	0.0006	-0.0124	-0.0008	0.0000
	Z	0.0000	0.0044	0.0000	0.0000	0.0000	0.0031
AT. 18	SI X	-0.0061	0.0000	0.0015	-0.0122	-0.0030	0.0000
	Y	0.0162	0.0000	0.0006	0.0124	-0.0008	0.0000
	Z	0.0000	-0.0044	0.0000	0.0000	0.0000	-0.0031
AT. 19	SI X	0.0090	0.0000	-0.0020	-0.0028	-0.0033	0.0000

	Y	0.0033	0.0000	0.0008	0.0085	-0.0100	0.0000
	Z	0.0000	0.0047	0.0000	0.0000	0.0000	0.0075
AT. 20	SI X	-0.0090	0.0000	-0.0020	0.0028	-0.0033	0.0000
	Y	-0.0033	0.0000	0.0008	-0.0085	-0.0100	0.0000
	Z	0.0000	-0.0047	0.0000	0.0000	0.0000	-0.0075
AT. 21	SI X	0.0090	0.0000	0.0020	-0.0028	-0.0033	0.0000
	Y	-0.0033	0.0000	0.0008	-0.0085	0.0100	0.0000
	Z	0.0000	0.0047	0.0000	0.0000	0.0000	-0.0075
AT. 22	SI X	-0.0090	0.0000	0.0020	0.0028	-0.0033	0.0000
	Y	0.0033	0.0000	0.0008	0.0085	0.0100	0.0000
	Z	0.0000	-0.0047	0.0000	0.0000	0.0000	0.0075
AT. 23	O X	-0.0032	0.0005	-0.0224	0.0106	-0.0090	-0.0006
	Y	-0.0071	0.0122	0.0089	-0.0141	-0.0101	0.0247
	Z	-0.0067	0.0001	-0.0204	-0.0011	-0.0058	-0.0033
AT. 24	O X	0.0032	0.0005	-0.0224	-0.0106	-0.0090	-0.0006
	Y	0.0071	0.0122	0.0089	0.0141	-0.0101	0.0247
	Z	-0.0067	-0.0001	0.0204	-0.0011	0.0058	0.0033
AT. 25	O X	-0.0032	-0.0005	0.0224	0.0106	-0.0090	-0.0006
	Y	0.0071	0.0122	0.0089	0.0141	0.0101	-0.0247
	Z	0.0067	0.0001	-0.0204	0.0011	0.0058	0.0033
AT. 26	O X	0.0032	-0.0005	0.0224	-0.0106	-0.0090	-0.0006
	Y	-0.0071	0.0122	0.0089	-0.0141	0.0101	-0.0247
	Z	0.0067	-0.0001	0.0204	0.0011	-0.0058	-0.0033
AT. 27	O X	0.0032	-0.0005	-0.0224	-0.0106	-0.0090	0.0006
	Y	0.0071	-0.0122	0.0089	0.0141	-0.0101	-0.0247
	Z	0.0067	-0.0001	-0.0204	0.0011	-0.0058	0.0033
AT. 28	O X	-0.0032	-0.0005	-0.0224	0.0106	-0.0090	0.0006
	Y	-0.0071	-0.0122	0.0089	-0.0141	-0.0101	-0.0247
	Z	0.0067	0.0001	0.0204	0.0011	0.0058	-0.0033
AT. 29	O X	0.0032	0.0005	0.0224	-0.0106	-0.0090	0.0006
	Y	-0.0071	-0.0122	0.0089	-0.0141	0.0101	0.0247
	Z	-0.0067	-0.0001	-0.0204	-0.0011	0.0058	-0.0033
AT. 30	O X	-0.0032	0.0005	0.0224	0.0106	-0.0090	0.0006
	Y	0.0071	-0.0122	0.0089	0.0141	0.0101	0.0247
	Z	-0.0067	0.0001	0.0204	-0.0011	-0.0058	0.0033
AT. 31	O X	0.0037	-0.0056	-0.0037	-0.0010	0.0216	0.0086
	Y	-0.0129	-0.0006	0.0011	0.0188	-0.0026	-0.0013
	Z	0.0033	-0.0037	-0.0019	-0.0141	0.0067	0.0004
AT. 32	O X	-0.0037	-0.0056	-0.0037	0.0010	0.0216	0.0086
	Y	0.0129	-0.0006	0.0011	-0.0188	-0.0026	-0.0013
	Z	0.0033	0.0037	0.0019	-0.0141	-0.0067	-0.0004
AT. 33	O X	0.0037	0.0056	0.0037	-0.0010	0.0216	0.0086
	Y	0.0129	-0.0006	0.0011	-0.0188	0.0026	0.0013
	Z	-0.0033	-0.0037	-0.0019	0.0141	-0.0067	-0.0004
AT. 34	O X	-0.0037	0.0056	0.0037	0.0010	0.0216	0.0086
	Y	-0.0129	-0.0006	0.0011	0.0188	0.0026	0.0013
	Z	-0.0033	0.0037	0.0019	0.0141	0.0067	0.0004
AT. 35	O X	-0.0037	0.0056	-0.0037	0.0010	0.0216	-0.0086
	Y	0.0129	0.0006	0.0011	-0.0188	-0.0026	0.0013
	Z	-0.0033	0.0037	-0.0019	0.0141	0.0067	-0.0004
AT. 36	O X	0.0037	0.0056	-0.0037	-0.0010	0.0216	-0.0086
	Y	-0.0129	0.0006	0.0011	0.0188	-0.0026	0.0013
	Z	-0.0033	-0.0037	0.0019	0.0141	-0.0067	0.0004
AT. 37	O X	-0.0037	-0.0056	0.0037	0.0010	0.0216	-0.0086

	Y	-0.0129	0.0006	0.0011	0.0188	0.0026	-0.0013
	Z	0.0033	0.0037	-0.0019	-0.0141	-0.0067	0.0004
AT. 38	O X	0.0037	-0.0056	0.0037	-0.0010	0.0216	-0.0086
	Y	0.0129	0.0006	0.0011	-0.0188	0.0026	-0.0013
	Z	0.0033	-0.0037	0.0019	-0.0141	0.0067	-0.0004
AT. 39	O X	0.0046	-0.0204	-0.0191	-0.0094	0.0006	0.0145
	Y	-0.0028	0.0144	-0.0124	-0.0113	0.0208	-0.0042
	Z	-0.0021	0.0002	0.0182	0.0190	-0.0098	0.0013
AT. 40	O X	-0.0046	-0.0204	-0.0191	0.0094	0.0006	0.0145
	Y	0.0028	0.0144	-0.0124	0.0113	0.0208	-0.0042
	Z	-0.0021	-0.0002	-0.0182	0.0190	0.0098	-0.0013
AT. 41	O X	0.0046	0.0204	0.0191	-0.0094	0.0006	0.0145
	Y	0.0028	0.0144	-0.0124	0.0113	-0.0208	0.0042
	Z	0.0021	0.0002	0.0182	-0.0190	0.0098	-0.0013
AT. 42	O X	-0.0046	0.0204	0.0191	0.0094	0.0006	0.0145
	Y	-0.0028	0.0144	-0.0124	-0.0113	-0.0208	0.0042
	Z	0.0021	-0.0002	-0.0182	-0.0190	-0.0098	0.0013
AT. 43	O X	-0.0046	0.0204	-0.0191	0.0094	0.0006	-0.0145
	Y	0.0028	-0.0144	-0.0124	0.0113	0.0208	0.0042
	Z	0.0021	-0.0002	0.0182	-0.0190	-0.0098	-0.0013
AT. 44	O X	0.0046	0.0204	-0.0191	-0.0094	0.0006	-0.0145
	Y	-0.0028	-0.0144	-0.0124	-0.0113	0.0208	0.0042
	Z	0.0021	0.0002	-0.0182	-0.0190	0.0098	0.0013
AT. 45	O X	-0.0046	-0.0204	0.0191	0.0094	0.0006	-0.0145
	Y	-0.0028	-0.0144	-0.0124	-0.0113	-0.0208	-0.0042
	Z	-0.0021	-0.0002	0.0182	0.0190	0.0098	0.0013
AT. 46	O X	0.0046	-0.0204	0.0191	-0.0094	0.0006	-0.0145
	Y	0.0028	-0.0144	-0.0124	0.0113	-0.0208	-0.0042
	Z	-0.0021	0.0002	-0.0182	0.0190	-0.0098	-0.0013
AT. 47	O X	0.0105	0.0000	-0.0045	0.0024	0.0003	0.0000
	Y	-0.0305	0.0000	0.0167	-0.0172	-0.0101	0.0000
	Z	0.0000	-0.0370	0.0000	0.0000	0.0000	-0.0179
AT. 48	O X	-0.0105	0.0000	-0.0045	-0.0024	0.0003	0.0000
	Y	0.0305	0.0000	0.0167	0.0172	-0.0101	0.0000
	Z	0.0000	0.0370	0.0000	0.0000	0.0000	0.0179
AT. 49	O X	0.0105	0.0000	0.0045	0.0024	0.0003	0.0000
	Y	0.0305	0.0000	0.0167	0.0172	0.0101	0.0000
	Z	0.0000	-0.0370	0.0000	0.0000	0.0000	0.0179
AT. 50	O X	-0.0105	0.0000	0.0045	-0.0024	0.0003	0.0000
	Y	-0.0305	0.0000	0.0167	-0.0172	0.0101	0.0000
	Z	0.0000	0.0370	0.0000	0.0000	0.0000	-0.0179
AT. 51	O X	0.0084	0.0000	-0.0150	-0.0039	0.0119	0.0000
	Y	0.0232	0.0000	-0.0147	-0.0087	0.0148	0.0000
	Z	0.0000	0.0102	0.0000	0.0000	0.0000	-0.0076
AT. 52	O X	-0.0084	0.0000	-0.0150	0.0039	0.0119	0.0000
	Y	-0.0232	0.0000	-0.0147	0.0087	0.0148	0.0000
	Z	0.0000	-0.0102	0.0000	0.0000	0.0000	0.0076
AT. 53	O X	0.0084	0.0000	0.0150	-0.0039	0.0119	0.0000
	Y	-0.0232	0.0000	-0.0147	0.0087	-0.0148	0.0000
	Z	0.0000	0.0102	0.0000	0.0000	0.0000	0.0076
AT. 54	O X	-0.0084	0.0000	0.0150	0.0039	0.0119	0.0000
	Y	0.0232	0.0000	-0.0147	-0.0087	-0.0148	0.0000
	Z	0.0000	-0.0102	0.0000	0.0000	0.0000	-0.0076
AT. 55	O X	0.0393	0.0000	-0.0288	-0.0119	-0.0221	0.0000

	Y	-0.0021	0.0000	0.0095	0.0142	0.0016	0.0000
	Z	0.0000	0.0073	0.0000	0.0000	0.0000	0.0307
AT. 56 O	X	-0.0393	0.0000	-0.0288	0.0119	-0.0221	0.0000
	Y	0.0021	0.0000	0.0095	-0.0142	0.0016	0.0000
	Z	0.0000	-0.0073	0.0000	0.0000	0.0000	-0.0307
AT. 57 O	X	0.0393	0.0000	0.0288	-0.0119	-0.0221	0.0000
	Y	0.0021	0.0000	0.0095	-0.0142	-0.0016	0.0000
	Z	0.0000	0.0073	0.0000	0.0000	0.0000	-0.0307
AT. 58 O	X	-0.0393	0.0000	0.0288	0.0119	-0.0221	0.0000
	Y	-0.0021	0.0000	0.0095	0.0142	-0.0016	0.0000
	Z	0.0000	-0.0073	0.0000	0.0000	0.0000	0.0307

FREQ(CM**-1) 351.77 358.02 376.21 377.01 377.15 378.77

AT. 1 FE	X	0.0000	0.0000	0.0001	-0.0031	0.0000	0.0000
	Y	-0.0020	-0.0050	0.0000	0.0000	-0.0009	0.0005
	Z	0.0035	-0.0056	0.0000	0.0000	-0.0029	0.0022
AT. 2 FE	X	0.0000	0.0000	-0.0001	-0.0031	0.0000	0.0000
	Y	0.0020	-0.0050	0.0000	0.0000	-0.0009	-0.0005
	Z	0.0035	0.0056	0.0000	0.0000	0.0029	0.0022
AT. 3 FE	X	0.0000	0.0000	0.0001	-0.0031	0.0000	0.0000
	Y	0.0020	-0.0050	0.0000	0.0000	-0.0009	0.0005
	Z	-0.0035	-0.0056	0.0000	0.0000	-0.0029	0.0022
AT. 4 FE	X	0.0000	0.0000	-0.0001	-0.0031	0.0000	0.0000
	Y	-0.0020	-0.0050	0.0000	0.0000	-0.0009	-0.0005
	Z	-0.0035	0.0056	0.0000	0.0000	0.0029	0.0022
AT. 5 AL	X	0.0000	-0.0047	0.0000	-0.0132	-0.0111	0.0000
	Y	0.0000	0.0013	0.0000	-0.0063	-0.0005	0.0000
	Z	-0.0132	0.0000	0.0262	0.0000	0.0000	0.0296
AT. 6 AL	X	0.0000	0.0047	0.0000	-0.0132	0.0111	0.0000
	Y	0.0000	0.0013	0.0000	0.0063	-0.0005	0.0000
	Z	-0.0132	0.0000	-0.0262	0.0000	0.0000	0.0296
AT. 7 AL	X	0.0000	-0.0047	0.0000	-0.0132	-0.0111	0.0000
	Y	0.0000	0.0013	0.0000	-0.0063	-0.0005	0.0000
	Z	0.0132	0.0000	0.0262	0.0000	0.0000	0.0296
AT. 8 AL	X	0.0000	0.0047	0.0000	-0.0132	0.0111	0.0000
	Y	0.0000	0.0013	0.0000	0.0063	-0.0005	0.0000
	Z	0.0132	0.0000	-0.0262	0.0000	0.0000	0.0296
AT. 9 AL	X	-0.0104	0.0078	0.0000	0.0030	-0.0216	0.0000
	Y	0.0081	-0.0200	0.0000	0.0131	-0.0092	0.0000
	Z	0.0000	0.0000	0.0132	0.0000	0.0000	0.0033
AT. 10 AL	X	0.0104	0.0078	0.0000	0.0030	-0.0216	0.0000
	Y	-0.0081	-0.0200	0.0000	0.0131	-0.0092	0.0000
	Z	0.0000	0.0000	0.0132	0.0000	0.0000	0.0033
AT. 11 AL	X	0.0104	-0.0078	0.0000	0.0030	0.0216	0.0000
	Y	0.0081	-0.0200	0.0000	-0.0131	-0.0092	0.0000
	Z	0.0000	0.0000	-0.0132	0.0000	0.0000	0.0033
AT. 12 AL	X	-0.0104	-0.0078	0.0000	0.0030	0.0216	0.0000
	Y	-0.0081	-0.0200	0.0000	-0.0131	-0.0092	0.0000
	Z	0.0000	0.0000	-0.0132	0.0000	0.0000	0.0033
AT. 13 SI	X	0.0000	0.0000	0.0000	0.0115	0.0000	0.0000
	Y	0.0000	0.0033	0.0000	0.0000	-0.0106	0.0000
	Z	0.0030	0.0000	0.0000	0.0000	0.0000	0.0051
AT. 14 SI	X	0.0000	0.0000	0.0000	0.0115	0.0000	0.0000

	Y	0.0000	0.0033	0.0000	0.0000	-0.0106	0.0000
	Z	-0.0030	0.0000	0.0000	0.0000	0.0000	0.0051
AT. 15	SI X	-0.0003	0.0159	0.0000	-0.0064	-0.0049	0.0000
	Y	0.0091	-0.0069	0.0000	0.0106	0.0051	0.0000
	Z	0.0000	0.0000	0.0050	0.0000	0.0000	0.0092
AT. 16	SI X	0.0003	0.0159	0.0000	-0.0064	-0.0049	0.0000
	Y	-0.0091	-0.0069	0.0000	0.0106	0.0051	0.0000
	Z	0.0000	0.0000	0.0050	0.0000	0.0000	0.0092
AT. 17	SI X	0.0003	-0.0159	0.0000	-0.0064	0.0049	0.0000
	Y	0.0091	-0.0069	0.0000	-0.0106	0.0051	0.0000
	Z	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0092
AT. 18	SI X	-0.0003	-0.0159	0.0000	-0.0064	0.0049	0.0000
	Y	-0.0091	-0.0069	0.0000	-0.0106	0.0051	0.0000
	Z	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0092
AT. 19	SI X	0.0063	-0.0014	0.0000	0.0093	-0.0101	0.0000
	Y	0.0024	0.0135	0.0000	0.0075	0.0005	0.0000
	Z	0.0000	0.0000	-0.0139	0.0000	0.0000	0.0007
AT. 20	SI X	-0.0063	-0.0014	0.0000	0.0093	-0.0101	0.0000
	Y	-0.0024	0.0135	0.0000	0.0075	0.0005	0.0000
	Z	0.0000	0.0000	-0.0139	0.0000	0.0000	0.0007
AT. 21	SI X	-0.0063	0.0014	0.0000	0.0093	0.0101	0.0000
	Y	0.0024	0.0135	0.0000	-0.0075	0.0005	0.0000
	Z	0.0000	0.0000	0.0139	0.0000	0.0000	0.0007
AT. 22	SI X	0.0063	0.0014	0.0000	0.0093	0.0101	0.0000
	Y	-0.0024	0.0135	0.0000	-0.0075	0.0005	0.0000
	Z	0.0000	0.0000	0.0139	0.0000	0.0000	0.0007
AT. 23	O X	-0.0230	-0.0003	0.0177	-0.0111	0.0070	-0.0138
	Y	0.0065	-0.0106	-0.0147	0.0006	0.0011	0.0180
	Z	-0.0170	0.0107	0.0078	-0.0027	0.0016	-0.0057
AT. 24	O X	0.0230	-0.0003	-0.0177	-0.0111	0.0070	0.0138
	Y	-0.0065	-0.0106	0.0147	0.0006	0.0011	-0.0180
	Z	-0.0170	-0.0107	0.0078	0.0027	-0.0016	-0.0057
AT. 25	O X	0.0230	0.0003	0.0177	-0.0111	-0.0070	0.0138
	Y	0.0065	-0.0106	0.0147	-0.0006	0.0011	0.0180
	Z	-0.0170	0.0107	-0.0078	0.0027	0.0016	-0.0057
AT. 26	O X	-0.0230	0.0003	-0.0177	-0.0111	-0.0070	-0.0138
	Y	-0.0065	-0.0106	-0.0147	-0.0006	0.0011	-0.0180
	Z	-0.0170	-0.0107	-0.0078	-0.0027	-0.0016	-0.0057
AT. 27	O X	0.0230	-0.0003	0.0177	-0.0111	0.0070	-0.0138
	Y	-0.0065	-0.0106	-0.0147	0.0006	0.0011	0.0180
	Z	0.0170	0.0107	0.0078	-0.0027	0.0016	-0.0057
AT. 28	O X	-0.0230	-0.0003	-0.0177	-0.0111	0.0070	0.0138
	Y	0.0065	-0.0106	0.0147	0.0006	0.0011	-0.0180
	Z	0.0170	-0.0107	0.0078	0.0027	-0.0016	-0.0057
AT. 29	O X	-0.0230	0.0003	0.0177	-0.0111	-0.0070	0.0138
	Y	-0.0065	-0.0106	0.0147	-0.0006	0.0011	0.0180
	Z	0.0170	0.0107	-0.0078	0.0027	0.0016	-0.0057
AT. 30	O X	0.0230	0.0003	-0.0177	-0.0111	-0.0070	-0.0138
	Y	0.0065	-0.0106	-0.0147	-0.0006	0.0011	-0.0180
	Z	0.0170	-0.0107	-0.0078	-0.0027	-0.0016	-0.0057
AT. 31	O X	-0.0015	0.0101	0.0056	0.0125	0.0128	0.0035
	Y	0.0140	0.0133	-0.0057	0.0028	-0.0058	0.0049
	Z	-0.0057	-0.0199	-0.0026	-0.0044	-0.0093	-0.0025
AT. 32	O X	0.0015	0.0101	-0.0056	0.0125	0.0128	-0.0035

	Y	-0.0140	0.0133	0.0057	0.0028	-0.0058	-0.0049
	Z	-0.0057	0.0199	-0.0026	0.0044	0.0093	-0.0025
AT. 33	O X	0.0015	-0.0101	0.0056	0.0125	-0.0128	-0.0035
	Y	0.0140	0.0133	0.0057	-0.0028	-0.0058	0.0049
	Z	-0.0057	-0.0199	0.0026	0.0044	-0.0093	-0.0025
AT. 34	O X	-0.0015	-0.0101	-0.0056	0.0125	-0.0128	0.0035
	Y	-0.0140	0.0133	-0.0057	-0.0028	-0.0058	-0.0049
	Z	-0.0057	0.0199	0.0026	-0.0044	0.0093	-0.0025
AT. 35	O X	0.0015	0.0101	0.0056	0.0125	0.0128	0.0035
	Y	-0.0140	0.0133	-0.0057	0.0028	-0.0058	0.0049
	Z	0.0057	-0.0199	-0.0026	-0.0044	-0.0093	-0.0025
AT. 36	O X	-0.0015	0.0101	-0.0056	0.0125	0.0128	-0.0035
	Y	0.0140	0.0133	0.0057	0.0028	-0.0058	-0.0049
	Z	0.0057	0.0199	-0.0026	0.0044	0.0093	-0.0025
AT. 37	O X	-0.0015	-0.0101	0.0056	0.0125	-0.0128	-0.0035
	Y	-0.0140	0.0133	0.0057	-0.0028	-0.0058	0.0049
	Z	0.0057	-0.0199	0.0026	0.0044	-0.0093	-0.0025
AT. 38	O X	0.0015	-0.0101	-0.0056	0.0125	-0.0128	0.0035
	Y	0.0140	0.0133	-0.0057	-0.0028	-0.0058	-0.0049
	Z	0.0057	0.0199	0.0026	-0.0044	0.0093	-0.0025
AT. 39	O X	0.0149	-0.0058	0.0188	-0.0136	-0.0159	0.0223
	Y	0.0185	0.0183	0.0150	-0.0119	-0.0044	-0.0020
	Z	-0.0159	0.0023	-0.0032	0.0103	0.0117	-0.0096
AT. 40	O X	-0.0149	-0.0058	-0.0188	-0.0136	-0.0159	-0.0223
	Y	-0.0185	0.0183	-0.0150	-0.0119	-0.0044	0.0020
	Z	-0.0159	-0.0023	-0.0032	-0.0103	-0.0117	-0.0096
AT. 41	O X	-0.0149	0.0058	0.0188	-0.0136	0.0159	-0.0223
	Y	0.0185	0.0183	-0.0150	0.0119	-0.0044	-0.0020
	Z	-0.0159	0.0023	0.0032	-0.0103	0.0117	-0.0096
AT. 42	O X	0.0149	0.0058	-0.0188	-0.0136	0.0159	0.0223
	Y	-0.0185	0.0183	0.0150	0.0119	-0.0044	0.0020
	Z	-0.0159	-0.0023	0.0032	0.0103	-0.0117	-0.0096
AT. 43	O X	-0.0149	-0.0058	0.0188	-0.0136	-0.0159	0.0223
	Y	-0.0185	0.0183	0.0150	-0.0119	-0.0044	-0.0020
	Z	0.0159	0.0023	-0.0032	0.0103	0.0117	-0.0096
AT. 44	O X	0.0149	-0.0058	-0.0188	-0.0136	-0.0159	-0.0223
	Y	0.0185	0.0183	-0.0150	-0.0119	-0.0044	0.0020
	Z	0.0159	-0.0023	-0.0032	-0.0103	-0.0117	-0.0096
AT. 45	O X	0.0149	0.0058	0.0188	-0.0136	0.0159	-0.0223
	Y	-0.0185	0.0183	-0.0150	0.0119	-0.0044	-0.0020
	Z	0.0159	0.0023	0.0032	-0.0103	0.0117	-0.0096
AT. 46	O X	-0.0149	0.0058	-0.0188	-0.0136	0.0159	0.0223
	Y	0.0185	0.0183	0.0150	0.0119	-0.0044	0.0020
	Z	0.0159	-0.0023	0.0032	0.0103	-0.0117	-0.0096
AT. 47	O X	0.0041	-0.0025	0.0000	0.0157	-0.0171	0.0000
	Y	0.0148	0.0098	0.0000	-0.0350	0.0190	0.0000
	Z	0.0000	0.0000	0.0206	0.0000	0.0000	-0.0203
AT. 48	O X	-0.0041	-0.0025	0.0000	0.0157	-0.0171	0.0000
	Y	-0.0148	0.0098	0.0000	-0.0350	0.0190	0.0000
	Z	0.0000	0.0000	0.0206	0.0000	0.0000	-0.0203
AT. 49	O X	-0.0041	0.0025	0.0000	0.0157	0.0171	0.0000
	Y	0.0148	0.0098	0.0000	0.0350	0.0190	0.0000
	Z	0.0000	0.0000	-0.0206	0.0000	0.0000	-0.0203
AT. 50	O X	0.0041	0.0025	0.0000	0.0157	0.0171	0.0000

	Y	-0.0148	0.0098	0.0000	0.0350	0.0190	0.0000
	Z	0.0000	0.0000	-0.0206	0.0000	0.0000	-0.0203
AT. 51 O	X	-0.0123	-0.0013	0.0000	-0.0037	0.0111	0.0000
	Y	-0.0022	-0.0249	0.0000	0.0088	0.0232	0.0000
	Z	0.0000	0.0000	-0.0150	0.0000	0.0000	-0.0079
AT. 52 O	X	0.0123	-0.0013	0.0000	-0.0037	0.0111	0.0000
	Y	0.0022	-0.0249	0.0000	0.0088	0.0232	0.0000
	Z	0.0000	0.0000	-0.0150	0.0000	0.0000	-0.0079
AT. 53 O	X	0.0123	0.0013	0.0000	-0.0037	-0.0111	0.0000
	Y	-0.0022	-0.0249	0.0000	-0.0088	0.0232	0.0000
	Z	0.0000	0.0000	0.0150	0.0000	0.0000	-0.0079
AT. 54 O	X	-0.0123	0.0013	0.0000	-0.0037	-0.0111	0.0000
	Y	0.0022	-0.0249	0.0000	-0.0088	0.0232	0.0000
	Z	0.0000	0.0000	0.0150	0.0000	0.0000	-0.0079
AT. 55 O	X	-0.0133	-0.0058	0.0000	0.0244	0.0246	0.0000
	Y	0.0096	0.0082	0.0000	0.0005	-0.0058	0.0000
	Z	0.0000	0.0000	-0.0047	0.0000	0.0000	-0.0210
AT. 56 O	X	0.0133	-0.0058	0.0000	0.0244	0.0246	0.0000
	Y	-0.0096	0.0082	0.0000	0.0005	-0.0058	0.0000
	Z	0.0000	0.0000	-0.0047	0.0000	0.0000	-0.0210
AT. 57 O	X	0.0133	0.0058	0.0000	0.0244	-0.0246	0.0000
	Y	0.0096	0.0082	0.0000	-0.0005	-0.0058	0.0000
	Z	0.0000	0.0000	0.0047	0.0000	0.0000	-0.0210
AT. 58 O	X	-0.0133	0.0058	0.0000	0.0244	-0.0246	0.0000
	Y	-0.0096	0.0082	0.0000	-0.0005	-0.0058	0.0000
	Z	0.0000	0.0000	0.0047	0.0000	0.0000	-0.0210

FREQ(CM**-1) 381.30 403.25 408.67 417.60 426.80 427.95

AT. 1 FE	X	-0.0005	0.0036	0.0028	0.0057	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0014	-0.0042
	Z	0.0000	0.0000	0.0000	0.0000	0.0011	0.0015
AT. 2 FE	X	0.0005	0.0036	0.0028	0.0057	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0014	-0.0042
	Z	0.0000	0.0000	0.0000	0.0000	0.0011	-0.0015
AT. 3 FE	X	0.0005	-0.0036	0.0028	0.0057	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0014	-0.0042
	Z	0.0000	0.0000	0.0000	0.0000	-0.0011	0.0015
AT. 4 FE	X	-0.0005	-0.0036	0.0028	0.0057	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0014	-0.0042
	Z	0.0000	0.0000	0.0000	0.0000	-0.0011	-0.0015
AT. 5 AL	X	0.0000	0.0052	-0.0012	-0.0080	0.0000	0.0016
	Y	0.0000	-0.0004	0.0059	0.0097	0.0000	0.0219
	Z	0.0007	0.0000	0.0000	0.0000	0.0263	0.0000
AT. 6 AL	X	0.0000	0.0052	-0.0012	-0.0080	0.0000	-0.0016
	Y	0.0000	0.0004	-0.0059	-0.0097	0.0000	0.0219
	Z	-0.0007	0.0000	0.0000	0.0000	0.0263	0.0000
AT. 7 AL	X	0.0000	-0.0052	-0.0012	-0.0080	0.0000	0.0016
	Y	0.0000	0.0004	0.0059	0.0097	0.0000	0.0219
	Z	-0.0007	0.0000	0.0000	0.0000	-0.0263	0.0000
AT. 8 AL	X	0.0000	-0.0052	-0.0012	-0.0080	0.0000	-0.0016
	Y	0.0000	-0.0004	-0.0059	-0.0097	0.0000	0.0219
	Z	0.0007	0.0000	0.0000	0.0000	-0.0263	0.0000
AT. 9 AL	X	0.0007	0.0000	0.0186	0.0181	0.0157	0.0124

	Y	-0.0044	0.0000	0.0180	-0.0134	0.0019	-0.0089
	Z	0.0000	-0.0402	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	-0.0007	0.0000	0.0186	0.0181	-0.0157	0.0124
	Y	0.0044	0.0000	0.0180	-0.0134	-0.0019	-0.0089
	Z	0.0000	0.0402	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0007	0.0000	0.0186	0.0181	-0.0157	-0.0124
	Y	0.0044	0.0000	-0.0180	0.0134	0.0019	-0.0089
	Z	0.0000	0.0402	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	-0.0007	0.0000	0.0186	0.0181	0.0157	-0.0124
	Y	-0.0044	0.0000	-0.0180	0.0134	-0.0019	-0.0089
	Z	0.0000	-0.0402	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0036	-0.0119	-0.0089	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0066
	Z	0.0000	0.0000	0.0000	0.0000	0.0187	0.0000
AT. 14	SI X	0.0000	-0.0036	-0.0119	-0.0089	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0066
	Z	0.0000	0.0000	0.0000	0.0000	-0.0187	0.0000
AT. 15	SI X	-0.0069	0.0000	-0.0027	0.0146	0.0097	-0.0035
	Y	-0.0017	0.0000	-0.0066	0.0032	-0.0034	-0.0105
	Z	0.0000	0.0065	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0069	0.0000	-0.0027	0.0146	-0.0097	-0.0035
	Y	0.0017	0.0000	-0.0066	0.0032	0.0034	-0.0105
	Z	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	-0.0069	0.0000	-0.0027	0.0146	-0.0097	0.0035
	Y	0.0017	0.0000	0.0066	-0.0032	-0.0034	-0.0105
	Z	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0069	0.0000	-0.0027	0.0146	0.0097	0.0035
	Y	-0.0017	0.0000	0.0066	-0.0032	0.0034	-0.0105
	Z	0.0000	0.0065	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0039	0.0000	0.0108	0.0075	-0.0039	0.0011
	Y	0.0032	0.0000	-0.0124	0.0155	-0.0009	-0.0199
	Z	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0039	0.0000	0.0108	0.0075	0.0039	0.0011
	Y	-0.0032	0.0000	-0.0124	0.0155	0.0009	-0.0199
	Z	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	-0.0039	0.0000	0.0108	0.0075	0.0039	-0.0011
	Y	-0.0032	0.0000	0.0124	-0.0155	-0.0009	-0.0199
	Z	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	0.0039	0.0000	0.0108	0.0075	-0.0039	-0.0011
	Y	0.0032	0.0000	0.0124	-0.0155	0.0009	-0.0199
	Z	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	-0.0190	0.0052	0.0090	-0.0172	0.0034	0.0113
	Y	0.0071	0.0021	-0.0084	0.0030	0.0048	0.0166
	Z	-0.0104	-0.0018	0.0087	-0.0192	0.0125	0.0015
AT. 24	O X	0.0190	0.0052	0.0090	-0.0172	-0.0034	0.0113
	Y	-0.0071	0.0021	-0.0084	0.0030	-0.0048	0.0166
	Z	-0.0104	0.0018	-0.0087	0.0192	0.0125	-0.0015
AT. 25	O X	-0.0190	0.0052	0.0090	-0.0172	-0.0034	-0.0113
	Y	-0.0071	-0.0021	0.0084	-0.0030	0.0048	0.0166
	Z	0.0104	0.0018	-0.0087	0.0192	0.0125	0.0015
AT. 26	O X	0.0190	0.0052	0.0090	-0.0172	0.0034	-0.0113
	Y	0.0071	-0.0021	0.0084	-0.0030	-0.0048	0.0166
	Z	0.0104	-0.0018	0.0087	-0.0192	0.0125	-0.0015
AT. 27	O X	0.0190	-0.0052	0.0090	-0.0172	-0.0034	0.0113

	Y	-0.0071	-0.0021	-0.0084	0.0030	-0.0048	0.0166
	Z	0.0104	0.0018	0.0087	-0.0192	-0.0125	0.0015
AT. 28 O	X	-0.0190	-0.0052	0.0090	-0.0172	0.0034	0.0113
	Y	0.0071	-0.0021	-0.0084	0.0030	0.0048	0.0166
	Z	0.0104	-0.0018	-0.0087	0.0192	-0.0125	-0.0015
AT. 29 O	X	0.0190	-0.0052	0.0090	-0.0172	0.0034	-0.0113
	Y	0.0071	0.0021	0.0084	-0.0030	-0.0048	0.0166
	Z	-0.0104	-0.0018	-0.0087	0.0192	-0.0125	0.0015
AT. 30 O	X	-0.0190	-0.0052	0.0090	-0.0172	-0.0034	-0.0113
	Y	-0.0071	0.0021	0.0084	-0.0030	0.0048	0.0166
	Z	-0.0104	0.0018	0.0087	-0.0192	-0.0125	-0.0015
AT. 31 O	X	-0.0036	-0.0161	-0.0026	-0.0114	-0.0013	-0.0021
	Y	0.0279	0.0174	0.0012	-0.0009	0.0055	0.0059
	Z	-0.0192	0.0037	-0.0098	0.0029	0.0095	-0.0084
AT. 32 O	X	0.0036	-0.0161	-0.0026	-0.0114	0.0013	-0.0021
	Y	-0.0279	0.0174	0.0012	-0.0009	-0.0055	0.0059
	Z	-0.0192	-0.0037	0.0098	-0.0029	0.0095	0.0084
AT. 33 O	X	-0.0036	-0.0161	-0.0026	-0.0114	0.0013	0.0021
	Y	-0.0279	-0.0174	-0.0012	0.0009	0.0055	0.0059
	Z	0.0192	-0.0037	0.0098	-0.0029	0.0095	-0.0084
AT. 34 O	X	0.0036	-0.0161	-0.0026	-0.0114	-0.0013	0.0021
	Y	0.0279	-0.0174	-0.0012	0.0009	-0.0055	0.0059
	Z	0.0192	0.0037	-0.0098	0.0029	0.0095	0.0084
AT. 35 O	X	0.0036	0.0161	-0.0026	-0.0114	0.0013	-0.0021
	Y	-0.0279	-0.0174	0.0012	-0.0009	-0.0055	0.0059
	Z	0.0192	-0.0037	-0.0098	0.0029	-0.0095	-0.0084
AT. 36 O	X	-0.0036	0.0161	-0.0026	-0.0114	-0.0013	-0.0021
	Y	0.0279	-0.0174	0.0012	-0.0009	0.0055	0.0059
	Z	0.0192	0.0037	0.0098	-0.0029	-0.0095	0.0084
AT. 37 O	X	0.0036	0.0161	-0.0026	-0.0114	-0.0013	0.0021
	Y	0.0279	0.0174	-0.0012	0.0009	-0.0055	0.0059
	Z	-0.0192	0.0037	0.0098	-0.0029	-0.0095	-0.0084
AT. 38 O	X	-0.0036	0.0161	-0.0026	-0.0114	0.0013	0.0021
	Y	-0.0279	0.0174	-0.0012	0.0009	0.0055	0.0059
	Z	-0.0192	-0.0037	-0.0098	0.0029	-0.0095	0.0084
AT. 39 O	X	0.0147	0.0012	-0.0164	-0.0042	0.0160	-0.0010
	Y	0.0137	-0.0025	0.0058	-0.0013	0.0045	-0.0060
	Z	-0.0115	-0.0003	0.0153	-0.0021	-0.0049	-0.0054
AT. 40 O	X	-0.0147	0.0012	-0.0164	-0.0042	-0.0160	-0.0010
	Y	-0.0137	-0.0025	0.0058	-0.0013	-0.0045	-0.0060
	Z	-0.0115	0.0003	-0.0153	0.0021	-0.0049	0.0054
AT. 41 O	X	0.0147	0.0012	-0.0164	-0.0042	-0.0160	0.0010
	Y	-0.0137	0.0025	-0.0058	0.0013	0.0045	-0.0060
	Z	0.0115	0.0003	-0.0153	0.0021	-0.0049	-0.0054
AT. 42 O	X	-0.0147	0.0012	-0.0164	-0.0042	0.0160	0.0010
	Y	0.0137	0.0025	-0.0058	0.0013	-0.0045	-0.0060
	Z	0.0115	-0.0003	0.0153	-0.0021	-0.0049	0.0054
AT. 43 O	X	-0.0147	-0.0012	-0.0164	-0.0042	-0.0160	-0.0010
	Y	-0.0137	0.0025	0.0058	-0.0013	-0.0045	-0.0060
	Z	0.0115	0.0003	0.0153	-0.0021	0.0049	-0.0054
AT. 44 O	X	0.0147	-0.0012	-0.0164	-0.0042	0.0160	-0.0010
	Y	0.0137	0.0025	0.0058	-0.0013	0.0045	-0.0060
	Z	0.0115	-0.0003	-0.0153	0.0021	0.0049	0.0054
AT. 45 O	X	-0.0147	-0.0012	-0.0164	-0.0042	0.0160	0.0010

	Y	0.0137	-0.0025	-0.0058	0.0013	-0.0045	-0.0060
	Z	-0.0115	-0.0003	-0.0153	0.0021	0.0049	-0.0054
AT. 46 O	X	0.0147	-0.0012	-0.0164	-0.0042	-0.0160	0.0010
	Y	-0.0137	-0.0025	-0.0058	0.0013	0.0045	-0.0060
	Z	-0.0115	0.0003	0.0153	-0.0021	0.0049	0.0054
AT. 47 O	X	0.0008	0.0000	0.0117	0.0088	-0.0120	-0.0010
	Y	-0.0145	0.0000	0.0033	-0.0012	0.0209	0.0175
	Z	0.0000	-0.0215	0.0000	0.0000	0.0000	0.0000
AT. 48 O	X	-0.0008	0.0000	0.0117	0.0088	0.0120	-0.0010
	Y	0.0145	0.0000	0.0033	-0.0012	-0.0209	0.0175
	Z	0.0000	0.0215	0.0000	0.0000	0.0000	0.0000
AT. 49 O	X	0.0008	0.0000	0.0117	0.0088	0.0120	0.0010
	Y	0.0145	0.0000	-0.0033	0.0012	0.0209	0.0175
	Z	0.0000	0.0215	0.0000	0.0000	0.0000	0.0000
AT. 50 O	X	-0.0008	0.0000	0.0117	0.0088	-0.0120	0.0010
	Y	-0.0145	0.0000	-0.0033	0.0012	-0.0209	0.0175
	Z	0.0000	-0.0215	0.0000	0.0000	0.0000	0.0000
AT. 51 O	X	0.0020	0.0000	-0.0063	0.0008	-0.0040	0.0136
	Y	0.0042	0.0000	-0.0090	-0.0160	-0.0171	0.0075
	Z	0.0000	0.0069	0.0000	0.0000	0.0000	0.0000
AT. 52 O	X	-0.0020	0.0000	-0.0063	0.0008	0.0040	0.0136
	Y	-0.0042	0.0000	-0.0090	-0.0160	0.0171	0.0075
	Z	0.0000	-0.0069	0.0000	0.0000	0.0000	0.0000
AT. 53 O	X	0.0020	0.0000	-0.0063	0.0008	0.0040	-0.0136
	Y	-0.0042	0.0000	0.0090	0.0160	-0.0171	0.0075
	Z	0.0000	-0.0069	0.0000	0.0000	0.0000	0.0000
AT. 54 O	X	-0.0020	0.0000	-0.0063	0.0008	-0.0040	-0.0136
	Y	0.0042	0.0000	0.0090	0.0160	0.0171	0.0075
	Z	0.0000	0.0069	0.0000	0.0000	0.0000	0.0000
AT. 55 O	X	0.0088	0.0000	-0.0262	-0.0103	-0.0127	-0.0205
	Y	-0.0041	0.0000	-0.0002	0.0133	0.0038	-0.0070
	Z	0.0000	-0.0023	0.0000	0.0000	0.0000	0.0000
AT. 56 O	X	-0.0088	0.0000	-0.0262	-0.0103	0.0127	-0.0205
	Y	0.0041	0.0000	-0.0002	0.0133	-0.0038	-0.0070
	Z	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
AT. 57 O	X	0.0088	0.0000	-0.0262	-0.0103	0.0127	0.0205
	Y	0.0041	0.0000	0.0002	-0.0133	0.0038	-0.0070
	Z	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	-0.0088	0.0000	-0.0262	-0.0103	-0.0127	0.0205
	Y	-0.0041	0.0000	0.0002	-0.0133	-0.0038	-0.0070
	Z	0.0000	-0.0023	0.0000	0.0000	0.0000	0.0000

FREQ(CM**-1) 436.22 436.56 461.58 462.71 464.04 473.41

AT. 1 FE	X	0.0000	0.0044	-0.0079	-0.0038	0.0000	0.0000
	Y	0.0039	0.0000	0.0000	0.0000	-0.0030	-0.0005
	Z	-0.0015	0.0000	0.0000	0.0000	0.0005	0.0007
AT. 2 FE	X	0.0000	-0.0044	0.0079	-0.0038	0.0000	0.0000
	Y	0.0039	0.0000	0.0000	0.0000	0.0030	-0.0005
	Z	0.0015	0.0000	0.0000	0.0000	0.0005	-0.0007
AT. 3 FE	X	0.0000	-0.0044	-0.0079	-0.0038	0.0000	0.0000
	Y	0.0039	0.0000	0.0000	0.0000	0.0030	0.0005
	Z	-0.0015	0.0000	0.0000	0.0000	-0.0005	-0.0007
AT. 4 FE	X	0.0000	0.0044	0.0079	-0.0038	0.0000	0.0000

	Y	0.0039	0.0000	0.0000	0.0000	-0.0030	0.0005
	Z	0.0015	0.0000	0.0000	0.0000	-0.0005	0.0007
AT. 5	AL X	0.0247	0.0000	0.0000	-0.0230	0.0000	0.0029
	Y	0.0079	0.0000	0.0000	-0.0079	0.0000	0.0048
	Z	0.0000	-0.0076	0.0066	0.0000	0.0131	0.0000
AT. 6	AL X	-0.0247	0.0000	0.0000	-0.0230	0.0000	-0.0029
	Y	0.0079	0.0000	0.0000	0.0079	0.0000	0.0048
	Z	0.0000	0.0076	-0.0066	0.0000	0.0131	0.0000
AT. 7	AL X	0.0247	0.0000	0.0000	-0.0230	0.0000	-0.0029
	Y	0.0079	0.0000	0.0000	-0.0079	0.0000	-0.0048
	Z	0.0000	0.0076	0.0066	0.0000	-0.0131	0.0000
AT. 8	AL X	-0.0247	0.0000	0.0000	-0.0230	0.0000	0.0029
	Y	0.0079	0.0000	0.0000	0.0079	0.0000	-0.0048
	Z	0.0000	-0.0076	-0.0066	0.0000	-0.0131	0.0000
AT. 9	AL X	0.0060	0.0012	0.0000	-0.0012	-0.0138	0.0000
	Y	-0.0002	0.0229	0.0000	0.0097	-0.0012	0.0000
	Z	0.0000	0.0000	-0.0321	0.0000	0.0000	-0.0004
AT. 10	AL X	0.0060	-0.0012	0.0000	-0.0012	0.0138	0.0000
	Y	-0.0002	-0.0229	0.0000	0.0097	0.0012	0.0000
	Z	0.0000	0.0000	-0.0321	0.0000	0.0000	0.0004
AT. 11	AL X	-0.0060	0.0012	0.0000	-0.0012	0.0138	0.0000
	Y	-0.0002	-0.0229	0.0000	-0.0097	-0.0012	0.0000
	Z	0.0000	0.0000	0.0321	0.0000	0.0000	-0.0004
AT. 12	AL X	-0.0060	-0.0012	0.0000	-0.0012	-0.0138	0.0000
	Y	-0.0002	0.0229	0.0000	-0.0097	0.0012	0.0000
	Z	0.0000	0.0000	0.0321	0.0000	0.0000	0.0004
AT. 13	SI X	0.0000	0.0000	0.0000	-0.0064	0.0000	0.0000
	Y	-0.0068	0.0000	0.0000	0.0000	0.0000	-0.0148
	Z	0.0000	0.0000	0.0000	0.0000	0.0118	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	-0.0064	0.0000	0.0000
	Y	-0.0068	0.0000	0.0000	0.0000	0.0000	0.0148
	Z	0.0000	0.0000	0.0000	0.0000	-0.0118	0.0000
AT. 15	SI X	0.0028	-0.0154	0.0000	0.0108	-0.0040	0.0000
	Y	0.0125	0.0039	0.0000	0.0073	-0.0104	0.0000
	Z	0.0000	0.0000	0.0095	0.0000	0.0000	0.0080
AT. 16	SI X	0.0028	0.0154	0.0000	0.0108	0.0040	0.0000
	Y	0.0125	-0.0039	0.0000	0.0073	0.0104	0.0000
	Z	0.0000	0.0000	0.0095	0.0000	0.0000	-0.0080
AT. 17	SI X	-0.0028	-0.0154	0.0000	0.0108	0.0040	0.0000
	Y	0.0125	-0.0039	0.0000	-0.0073	-0.0104	0.0000
	Z	0.0000	0.0000	-0.0095	0.0000	0.0000	0.0080
AT. 18	SI X	-0.0028	0.0154	0.0000	0.0108	-0.0040	0.0000
	Y	0.0125	0.0039	0.0000	-0.0073	0.0104	0.0000
	Z	0.0000	0.0000	-0.0095	0.0000	0.0000	-0.0080
AT. 19	SI X	0.0029	-0.0081	0.0000	0.0001	0.0052	0.0000
	Y	0.0071	-0.0081	0.0000	0.0099	-0.0202	0.0000
	Z	0.0000	0.0000	0.0047	0.0000	0.0000	0.0097
AT. 20	SI X	0.0029	0.0081	0.0000	0.0001	-0.0052	0.0000
	Y	0.0071	0.0081	0.0000	0.0099	0.0202	0.0000
	Z	0.0000	0.0000	0.0047	0.0000	0.0000	-0.0097
AT. 21	SI X	-0.0029	-0.0081	0.0000	0.0001	-0.0052	0.0000
	Y	0.0071	0.0081	0.0000	-0.0099	-0.0202	0.0000
	Z	0.0000	0.0000	-0.0047	0.0000	0.0000	0.0097
AT. 22	SI X	-0.0029	0.0081	0.0000	0.0001	0.0052	0.0000

	Y	0.0071	-0.0081	0.0000	-0.0099	0.0202	0.0000
	Z	0.0000	0.0000	-0.0047	0.0000	0.0000	-0.0097
AT. 23	O X	0.0136	0.0122	0.0105	0.0176	-0.0106	-0.0073
	Y	-0.0078	-0.0082	-0.0008	0.0053	-0.0004	-0.0016
	Z	0.0164	0.0183	-0.0018	0.0077	-0.0048	0.0023
AT. 24	O X	0.0136	-0.0122	-0.0105	0.0176	0.0106	-0.0073
	Y	-0.0078	0.0082	0.0008	0.0053	0.0004	-0.0016
	Z	-0.0164	0.0183	-0.0018	-0.0077	-0.0048	-0.0023
AT. 25	O X	-0.0136	0.0122	0.0105	0.0176	0.0106	0.0073
	Y	-0.0078	0.0082	0.0008	-0.0053	-0.0004	-0.0016
	Z	0.0164	-0.0183	0.0018	-0.0077	-0.0048	0.0023
AT. 26	O X	-0.0136	-0.0122	-0.0105	0.0176	-0.0106	0.0073
	Y	-0.0078	-0.0082	-0.0008	-0.0053	0.0004	-0.0016
	Z	-0.0164	-0.0183	0.0018	0.0077	-0.0048	-0.0023
AT. 27	O X	0.0136	-0.0122	0.0105	0.0176	0.0106	0.0073
	Y	-0.0078	0.0082	-0.0008	0.0053	0.0004	0.0016
	Z	0.0164	-0.0183	-0.0018	0.0077	0.0048	-0.0023
AT. 28	O X	0.0136	0.0122	-0.0105	0.0176	-0.0106	0.0073
	Y	-0.0078	-0.0082	0.0008	0.0053	-0.0004	0.0016
	Z	-0.0164	-0.0183	-0.0018	-0.0077	0.0048	0.0023
AT. 29	O X	-0.0136	-0.0122	0.0105	0.0176	-0.0106	-0.0073
	Y	-0.0078	-0.0082	0.0008	-0.0053	0.0004	0.0016
	Z	0.0164	0.0183	0.0018	-0.0077	0.0048	-0.0023
AT. 30	O X	-0.0136	0.0122	-0.0105	0.0176	0.0106	-0.0073
	Y	-0.0078	0.0082	-0.0008	-0.0053	-0.0004	0.0016
	Z	-0.0164	0.0183	0.0018	0.0077	0.0048	0.0023
AT. 31	O X	-0.0003	-0.0011	-0.0132	0.0011	0.0062	-0.0326
	Y	-0.0005	0.0103	0.0191	-0.0032	0.0103	0.0176
	Z	-0.0009	-0.0153	0.0042	-0.0017	-0.0037	-0.0051
AT. 32	O X	-0.0003	0.0011	0.0132	0.0011	-0.0062	-0.0326
	Y	-0.0005	-0.0103	-0.0191	-0.0032	-0.0103	0.0176
	Z	0.0009	-0.0153	0.0042	0.0017	-0.0037	0.0051
AT. 33	O X	0.0003	-0.0011	-0.0132	0.0011	-0.0062	0.0326
	Y	-0.0005	-0.0103	-0.0191	0.0032	0.0103	0.0176
	Z	-0.0009	0.0153	-0.0042	0.0017	-0.0037	-0.0051
AT. 34	O X	0.0003	0.0011	0.0132	0.0011	0.0062	0.0326
	Y	-0.0005	0.0103	0.0191	0.0032	-0.0103	0.0176
	Z	0.0009	0.0153	-0.0042	-0.0017	-0.0037	0.0051
AT. 35	O X	-0.0003	0.0011	-0.0132	0.0011	-0.0062	0.0326
	Y	-0.0005	-0.0103	0.0191	-0.0032	-0.0103	-0.0176
	Z	-0.0009	0.0153	0.0042	-0.0017	0.0037	0.0051
AT. 36	O X	-0.0003	-0.0011	0.0132	0.0011	0.0062	0.0326
	Y	-0.0005	0.0103	-0.0191	-0.0032	0.0103	-0.0176
	Z	0.0009	0.0153	0.0042	0.0017	0.0037	-0.0051
AT. 37	O X	0.0003	0.0011	-0.0132	0.0011	0.0062	-0.0326
	Y	-0.0005	0.0103	-0.0191	0.0032	-0.0103	-0.0176
	Z	-0.0009	-0.0153	-0.0042	0.0017	0.0037	0.0051
AT. 38	O X	0.0003	-0.0011	0.0132	0.0011	-0.0062	-0.0326
	Y	-0.0005	-0.0103	0.0191	0.0032	0.0103	-0.0176
	Z	0.0009	-0.0153	-0.0042	-0.0017	0.0037	-0.0051
AT. 39	O X	-0.0073	0.0027	0.0005	0.0058	-0.0105	-0.0025
	Y	-0.0179	-0.0090	0.0017	0.0128	-0.0034	-0.0085
	Z	0.0178	-0.0004	-0.0027	-0.0173	0.0206	-0.0018
AT. 40	O X	-0.0073	-0.0027	-0.0005	0.0058	0.0105	-0.0025

	Y	-0.0179	0.0090	-0.0017	0.0128	0.0034	-0.0085
	Z	-0.0178	-0.0004	-0.0027	0.0173	0.0206	0.0018
AT. 41	O X	0.0073	0.0027	0.0005	0.0058	0.0105	0.0025
	Y	-0.0179	0.0090	-0.0017	-0.0128	-0.0034	-0.0085
	Z	0.0178	0.0004	0.0027	0.0173	0.0206	-0.0018
AT. 42	O X	0.0073	-0.0027	-0.0005	0.0058	-0.0105	0.0025
	Y	-0.0179	-0.0090	0.0017	-0.0128	0.0034	-0.0085
	Z	-0.0178	0.0004	0.0027	-0.0173	0.0206	0.0018
AT. 43	O X	-0.0073	-0.0027	0.0005	0.0058	0.0105	0.0025
	Y	-0.0179	0.0090	0.0017	0.0128	0.0034	0.0085
	Z	0.0178	0.0004	-0.0027	-0.0173	-0.0206	0.0018
AT. 44	O X	-0.0073	0.0027	-0.0005	0.0058	-0.0105	0.0025
	Y	-0.0179	-0.0090	-0.0017	0.0128	-0.0034	0.0085
	Z	-0.0178	0.0004	-0.0027	0.0173	-0.0206	-0.0018
AT. 45	O X	0.0073	-0.0027	0.0005	0.0058	-0.0105	-0.0025
	Y	-0.0179	-0.0090	-0.0017	-0.0128	0.0034	0.0085
	Z	0.0178	-0.0004	0.0027	0.0173	-0.0206	0.0018
AT. 46	O X	0.0073	0.0027	-0.0005	0.0058	0.0105	-0.0025
	Y	-0.0179	0.0090	0.0017	-0.0128	-0.0034	0.0085
	Z	-0.0178	-0.0004	0.0027	-0.0173	-0.0206	-0.0018
AT. 47	O X	0.0059	-0.0118	0.0000	0.0049	0.0042	0.0000
	Y	-0.0078	0.0125	0.0000	-0.0105	0.0132	0.0000
	Z	0.0000	0.0000	0.0199	0.0000	0.0000	0.0080
AT. 48	O X	0.0059	0.0118	0.0000	0.0049	-0.0042	0.0000
	Y	-0.0078	-0.0125	0.0000	-0.0105	-0.0132	0.0000
	Z	0.0000	0.0000	0.0199	0.0000	0.0000	-0.0080
AT. 49	O X	-0.0059	-0.0118	0.0000	0.0049	-0.0042	0.0000
	Y	-0.0078	-0.0125	0.0000	0.0105	0.0132	0.0000
	Z	0.0000	0.0000	-0.0199	0.0000	0.0000	0.0080
AT. 50	O X	-0.0059	0.0118	0.0000	0.0049	0.0042	0.0000
	Y	-0.0078	0.0125	0.0000	0.0105	-0.0132	0.0000
	Z	0.0000	0.0000	-0.0199	0.0000	0.0000	-0.0080
AT. 51	O X	-0.0026	-0.0076	0.0000	-0.0105	0.0022	0.0000
	Y	-0.0003	0.0123	0.0000	-0.0141	0.0034	0.0000
	Z	0.0000	0.0000	0.0041	0.0000	0.0000	-0.0092
AT. 52	O X	-0.0026	0.0076	0.0000	-0.0105	-0.0022	0.0000
	Y	-0.0003	-0.0123	0.0000	-0.0141	-0.0034	0.0000
	Z	0.0000	0.0000	0.0041	0.0000	0.0000	0.0092
AT. 53	O X	0.0026	-0.0076	0.0000	-0.0105	-0.0022	0.0000
	Y	-0.0003	-0.0123	0.0000	0.0141	0.0034	0.0000
	Z	0.0000	0.0000	-0.0041	0.0000	0.0000	-0.0092
AT. 54	O X	0.0026	0.0076	0.0000	-0.0105	0.0022	0.0000
	Y	-0.0003	0.0123	0.0000	0.0141	-0.0034	0.0000
	Z	0.0000	0.0000	-0.0041	0.0000	0.0000	0.0092
AT. 55	O X	-0.0056	0.0076	0.0000	-0.0027	-0.0184	0.0000
	Y	0.0087	-0.0077	0.0000	0.0091	-0.0091	0.0000
	Z	0.0000	0.0000	-0.0089	0.0000	0.0000	-0.0148
AT. 56	O X	-0.0056	-0.0076	0.0000	-0.0027	0.0184	0.0000
	Y	0.0087	0.0077	0.0000	0.0091	0.0091	0.0000
	Z	0.0000	0.0000	-0.0089	0.0000	0.0000	0.0148
AT. 57	O X	0.0056	0.0076	0.0000	-0.0027	0.0184	0.0000
	Y	0.0087	0.0077	0.0000	-0.0091	-0.0091	0.0000
	Z	0.0000	0.0000	0.0089	0.0000	0.0000	-0.0148
AT. 58	O X	0.0056	-0.0076	0.0000	-0.0027	-0.0184	0.0000

Y	0.0087	-0.0077	0.0000	-0.0091	0.0091	0.0000
Z	0.0000	0.0000	0.0089	0.0000	0.0000	0.0148

FREQ(CM**-1) 476.46 479.87 488.71 490.03 491.67 494.29

AT. 1 FE X	0.0011	-0.0015	0.0000	0.0000	0.0000	0.0038
Y	0.0000	0.0000	0.0003	-0.0036	-0.0002	0.0000
Z	0.0000	0.0000	-0.0020	-0.0020	-0.0005	0.0000
AT. 2 FE X	0.0011	0.0015	0.0000	0.0000	0.0000	-0.0038
Y	0.0000	0.0000	0.0003	0.0036	-0.0002	0.0000
Z	0.0000	0.0000	0.0020	-0.0020	0.0005	0.0000
AT. 3 FE X	-0.0011	-0.0015	0.0000	0.0000	0.0000	-0.0038
Y	0.0000	0.0000	-0.0003	-0.0036	-0.0002	0.0000
Z	0.0000	0.0000	0.0020	-0.0020	-0.0005	0.0000
AT. 4 FE X	-0.0011	0.0015	0.0000	0.0000	0.0000	0.0038
Y	0.0000	0.0000	-0.0003	0.0036	-0.0002	0.0000
Z	0.0000	0.0000	-0.0020	-0.0020	0.0005	0.0000
AT. 5 AL X	0.0045	0.0000	-0.0040	0.0000	-0.0032	0.0000
Y	-0.0002	0.0000	-0.0040	0.0000	0.0164	0.0000
Z	0.0000	-0.0134	0.0000	-0.0027	0.0000	-0.0140
AT. 6 AL X	0.0045	0.0000	0.0040	0.0000	0.0032	0.0000
Y	0.0002	0.0000	-0.0040	0.0000	0.0164	0.0000
Z	0.0000	0.0134	0.0000	-0.0027	0.0000	0.0140
AT. 7 AL X	-0.0045	0.0000	0.0040	0.0000	-0.0032	0.0000
Y	0.0002	0.0000	0.0040	0.0000	0.0164	0.0000
Z	0.0000	-0.0134	0.0000	-0.0027	0.0000	0.0140
AT. 8 AL X	-0.0045	0.0000	-0.0040	0.0000	0.0032	0.0000
Y	-0.0002	0.0000	0.0040	0.0000	0.0164	0.0000
Z	0.0000	0.0134	0.0000	-0.0027	0.0000	-0.0140
AT. 9 AL X	0.0000	0.0000	0.0000	0.0000	-0.0075	0.0149
Y	0.0000	0.0000	0.0000	0.0000	0.0027	0.0082
Z	0.0003	-0.0015	-0.0010	-0.0006	0.0000	0.0000
AT. 10 AL X	0.0000	0.0000	0.0000	0.0000	-0.0075	-0.0149
Y	0.0000	0.0000	0.0000	0.0000	0.0027	-0.0082
Z	-0.0003	-0.0015	0.0010	-0.0006	0.0000	0.0000
AT. 11 AL X	0.0000	0.0000	0.0000	0.0000	0.0075	0.0149
Y	0.0000	0.0000	0.0000	0.0000	0.0027	-0.0082
Z	-0.0003	0.0015	-0.0010	-0.0006	0.0000	0.0000
AT. 12 AL X	0.0000	0.0000	0.0000	0.0000	0.0075	-0.0149
Y	0.0000	0.0000	0.0000	0.0000	0.0027	0.0082
Z	0.0003	0.0015	0.0010	-0.0006	0.0000	0.0000
AT. 13 SI X	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	0.0000	0.0072	0.0000	0.0292	0.0000
Z	0.0000	0.0000	0.0000	0.0050	0.0000	0.0000
AT. 14 SI X	-0.0026	0.0000	0.0000	0.0000	0.0000	0.0000
Y	0.0000	0.0000	-0.0072	0.0000	0.0292	0.0000
Z	0.0000	0.0000	0.0000	0.0050	0.0000	0.0000
AT. 15 SI X	0.0000	0.0000	0.0000	0.0000	0.0118	0.0002
Y	0.0000	0.0000	0.0000	0.0000	-0.0088	-0.0019
Z	-0.0163	0.0130	0.0144	-0.0003	0.0000	0.0000
AT. 16 SI X	0.0000	0.0000	0.0000	0.0000	0.0118	-0.0002
Y	0.0000	0.0000	0.0000	0.0000	-0.0088	0.0019
Z	0.0163	0.0130	-0.0144	-0.0003	0.0000	0.0000
AT. 17 SI X	0.0000	0.0000	0.0000	0.0000	-0.0118	0.0002

	Y	0.0000	0.0000	0.0000	0.0000	-0.0088	0.0019
	Z	0.0163	-0.0130	0.0144	-0.0003	0.0000	0.0000
AT. 18 SI	X	0.0000	0.0000	0.0000	0.0000	-0.0118	-0.0002
	Y	0.0000	0.0000	0.0000	0.0000	-0.0088	-0.0019
	Z	-0.0163	-0.0130	-0.0144	-0.0003	0.0000	0.0000
AT. 19 SI	X	0.0000	0.0000	0.0000	0.0000	-0.0082	0.0009
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0171
	Z	0.0227	-0.0103	-0.0042	0.0200	0.0000	0.0000
AT. 20 SI	X	0.0000	0.0000	0.0000	0.0000	-0.0082	-0.0009
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	-0.0171
	Z	-0.0227	-0.0103	0.0042	0.0200	0.0000	0.0000
AT. 21 SI	X	0.0000	0.0000	0.0000	0.0000	0.0082	0.0009
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	-0.0171
	Z	-0.0227	0.0103	-0.0042	0.0200	0.0000	0.0000
AT. 22 SI	X	0.0000	0.0000	0.0000	0.0000	0.0082	-0.0009
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0171
	Z	0.0227	0.0103	0.0042	0.0200	0.0000	0.0000
AT. 23 O	X	-0.0062	0.0098	-0.0260	-0.0059	-0.0033	-0.0085
	Y	0.0021	0.0151	-0.0140	-0.0131	-0.0031	0.0086
	Z	0.0045	-0.0089	0.0011	0.0019	0.0105	-0.0044
AT. 24 O	X	-0.0062	-0.0098	-0.0260	0.0059	-0.0033	0.0085
	Y	0.0021	-0.0151	-0.0140	0.0131	-0.0031	-0.0086
	Z	-0.0045	-0.0089	-0.0011	0.0019	-0.0105	-0.0044
AT. 25 O	X	-0.0062	0.0098	0.0260	0.0059	0.0033	-0.0085
	Y	-0.0021	-0.0151	-0.0140	-0.0131	-0.0031	-0.0086
	Z	-0.0045	0.0089	0.0011	0.0019	0.0105	0.0044
AT. 26 O	X	-0.0062	-0.0098	0.0260	-0.0059	0.0033	0.0085
	Y	-0.0021	0.0151	-0.0140	0.0131	-0.0031	0.0086
	Z	0.0045	0.0089	-0.0011	0.0019	-0.0105	0.0044
AT. 27 O	X	0.0062	0.0098	0.0260	-0.0059	-0.0033	0.0085
	Y	-0.0021	0.0151	0.0140	-0.0131	-0.0031	-0.0086
	Z	-0.0045	-0.0089	-0.0011	0.0019	0.0105	0.0044
AT. 28 O	X	0.0062	-0.0098	0.0260	0.0059	-0.0033	-0.0085
	Y	-0.0021	-0.0151	0.0140	0.0131	-0.0031	0.0086
	Z	0.0045	-0.0089	0.0011	0.0019	-0.0105	0.0044
AT. 29 O	X	0.0062	0.0098	-0.0260	0.0059	0.0033	0.0085
	Y	0.0021	-0.0151	0.0140	-0.0131	-0.0031	0.0086
	Z	0.0045	0.0089	-0.0011	0.0019	0.0105	-0.0044
AT. 30 O	X	0.0062	-0.0098	-0.0260	-0.0059	0.0033	-0.0085
	Y	0.0021	0.0151	0.0140	0.0131	-0.0031	-0.0086
	Z	-0.0045	0.0089	0.0011	0.0019	-0.0105	-0.0044
AT. 31 O	X	0.0002	0.0048	0.0025	0.0043	0.0048	0.0115
	Y	0.0008	-0.0014	-0.0011	0.0030	-0.0078	-0.0004
	Z	0.0004	-0.0010	0.0022	-0.0028	0.0230	-0.0084
AT. 32 O	X	0.0002	-0.0048	0.0025	-0.0043	0.0048	-0.0115
	Y	0.0008	0.0014	-0.0011	-0.0030	-0.0078	0.0004
	Z	-0.0004	-0.0010	-0.0022	-0.0028	-0.0230	-0.0084
AT. 33 O	X	0.0002	0.0048	-0.0025	-0.0043	-0.0048	0.0115
	Y	-0.0008	0.0014	-0.0011	0.0030	-0.0078	0.0004
	Z	-0.0004	0.0010	0.0022	-0.0028	0.0230	0.0084
AT. 34 O	X	0.0002	-0.0048	-0.0025	0.0043	-0.0048	-0.0115
	Y	-0.0008	-0.0014	-0.0011	-0.0030	-0.0078	-0.0004
	Z	0.0004	0.0010	-0.0022	-0.0028	-0.0230	0.0084
AT. 35 O	X	-0.0002	0.0048	-0.0025	0.0043	0.0048	-0.0115

	Y	-0.0008	-0.0014	0.0011	0.0030	-0.0078	0.0004
	Z	-0.0004	-0.0010	-0.0022	-0.0028	0.0230	0.0084
AT. 36	O X	-0.0002	-0.0048	-0.0025	-0.0043	0.0048	0.0115
	Y	-0.0008	0.0014	0.0011	-0.0030	-0.0078	-0.0004
	Z	0.0004	-0.0010	0.0022	-0.0028	-0.0230	0.0084
AT. 37	O X	-0.0002	0.0048	0.0025	-0.0043	-0.0048	-0.0115
	Y	0.0008	0.0014	0.0011	0.0030	-0.0078	-0.0004
	Z	0.0004	0.0010	-0.0022	-0.0028	0.0230	-0.0084
AT. 38	O X	-0.0002	-0.0048	0.0025	0.0043	-0.0048	0.0115
	Y	0.0008	-0.0014	0.0011	-0.0030	-0.0078	0.0004
	Z	-0.0004	0.0010	0.0022	-0.0028	-0.0230	-0.0084
AT. 39	O X	0.0034	-0.0131	-0.0018	-0.0031	-0.0081	-0.0205
	Y	0.0289	0.0249	0.0210	0.0283	0.0017	0.0053
	Z	0.0042	0.0083	-0.0012	0.0090	0.0052	0.0140
AT. 40	O X	0.0034	0.0131	-0.0018	0.0031	-0.0081	0.0205
	Y	0.0289	-0.0249	0.0210	-0.0283	0.0017	-0.0053
	Z	-0.0042	0.0083	0.0012	0.0090	-0.0052	0.0140
AT. 41	O X	0.0034	-0.0131	0.0018	0.0031	0.0081	-0.0205
	Y	-0.0289	-0.0249	0.0210	0.0283	0.0017	-0.0053
	Z	-0.0042	-0.0083	-0.0012	0.0090	0.0052	-0.0140
AT. 42	O X	0.0034	0.0131	0.0018	-0.0031	0.0081	0.0205
	Y	-0.0289	0.0249	0.0210	-0.0283	0.0017	0.0053
	Z	0.0042	-0.0083	0.0012	0.0090	-0.0052	-0.0140
AT. 43	O X	-0.0034	-0.0131	0.0018	-0.0031	-0.0081	0.0205
	Y	-0.0289	0.0249	-0.0210	0.0283	0.0017	-0.0053
	Z	-0.0042	0.0083	0.0012	0.0090	0.0052	-0.0140
AT. 44	O X	-0.0034	0.0131	0.0018	0.0031	-0.0081	-0.0205
	Y	-0.0289	-0.0249	-0.0210	-0.0283	0.0017	0.0053
	Z	0.0042	0.0083	-0.0012	0.0090	-0.0052	-0.0140
AT. 45	O X	-0.0034	-0.0131	-0.0018	0.0031	0.0081	0.0205
	Y	0.0289	-0.0249	-0.0210	0.0283	0.0017	0.0053
	Z	0.0042	-0.0083	0.0012	0.0090	0.0052	0.0140
AT. 46	O X	-0.0034	0.0131	-0.0018	-0.0031	0.0081	-0.0205
	Y	0.0289	0.0249	-0.0210	-0.0283	0.0017	-0.0053
	Z	-0.0042	-0.0083	-0.0012	0.0090	-0.0052	0.0140
AT. 47	O X	0.0000	0.0000	0.0000	0.0000	-0.0094	-0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0029	0.0060
	Z	-0.0155	0.0030	0.0039	-0.0123	0.0000	0.0000
AT. 48	O X	0.0000	0.0000	0.0000	0.0000	-0.0094	0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0029	-0.0060
	Z	0.0155	0.0030	-0.0039	-0.0123	0.0000	0.0000
AT. 49	O X	0.0000	0.0000	0.0000	0.0000	0.0094	-0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0029	-0.0060
	Z	0.0155	-0.0030	0.0039	-0.0123	0.0000	0.0000
AT. 50	O X	0.0000	0.0000	0.0000	0.0000	0.0094	0.0064
	Y	0.0000	0.0000	0.0000	0.0000	0.0029	0.0060
	Z	-0.0155	-0.0030	-0.0039	-0.0123	0.0000	0.0000
AT. 51	O X	0.0000	0.0000	0.0000	0.0000	0.0018	-0.0028
	Y	0.0000	0.0000	0.0000	0.0000	-0.0095	-0.0065
	Z	0.0087	-0.0159	-0.0250	-0.0070	0.0000	0.0000
AT. 52	O X	0.0000	0.0000	0.0000	0.0000	0.0018	0.0028
	Y	0.0000	0.0000	0.0000	0.0000	-0.0095	0.0065
	Z	-0.0087	-0.0159	0.0250	-0.0070	0.0000	0.0000
AT. 53	O X	0.0000	0.0000	0.0000	0.0000	-0.0018	-0.0028

	Y	0.0000	0.0000	0.0000	0.0000	-0.0095	0.0065
	Z	-0.0087	0.0159	-0.0250	-0.0070	0.0000	0.0000
AT. 54 O	X	0.0000	0.0000	0.0000	0.0000	-0.0018	0.0028
	Y	0.0000	0.0000	0.0000	0.0000	-0.0095	-0.0065
	Z	0.0087	0.0159	0.0250	-0.0070	0.0000	0.0000
AT. 55 O	X	0.0000	0.0000	0.0000	0.0000	-0.0063	0.0157
	Y	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0033
	Z	-0.0192	0.0168	0.0066	-0.0239	0.0000	0.0000
AT. 56 O	X	0.0000	0.0000	0.0000	0.0000	-0.0063	-0.0157
	Y	0.0000	0.0000	0.0000	0.0000	-0.0053	-0.0033
	Z	0.0192	0.0168	-0.0066	-0.0239	0.0000	0.0000
AT. 57 O	X	0.0000	0.0000	0.0000	0.0000	0.0063	0.0157
	Y	0.0000	0.0000	0.0000	0.0000	-0.0053	-0.0033
	Z	0.0192	-0.0168	0.0066	-0.0239	0.0000	0.0000
AT. 58 O	X	0.0000	0.0000	0.0000	0.0000	0.0063	-0.0157
	Y	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0033
	Z	-0.0192	-0.0168	-0.0066	-0.0239	0.0000	0.0000

FREQ(CM**-1) 498.33 501.01 502.05 506.57 508.19 513.05

AT. 1 FE	X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0034
	Y	-0.0035	0.0020	-0.0034	0.0041	-0.0032	0.0000
	Z	0.0007	-0.0027	0.0002	-0.0009	-0.0002	0.0000
AT. 2 FE	X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0034
	Y	0.0035	-0.0020	-0.0034	-0.0041	-0.0032	0.0000
	Z	0.0007	-0.0027	-0.0002	-0.0009	0.0002	0.0000
AT. 3 FE	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034
	Y	0.0035	0.0020	0.0034	0.0041	-0.0032	0.0000
	Z	-0.0007	-0.0027	-0.0002	-0.0009	-0.0002	0.0000
AT. 4 FE	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034
	Y	-0.0035	-0.0020	0.0034	-0.0041	-0.0032	0.0000
	Z	-0.0007	-0.0027	0.0002	-0.0009	0.0002	0.0000
AT. 5 AL	X	0.0000	0.0000	0.0030	0.0000	0.0014	-0.0010
	Y	0.0000	0.0000	-0.0077	0.0000	0.0056	0.0024
	Z	0.0107	0.0011	0.0000	-0.0059	0.0000	0.0000
AT. 6 AL	X	0.0000	0.0000	-0.0030	0.0000	-0.0014	-0.0010
	Y	0.0000	0.0000	-0.0077	0.0000	0.0056	-0.0024
	Z	0.0107	0.0011	0.0000	-0.0059	0.0000	0.0000
AT. 7 AL	X	0.0000	0.0000	-0.0030	0.0000	0.0014	0.0010
	Y	0.0000	0.0000	0.0077	0.0000	0.0056	-0.0024
	Z	-0.0107	0.0011	0.0000	-0.0059	0.0000	0.0000
AT. 8 AL	X	0.0000	0.0000	0.0030	0.0000	-0.0014	0.0010
	Y	0.0000	0.0000	0.0077	0.0000	0.0056	0.0024
	Z	-0.0107	0.0011	0.0000	-0.0059	0.0000	0.0000
AT. 9 AL	X	0.0108	0.0000	0.0000	0.0000	-0.0071	0.0000
	Y	0.0011	0.0000	0.0000	0.0000	0.0032	0.0000
	Z	0.0000	0.0048	-0.0007	-0.0022	0.0000	0.0023
AT. 10 AL	X	-0.0108	0.0000	0.0000	0.0000	-0.0071	0.0000
	Y	-0.0011	0.0000	0.0000	0.0000	0.0032	0.0000
	Z	0.0000	0.0048	0.0007	-0.0022	0.0000	-0.0023
AT. 11 AL	X	-0.0108	0.0000	0.0000	0.0000	0.0071	0.0000
	Y	0.0011	0.0000	0.0000	0.0000	0.0032	0.0000
	Z	0.0000	0.0048	-0.0007	-0.0022	0.0000	-0.0023
AT. 12 AL	X	0.0108	0.0000	0.0000	0.0000	0.0071	0.0000

	Y	-0.0011	0.0000	0.0000	0.0000	0.0032	0.0000
	Z	0.0000	0.0048	0.0007	-0.0022	0.0000	0.0023
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0031
	Y	0.0000	0.0000	-0.0064	0.0000	-0.0121	0.0000
	Z	-0.0202	-0.0238	0.0000	0.0121	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0031
	Y	0.0000	0.0000	0.0064	0.0000	-0.0121	0.0000
	Z	0.0202	-0.0238	0.0000	0.0121	0.0000	0.0000
AT. 15	SI X	-0.0114	0.0000	0.0000	0.0000	0.0002	0.0000
	Y	0.0114	0.0000	0.0000	0.0000	-0.0050	0.0000
	Z	0.0000	0.0097	-0.0140	0.0187	0.0000	0.0154
AT. 16	SI X	0.0114	0.0000	0.0000	0.0000	0.0002	0.0000
	Y	-0.0114	0.0000	0.0000	0.0000	-0.0050	0.0000
	Z	0.0000	0.0097	0.0140	0.0187	0.0000	-0.0154
AT. 17	SI X	0.0114	0.0000	0.0000	0.0000	-0.0002	0.0000
	Y	0.0114	0.0000	0.0000	0.0000	-0.0050	0.0000
	Z	0.0000	0.0097	-0.0140	0.0187	0.0000	-0.0154
AT. 18	SI X	-0.0114	0.0000	0.0000	0.0000	-0.0002	0.0000
	Y	-0.0114	0.0000	0.0000	0.0000	-0.0050	0.0000
	Z	0.0000	0.0097	0.0140	0.0187	0.0000	0.0154
AT. 19	SI X	-0.0068	0.0000	0.0000	0.0000	-0.0157	0.0000
	Y	-0.0117	0.0000	0.0000	0.0000	-0.0019	0.0000
	Z	0.0000	-0.0043	-0.0171	-0.0089	0.0000	-0.0033
AT. 20	SI X	0.0068	0.0000	0.0000	0.0000	-0.0157	0.0000
	Y	0.0117	0.0000	0.0000	0.0000	-0.0019	0.0000
	Z	0.0000	-0.0043	0.0171	-0.0089	0.0000	0.0033
AT. 21	SI X	0.0068	0.0000	0.0000	0.0000	0.0157	0.0000
	Y	-0.0117	0.0000	0.0000	0.0000	-0.0019	0.0000
	Z	0.0000	-0.0043	-0.0171	-0.0089	0.0000	0.0033
AT. 22	SI X	-0.0068	0.0000	0.0000	0.0000	0.0157	0.0000
	Y	0.0117	0.0000	0.0000	0.0000	-0.0019	0.0000
	Z	0.0000	-0.0043	0.0171	-0.0089	0.0000	-0.0033
AT. 23	O X	0.0021	-0.0099	0.0098	-0.0219	-0.0021	0.0268
	Y	0.0220	-0.0034	-0.0006	-0.0129	-0.0033	0.0146
	Z	-0.0101	0.0030	-0.0030	0.0080	0.0031	-0.0016
AT. 24	O X	-0.0021	0.0099	0.0098	0.0219	-0.0021	0.0268
	Y	-0.0220	0.0034	-0.0006	0.0129	-0.0033	0.0146
	Z	-0.0101	0.0030	0.0030	0.0080	-0.0031	0.0016
AT. 25	O X	-0.0021	0.0099	-0.0098	0.0219	0.0021	0.0268
	Y	0.0220	-0.0034	-0.0006	-0.0129	-0.0033	-0.0146
	Z	-0.0101	0.0030	-0.0030	0.0080	0.0031	0.0016
AT. 26	O X	0.0021	-0.0099	-0.0098	-0.0219	0.0021	0.0268
	Y	-0.0220	0.0034	-0.0006	0.0129	-0.0033	-0.0146
	Z	-0.0101	0.0030	0.0030	0.0080	-0.0031	-0.0016
AT. 27	O X	-0.0021	-0.0099	-0.0098	-0.0219	-0.0021	-0.0268
	Y	-0.0220	-0.0034	0.0006	-0.0129	-0.0033	-0.0146
	Z	0.0101	0.0030	0.0030	0.0080	0.0031	0.0016
AT. 28	O X	0.0021	0.0099	-0.0098	0.0219	-0.0021	-0.0268
	Y	0.0220	0.0034	0.0006	0.0129	-0.0033	-0.0146
	Z	0.0101	0.0030	-0.0030	0.0080	-0.0031	-0.0016
AT. 29	O X	0.0021	0.0099	0.0098	0.0219	0.0021	-0.0268
	Y	-0.0220	-0.0034	0.0006	-0.0129	-0.0033	0.0146
	Z	0.0101	0.0030	0.0030	0.0080	0.0031	-0.0016
AT. 30	O X	-0.0021	-0.0099	0.0098	-0.0219	0.0021	-0.0268

	Y	0.0220	0.0034	0.0006	0.0129	-0.0033	0.0146
	Z	0.0101	0.0030	-0.0030	0.0080	-0.0031	0.0016
AT. 31	O X	-0.0033	-0.0310	-0.0157	0.0093	-0.0299	0.0010
	Y	-0.0125	-0.0106	0.0075	0.0062	0.0145	-0.0016
	Z	-0.0001	0.0141	-0.0013	-0.0048	-0.0015	-0.0004
AT. 32	O X	0.0033	0.0310	-0.0157	-0.0093	-0.0299	0.0010
	Y	0.0125	0.0106	0.0075	-0.0062	0.0145	-0.0016
	Z	-0.0001	0.0141	0.0013	-0.0048	0.0015	0.0004
AT. 33	O X	0.0033	0.0310	0.0157	-0.0093	0.0299	0.0010
	Y	-0.0125	-0.0106	0.0075	0.0062	0.0145	0.0016
	Z	-0.0001	0.0141	-0.0013	-0.0048	-0.0015	0.0004
AT. 34	O X	-0.0033	-0.0310	0.0157	0.0093	0.0299	0.0010
	Y	0.0125	0.0106	0.0075	-0.0062	0.0145	0.0016
	Z	-0.0001	0.0141	0.0013	-0.0048	0.0015	-0.0004
AT. 35	O X	0.0033	-0.0310	0.0157	0.0093	-0.0299	-0.0010
	Y	0.0125	-0.0106	-0.0075	0.0062	0.0145	0.0016
	Z	0.0001	0.0141	0.0013	-0.0048	-0.0015	0.0004
AT. 36	O X	-0.0033	0.0310	0.0157	-0.0093	-0.0299	-0.0010
	Y	-0.0125	0.0106	-0.0075	-0.0062	0.0145	0.0016
	Z	0.0001	0.0141	-0.0013	-0.0048	0.0015	-0.0004
AT. 37	O X	-0.0033	0.0310	-0.0157	-0.0093	0.0299	-0.0010
	Y	0.0125	-0.0106	-0.0075	0.0062	0.0145	-0.0016
	Z	0.0001	0.0141	0.0013	-0.0048	-0.0015	-0.0004
AT. 38	O X	0.0033	-0.0310	-0.0157	0.0093	0.0299	-0.0010
	Y	-0.0125	0.0106	-0.0075	-0.0062	0.0145	-0.0016
	Z	0.0001	0.0141	-0.0013	-0.0048	0.0015	0.0004
AT. 39	O X	-0.0015	-0.0036	0.0034	-0.0070	-0.0071	-0.0048
	Y	0.0108	0.0031	0.0205	-0.0100	0.0077	0.0144
	Z	0.0040	-0.0009	0.0033	-0.0016	0.0061	-0.0017
AT. 40	O X	0.0015	0.0036	0.0034	0.0070	-0.0071	-0.0048
	Y	-0.0108	-0.0031	0.0205	0.0100	0.0077	0.0144
	Z	0.0040	-0.0009	-0.0033	-0.0016	-0.0061	0.0017
AT. 41	O X	0.0015	0.0036	-0.0034	0.0070	0.0071	-0.0048
	Y	0.0108	0.0031	0.0205	-0.0100	0.0077	-0.0144
	Z	0.0040	-0.0009	0.0033	-0.0016	0.0061	0.0017
AT. 42	O X	-0.0015	-0.0036	-0.0034	-0.0070	0.0071	-0.0048
	Y	-0.0108	-0.0031	0.0205	0.0100	0.0077	-0.0144
	Z	0.0040	-0.0009	-0.0033	-0.0016	-0.0061	-0.0017
AT. 43	O X	0.0015	-0.0036	-0.0034	-0.0070	-0.0071	0.0048
	Y	-0.0108	0.0031	-0.0205	-0.0100	0.0077	-0.0144
	Z	-0.0040	-0.0009	-0.0033	-0.0016	0.0061	0.0017
AT. 44	O X	-0.0015	0.0036	-0.0034	0.0070	-0.0071	0.0048
	Y	0.0108	-0.0031	-0.0205	0.0100	0.0077	-0.0144
	Z	-0.0040	-0.0009	0.0033	-0.0016	-0.0061	-0.0017
AT. 45	O X	-0.0015	0.0036	0.0034	0.0070	0.0071	0.0048
	Y	-0.0108	0.0031	-0.0205	-0.0100	0.0077	0.0144
	Z	-0.0040	-0.0009	-0.0033	-0.0016	0.0061	-0.0017
AT. 46	O X	0.0015	-0.0036	0.0034	-0.0070	0.0071	0.0048
	Y	0.0108	-0.0031	-0.0205	0.0100	0.0077	0.0144
	Z	-0.0040	-0.0009	0.0033	-0.0016	-0.0061	0.0017
AT. 47	O X	-0.0099	0.0000	0.0000	0.0000	-0.0073	0.0000
	Y	0.0058	0.0000	0.0000	0.0000	-0.0141	0.0000
	Z	0.0000	-0.0064	0.0166	0.0102	0.0000	0.0011
AT. 48	O X	0.0099	0.0000	0.0000	0.0000	-0.0073	0.0000

	Y	-0.0058	0.0000	0.0000	0.0000	-0.0141	0.0000
	Z	0.0000	-0.0064	-0.0166	0.0102	0.0000	-0.0011
AT. 49 O	X	0.0099	0.0000	0.0000	0.0000	0.0073	0.0000
	Y	0.0058	0.0000	0.0000	0.0000	-0.0141	0.0000
	Z	0.0000	-0.0064	0.0166	0.0102	0.0000	-0.0011
AT. 50 O	X	-0.0099	0.0000	0.0000	0.0000	0.0073	0.0000
	Y	-0.0058	0.0000	0.0000	0.0000	-0.0141	0.0000
	Z	0.0000	-0.0064	-0.0166	0.0102	0.0000	0.0011
AT. 51 O	X	0.0013	0.0000	0.0000	0.0000	0.0015	0.0000
	Y	0.0166	0.0000	0.0000	0.0000	0.0018	0.0000
	Z	0.0000	-0.0084	0.0092	-0.0241	0.0000	-0.0236
AT. 52 O	X	-0.0013	0.0000	0.0000	0.0000	0.0015	0.0000
	Y	-0.0166	0.0000	0.0000	0.0000	0.0018	0.0000
	Z	0.0000	-0.0084	-0.0092	-0.0241	0.0000	0.0236
AT. 53 O	X	-0.0013	0.0000	0.0000	0.0000	-0.0015	0.0000
	Y	0.0166	0.0000	0.0000	0.0000	0.0018	0.0000
	Z	0.0000	-0.0084	0.0092	-0.0241	0.0000	0.0236
AT. 54 O	X	0.0013	0.0000	0.0000	0.0000	-0.0015	0.0000
	Y	-0.0166	0.0000	0.0000	0.0000	0.0018	0.0000
	Z	0.0000	-0.0084	-0.0092	-0.0241	0.0000	-0.0236
AT. 55 O	X	0.0010	0.0000	0.0000	0.0000	0.0062	0.0000
	Y	-0.0036	0.0000	0.0000	0.0000	-0.0063	0.0000
	Z	0.0000	-0.0060	0.0252	-0.0010	0.0000	-0.0166
AT. 56 O	X	-0.0010	0.0000	0.0000	0.0000	0.0062	0.0000
	Y	0.0036	0.0000	0.0000	0.0000	-0.0063	0.0000
	Z	0.0000	-0.0060	-0.0252	-0.0010	0.0000	0.0166
AT. 57 O	X	-0.0010	0.0000	0.0000	0.0000	-0.0062	0.0000
	Y	-0.0036	0.0000	0.0000	0.0000	-0.0063	0.0000
	Z	0.0000	-0.0060	0.0252	-0.0010	0.0000	0.0166
AT. 58 O	X	0.0010	0.0000	0.0000	0.0000	-0.0062	0.0000
	Y	0.0036	0.0000	0.0000	0.0000	-0.0063	0.0000
	Z	0.0000	-0.0060	-0.0252	-0.0010	0.0000	-0.0166

FREQ(CM**-1) 538.07 554.26 563.97 566.78 572.49 581.71

AT. 1 FE	X	0.0012	-0.0023	0.0000	-0.0012	0.0014	0.0000
	Y	0.0000	0.0000	-0.0002	0.0000	0.0000	-0.0005
	Z	0.0000	0.0000	-0.0025	0.0000	0.0000	-0.0008
AT. 2 FE	X	0.0012	0.0023	0.0000	0.0012	0.0014	0.0000
	Y	0.0000	0.0000	0.0002	0.0000	0.0000	0.0005
	Z	0.0000	0.0000	-0.0025	0.0000	0.0000	-0.0008
AT. 3 FE	X	0.0012	-0.0023	0.0000	0.0012	0.0014	0.0000
	Y	0.0000	0.0000	0.0002	0.0000	0.0000	0.0005
	Z	0.0000	0.0000	0.0025	0.0000	0.0000	0.0008
AT. 4 FE	X	0.0012	0.0023	0.0000	-0.0012	0.0014	0.0000
	Y	0.0000	0.0000	-0.0002	0.0000	0.0000	-0.0005
	Z	0.0000	0.0000	0.0025	0.0000	0.0000	0.0008
AT. 5 AL	X	-0.0150	0.0000	0.0000	0.0000	-0.0015	0.0000
	Y	-0.0081	0.0000	0.0000	0.0000	0.0103	0.0000
	Z	0.0000	-0.0005	-0.0004	0.0068	0.0000	0.0026
AT. 6 AL	X	-0.0150	0.0000	0.0000	0.0000	-0.0015	0.0000
	Y	0.0081	0.0000	0.0000	0.0000	-0.0103	0.0000
	Z	0.0000	0.0005	-0.0004	-0.0068	0.0000	0.0026
AT. 7 AL	X	-0.0150	0.0000	0.0000	0.0000	-0.0015	0.0000

	Y	-0.0081	0.0000	0.0000	0.0000	0.0103	0.0000
	Z	0.0000	-0.0005	0.0004	-0.0068	0.0000	-0.0026
AT. 8	AL X	-0.0150	0.0000	0.0000	0.0000	-0.0015	0.0000
	Y	0.0081	0.0000	0.0000	0.0000	-0.0103	0.0000
	Z	0.0000	0.0005	0.0004	0.0068	0.0000	-0.0026
AT. 9	AL X	0.0134	0.0000	-0.0052	-0.0160	0.0062	-0.0049
	Y	-0.0155	0.0000	-0.0013	0.0203	0.0140	0.0030
	Z	0.0000	0.0077	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0134	0.0000	0.0052	0.0160	0.0062	0.0049
	Y	-0.0155	0.0000	0.0013	-0.0203	0.0140	-0.0030
	Z	0.0000	0.0077	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0134	0.0000	0.0052	-0.0160	0.0062	0.0049
	Y	0.0155	0.0000	-0.0013	-0.0203	-0.0140	0.0030
	Z	0.0000	-0.0077	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0134	0.0000	-0.0052	0.0160	0.0062	-0.0049
	Y	0.0155	0.0000	0.0013	0.0203	-0.0140	-0.0030
	Z	0.0000	-0.0077	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	-0.0021	0.0000	0.0000	0.0000	-0.0129	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0040	0.0000	0.0000	-0.0011
AT. 14	SI X	-0.0021	0.0000	0.0000	0.0000	-0.0129	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0040	0.0000	0.0000	0.0011
AT. 15	SI X	-0.0131	0.0000	0.0018	0.0070	0.0051	0.0133
	Y	-0.0066	0.0000	0.0040	-0.0061	-0.0187	0.0151
	Z	0.0000	0.0138	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	-0.0131	0.0000	-0.0018	-0.0070	0.0051	-0.0133
	Y	-0.0066	0.0000	-0.0040	0.0061	-0.0187	-0.0151
	Z	0.0000	0.0138	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	-0.0131	0.0000	-0.0018	0.0070	0.0051	-0.0133
	Y	0.0066	0.0000	0.0040	0.0061	0.0187	0.0151
	Z	0.0000	-0.0138	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	-0.0131	0.0000	0.0018	-0.0070	0.0051	0.0133
	Y	0.0066	0.0000	-0.0040	-0.0061	0.0187	-0.0151
	Z	0.0000	-0.0138	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	0.0061	0.0000	0.0094	0.0005	-0.0168	-0.0085
	Y	0.0016	0.0000	0.0015	0.0030	0.0027	0.0012
	Z	0.0000	0.0102	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0061	0.0000	-0.0094	-0.0005	-0.0168	0.0085
	Y	0.0016	0.0000	-0.0015	-0.0030	0.0027	-0.0012
	Z	0.0000	0.0102	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0061	0.0000	-0.0094	0.0005	-0.0168	0.0085
	Y	-0.0016	0.0000	0.0015	-0.0030	-0.0027	0.0012
	Z	0.0000	-0.0102	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	0.0061	0.0000	0.0094	-0.0005	-0.0168	-0.0085
	Y	-0.0016	0.0000	-0.0015	0.0030	-0.0027	-0.0012
	Z	0.0000	-0.0102	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	-0.0045	0.0202	-0.0020	0.0094	-0.0027	0.0017
	Y	-0.0164	0.0098	-0.0088	0.0240	-0.0052	-0.0032
	Z	0.0187	-0.0051	0.0022	-0.0111	-0.0026	0.0120
AT. 24	O X	-0.0045	-0.0202	0.0020	-0.0094	-0.0027	-0.0017
	Y	-0.0164	-0.0098	0.0088	-0.0240	-0.0052	0.0032
	Z	-0.0187	-0.0051	0.0022	-0.0111	0.0026	0.0120
AT. 25	O X	-0.0045	0.0202	0.0020	0.0094	-0.0027	-0.0017

	Y	0.0164	-0.0098	-0.0088	-0.0240	0.0052	-0.0032
	Z	-0.0187	0.0051	0.0022	0.0111	0.0026	0.0120
AT. 26	O X	-0.0045	-0.0202	-0.0020	-0.0094	-0.0027	0.0017
	Y	0.0164	0.0098	0.0088	0.0240	0.0052	0.0032
	Z	0.0187	0.0051	0.0022	0.0111	-0.0026	0.0120
AT. 27	O X	-0.0045	0.0202	0.0020	-0.0094	-0.0027	-0.0017
	Y	-0.0164	0.0098	0.0088	-0.0240	-0.0052	0.0032
	Z	0.0187	-0.0051	-0.0022	0.0111	-0.0026	-0.0120
AT. 28	O X	-0.0045	-0.0202	-0.0020	0.0094	-0.0027	0.0017
	Y	-0.0164	-0.0098	-0.0088	0.0240	-0.0052	-0.0032
	Z	-0.0187	-0.0051	-0.0022	0.0111	0.0026	-0.0120
AT. 29	O X	-0.0045	0.0202	-0.0020	-0.0094	-0.0027	0.0017
	Y	0.0164	-0.0098	0.0088	0.0240	0.0052	0.0032
	Z	-0.0187	0.0051	-0.0022	-0.0111	0.0026	-0.0120
AT. 30	O X	-0.0045	-0.0202	0.0020	0.0094	-0.0027	-0.0017
	Y	0.0164	0.0098	-0.0088	-0.0240	0.0052	-0.0032
	Z	0.0187	0.0051	-0.0022	-0.0111	-0.0026	-0.0120
AT. 31	O X	-0.0046	0.0012	-0.0287	-0.0018	0.0049	0.0101
	Y	0.0005	-0.0044	-0.0065	0.0001	-0.0056	0.0012
	Z	0.0040	0.0000	0.0175	-0.0050	-0.0087	-0.0077
AT. 32	O X	-0.0046	-0.0012	0.0287	0.0018	0.0049	-0.0101
	Y	0.0005	0.0044	0.0065	-0.0001	-0.0056	-0.0012
	Z	-0.0040	0.0000	0.0175	-0.0050	0.0087	-0.0077
AT. 33	O X	-0.0046	0.0012	0.0287	-0.0018	0.0049	-0.0101
	Y	-0.0005	0.0044	-0.0065	-0.0001	0.0056	0.0012
	Z	-0.0040	0.0000	0.0175	0.0050	0.0087	-0.0077
AT. 34	O X	-0.0046	-0.0012	-0.0287	0.0018	0.0049	0.0101
	Y	-0.0005	-0.0044	0.0065	0.0001	0.0056	-0.0012
	Z	0.0040	0.0000	0.0175	0.0050	-0.0087	-0.0077
AT. 35	O X	-0.0046	0.0012	0.0287	0.0018	0.0049	-0.0101
	Y	0.0005	-0.0044	0.0065	-0.0001	-0.0056	-0.0012
	Z	0.0040	0.0000	-0.0175	0.0050	-0.0087	0.0077
AT. 36	O X	-0.0046	-0.0012	-0.0287	-0.0018	0.0049	0.0101
	Y	0.0005	0.0044	-0.0065	0.0001	-0.0056	0.0012
	Z	-0.0040	0.0000	-0.0175	0.0050	0.0087	0.0077
AT. 37	O X	-0.0046	0.0012	-0.0287	0.0018	0.0049	0.0101
	Y	-0.0005	0.0044	0.0065	0.0001	0.0056	-0.0012
	Z	-0.0040	0.0000	-0.0175	-0.0050	0.0087	0.0077
AT. 38	O X	-0.0046	-0.0012	0.0287	-0.0018	0.0049	-0.0101
	Y	-0.0005	-0.0044	-0.0065	-0.0001	0.0056	0.0012
	Z	0.0040	0.0000	-0.0175	-0.0050	-0.0087	0.0077
AT. 39	O X	0.0057	-0.0023	-0.0090	0.0043	0.0051	-0.0168
	Y	-0.0067	-0.0175	0.0085	-0.0059	-0.0145	0.0203
	Z	-0.0084	-0.0033	0.0058	0.0017	-0.0101	0.0046
AT. 40	O X	0.0057	0.0023	0.0090	-0.0043	0.0051	0.0168
	Y	-0.0067	0.0175	-0.0085	0.0059	-0.0145	-0.0203
	Z	0.0084	-0.0033	0.0058	0.0017	0.0101	0.0046
AT. 41	O X	0.0057	-0.0023	0.0090	0.0043	0.0051	0.0168
	Y	0.0067	0.0175	0.0085	0.0059	0.0145	0.0203
	Z	0.0084	0.0033	0.0058	-0.0017	0.0101	0.0046
AT. 42	O X	0.0057	0.0023	-0.0090	-0.0043	0.0051	-0.0168
	Y	0.0067	-0.0175	-0.0085	-0.0059	0.0145	-0.0203
	Z	-0.0084	0.0033	0.0058	-0.0017	-0.0101	0.0046
AT. 43	O X	0.0057	-0.0023	0.0090	-0.0043	0.0051	0.0168

	Y	-0.0067	-0.0175	-0.0085	0.0059	-0.0145	-0.0203
	Z	-0.0084	-0.0033	-0.0058	-0.0017	-0.0101	-0.0046
AT. 44 O	X	0.0057	0.0023	-0.0090	0.0043	0.0051	-0.0168
	Y	-0.0067	0.0175	0.0085	-0.0059	-0.0145	0.0203
	Z	0.0084	-0.0033	-0.0058	-0.0017	0.0101	-0.0046
AT. 45 O	X	0.0057	-0.0023	-0.0090	-0.0043	0.0051	-0.0168
	Y	0.0067	0.0175	-0.0085	-0.0059	0.0145	-0.0203
	Z	0.0084	0.0033	-0.0058	0.0017	0.0101	-0.0046
AT. 46 O	X	0.0057	0.0023	0.0090	0.0043	0.0051	0.0168
	Y	0.0067	-0.0175	0.0085	0.0059	0.0145	0.0203
	Z	-0.0084	0.0033	-0.0058	0.0017	-0.0101	-0.0046
AT. 47 O	X	0.0077	0.0000	0.0044	0.0031	-0.0058	-0.0033
	Y	0.0041	0.0000	0.0097	0.0027	-0.0112	-0.0076
	Z	0.0000	-0.0122	0.0000	0.0000	0.0000	0.0000
AT. 48 O	X	0.0077	0.0000	-0.0044	-0.0031	-0.0058	0.0033
	Y	0.0041	0.0000	-0.0097	-0.0027	-0.0112	0.0076
	Z	0.0000	-0.0122	0.0000	0.0000	0.0000	0.0000
AT. 49 O	X	0.0077	0.0000	-0.0044	0.0031	-0.0058	0.0033
	Y	-0.0041	0.0000	0.0097	-0.0027	0.0112	-0.0076
	Z	0.0000	0.0122	0.0000	0.0000	0.0000	0.0000
AT. 50 O	X	0.0077	0.0000	0.0044	-0.0031	-0.0058	-0.0033
	Y	-0.0041	0.0000	-0.0097	0.0027	0.0112	0.0076
	Z	0.0000	0.0122	0.0000	0.0000	0.0000	0.0000
AT. 51 O	X	0.0086	0.0000	-0.0027	-0.0083	0.0072	-0.0074
	Y	0.0056	0.0000	-0.0011	-0.0088	-0.0057	-0.0061
	Z	0.0000	-0.0203	0.0000	0.0000	0.0000	0.0000
AT. 52 O	X	0.0086	0.0000	0.0027	0.0083	0.0072	0.0074
	Y	0.0056	0.0000	0.0011	0.0088	-0.0057	0.0061
	Z	0.0000	-0.0203	0.0000	0.0000	0.0000	0.0000
AT. 53 O	X	0.0086	0.0000	0.0027	-0.0083	0.0072	0.0074
	Y	-0.0056	0.0000	-0.0011	0.0088	0.0057	-0.0061
	Z	0.0000	0.0203	0.0000	0.0000	0.0000	0.0000
AT. 54 O	X	0.0086	0.0000	-0.0027	0.0083	0.0072	-0.0074
	Y	-0.0056	0.0000	0.0011	-0.0088	0.0057	0.0061
	Z	0.0000	0.0203	0.0000	0.0000	0.0000	0.0000
AT. 55 O	X	0.0036	0.0000	-0.0059	-0.0057	0.0028	-0.0052
	Y	-0.0025	0.0000	0.0039	-0.0013	-0.0110	0.0086
	Z	0.0000	-0.0214	0.0000	0.0000	0.0000	0.0000
AT. 56 O	X	0.0036	0.0000	0.0059	0.0057	0.0028	0.0052
	Y	-0.0025	0.0000	-0.0039	0.0013	-0.0110	-0.0086
	Z	0.0000	-0.0214	0.0000	0.0000	0.0000	0.0000
AT. 57 O	X	0.0036	0.0000	0.0059	-0.0057	0.0028	0.0052
	Y	0.0025	0.0000	0.0039	0.0013	0.0110	0.0086
	Z	0.0000	0.0214	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	0.0036	0.0000	-0.0059	0.0057	0.0028	-0.0052
	Y	0.0025	0.0000	-0.0039	-0.0013	0.0110	-0.0086
	Z	0.0000	0.0214	0.0000	0.0000	0.0000	0.0000

FREQ(CM**-1) 582.76 585.36 586.86 596.36 601.03 603.35

AT. 1 FE	X	0.0000	0.0017	0.0000	0.0000	0.0000	-0.0012
	Y	0.0007	0.0000	0.0013	-0.0003	0.0018	0.0000
	Z	0.0002	0.0000	-0.0002	0.0012	-0.0007	0.0000
AT. 2 FE	X	0.0000	-0.0017	0.0000	0.0000	0.0000	0.0012

	Y	0.0007	0.0000	-0.0013	-0.0003	-0.0018	0.0000
	Z	-0.0002	0.0000	-0.0002	-0.0012	-0.0007	0.0000
AT. 3	FE X	0.0000	0.0017	0.0000	0.0000	0.0000	0.0012
	Y	0.0007	0.0000	0.0013	-0.0003	-0.0018	0.0000
	Z	0.0002	0.0000	-0.0002	0.0012	0.0007	0.0000
AT. 4	FE X	0.0000	-0.0017	0.0000	0.0000	0.0000	-0.0012
	Y	0.0007	0.0000	-0.0013	-0.0003	0.0018	0.0000
	Z	-0.0002	0.0000	-0.0002	-0.0012	0.0007	0.0000
AT. 5	AL X	0.0092	0.0000	0.0000	0.0135	0.0000	0.0000
	Y	-0.0089	0.0000	0.0000	0.0079	0.0000	0.0000
	Z	0.0000	0.0026	0.0010	0.0000	0.0091	0.0018
AT. 6	AL X	-0.0092	0.0000	0.0000	-0.0135	0.0000	0.0000
	Y	-0.0089	0.0000	0.0000	0.0079	0.0000	0.0000
	Z	0.0000	-0.0026	0.0010	0.0000	0.0091	-0.0018
AT. 7	AL X	0.0092	0.0000	0.0000	0.0135	0.0000	0.0000
	Y	-0.0089	0.0000	0.0000	0.0079	0.0000	0.0000
	Z	0.0000	0.0026	0.0010	0.0000	-0.0091	-0.0018
AT. 8	AL X	-0.0092	0.0000	0.0000	-0.0135	0.0000	0.0000
	Y	-0.0089	0.0000	0.0000	0.0079	0.0000	0.0000
	Z	0.0000	-0.0026	0.0010	0.0000	-0.0091	0.0018
AT. 9	AL X	0.0139	0.0000	0.0000	0.0026	-0.0032	-0.0025
	Y	-0.0143	0.0000	0.0000	0.0209	0.0263	0.0042
	Z	0.0000	-0.0139	0.0069	0.0000	0.0000	0.0000
AT. 10	AL X	0.0139	0.0000	0.0000	0.0026	0.0032	0.0025
	Y	-0.0143	0.0000	0.0000	0.0209	-0.0263	-0.0042
	Z	0.0000	-0.0139	0.0069	0.0000	0.0000	0.0000
AT. 11	AL X	-0.0139	0.0000	0.0000	-0.0026	0.0032	-0.0025
	Y	-0.0143	0.0000	0.0000	0.0209	0.0263	-0.0042
	Z	0.0000	0.0139	0.0069	0.0000	0.0000	0.0000
AT. 12	AL X	-0.0139	0.0000	0.0000	-0.0026	-0.0032	0.0025
	Y	-0.0143	0.0000	0.0000	0.0209	-0.0263	0.0042
	Z	0.0000	0.0139	0.0069	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0161	0.0000	0.0000	-0.0149	0.0000	0.0000
	Z	0.0000	0.0000	-0.0071	0.0000	-0.0225	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0161	0.0000	0.0000	-0.0149	0.0000	0.0000
	Z	0.0000	0.0000	-0.0071	0.0000	0.0225	0.0000
AT. 15	SI X	-0.0130	0.0000	0.0000	-0.0093	-0.0037	-0.0047
	Y	-0.0110	0.0000	0.0000	-0.0144	-0.0034	-0.0057
	Z	0.0000	0.0078	-0.0150	0.0000	0.0000	0.0000
AT. 16	SI X	-0.0130	0.0000	0.0000	-0.0093	0.0037	0.0047
	Y	-0.0110	0.0000	0.0000	-0.0144	0.0034	0.0057
	Z	0.0000	0.0078	-0.0150	0.0000	0.0000	0.0000
AT. 17	SI X	0.0130	0.0000	0.0000	0.0093	0.0037	-0.0047
	Y	-0.0110	0.0000	0.0000	-0.0144	-0.0034	0.0057
	Z	0.0000	-0.0078	-0.0150	0.0000	0.0000	0.0000
AT. 18	SI X	0.0130	0.0000	0.0000	0.0093	-0.0037	0.0047
	Y	-0.0110	0.0000	0.0000	-0.0144	0.0034	-0.0057
	Z	0.0000	-0.0078	-0.0150	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0056	0.0000	0.0000	0.0021	-0.0018	-0.0128
	Y	0.0109	0.0000	0.0000	-0.0015	-0.0005	0.0031
	Z	0.0000	0.0124	0.0137	0.0000	0.0000	0.0000
AT. 20	SI X	-0.0056	0.0000	0.0000	0.0021	0.0018	0.0128

	Y	0.0109	0.0000	0.0000	-0.0015	0.0005	-0.0031
	Z	0.0000	0.0124	0.0137	0.0000	0.0000	0.0000
AT. 21	SI X	0.0056	0.0000	0.0000	-0.0021	0.0018	-0.0128
	Y	0.0109	0.0000	0.0000	-0.0015	-0.0005	-0.0031
	Z	0.0000	-0.0124	0.0137	0.0000	0.0000	0.0000
AT. 22	SI X	0.0056	0.0000	0.0000	-0.0021	-0.0018	0.0128
	Y	0.0109	0.0000	0.0000	-0.0015	0.0005	0.0031
	Z	0.0000	-0.0124	0.0137	0.0000	0.0000	0.0000
AT. 23	O X	0.0085	-0.0015	-0.0062	-0.0065	-0.0108	0.0014
	Y	0.0076	-0.0152	-0.0227	-0.0064	-0.0149	0.0015
	Z	-0.0103	0.0003	-0.0013	-0.0012	0.0052	0.0019
AT. 24	O X	0.0085	0.0015	0.0062	-0.0065	0.0108	-0.0014
	Y	0.0076	0.0152	0.0227	-0.0064	0.0149	-0.0015
	Z	0.0103	0.0003	-0.0013	0.0012	0.0052	0.0019
AT. 25	O X	-0.0085	-0.0015	0.0062	0.0065	0.0108	0.0014
	Y	0.0076	0.0152	-0.0227	-0.0064	-0.0149	-0.0015
	Z	-0.0103	-0.0003	-0.0013	-0.0012	0.0052	-0.0019
AT. 26	O X	-0.0085	0.0015	-0.0062	0.0065	-0.0108	-0.0014
	Y	0.0076	-0.0152	0.0227	-0.0064	0.0149	0.0015
	Z	0.0103	-0.0003	-0.0013	0.0012	0.0052	-0.0019
AT. 27	O X	0.0085	-0.0015	-0.0062	-0.0065	0.0108	-0.0014
	Y	0.0076	-0.0152	-0.0227	-0.0064	0.0149	-0.0015
	Z	-0.0103	0.0003	-0.0013	-0.0012	-0.0052	-0.0019
AT. 28	O X	0.0085	0.0015	0.0062	-0.0065	-0.0108	0.0014
	Y	0.0076	0.0152	0.0227	-0.0064	-0.0149	0.0015
	Z	0.0103	0.0003	-0.0013	0.0012	-0.0052	-0.0019
AT. 29	O X	-0.0085	-0.0015	0.0062	0.0065	-0.0108	-0.0014
	Y	0.0076	0.0152	-0.0227	-0.0064	0.0149	0.0015
	Z	-0.0103	-0.0003	-0.0013	-0.0012	-0.0052	0.0019
AT. 30	O X	-0.0085	0.0015	-0.0062	0.0065	0.0108	0.0014
	Y	0.0076	-0.0152	0.0227	-0.0064	-0.0149	-0.0015
	Z	0.0103	-0.0003	-0.0013	0.0012	-0.0052	0.0019
AT. 31	O X	-0.0003	0.0276	-0.0006	0.0121	0.0027	-0.0275
	Y	-0.0003	-0.0022	-0.0033	-0.0063	-0.0120	0.0031
	Z	0.0098	-0.0085	-0.0008	-0.0068	-0.0049	0.0126
AT. 32	O X	-0.0003	-0.0276	0.0006	0.0121	-0.0027	0.0275
	Y	-0.0003	0.0022	0.0033	-0.0063	0.0120	-0.0031
	Z	-0.0098	-0.0085	-0.0008	0.0068	-0.0049	0.0126
AT. 33	O X	0.0003	0.0276	0.0006	-0.0121	-0.0027	-0.0275
	Y	-0.0003	0.0022	-0.0033	-0.0063	-0.0120	-0.0031
	Z	0.0098	0.0085	-0.0008	-0.0068	-0.0049	-0.0126
AT. 34	O X	0.0003	-0.0276	-0.0006	-0.0121	0.0027	0.0275
	Y	-0.0003	-0.0022	0.0033	-0.0063	0.0120	0.0031
	Z	-0.0098	0.0085	-0.0008	0.0068	-0.0049	-0.0126
AT. 35	O X	-0.0003	0.0276	-0.0006	0.0121	-0.0027	0.0275
	Y	-0.0003	-0.0022	-0.0033	-0.0063	0.0120	-0.0031
	Z	0.0098	-0.0085	-0.0008	-0.0068	0.0049	-0.0126
AT. 36	O X	-0.0003	-0.0276	0.0006	0.0121	0.0027	-0.0275
	Y	-0.0003	0.0022	0.0033	-0.0063	-0.0120	0.0031
	Z	-0.0098	-0.0085	-0.0008	0.0068	0.0049	-0.0126
AT. 37	O X	0.0003	0.0276	0.0006	-0.0121	0.0027	0.0275
	Y	-0.0003	0.0022	-0.0033	-0.0063	0.0120	0.0031
	Z	0.0098	0.0085	-0.0008	-0.0068	0.0049	0.0126
AT. 38	O X	0.0003	-0.0276	-0.0006	-0.0121	-0.0027	-0.0275

	Y	-0.0003	-0.0022	0.0033	-0.0063	-0.0120	-0.0031
	Z	-0.0098	0.0085	-0.0008	0.0068	0.0049	0.0126
AT. 39	O X	-0.0029	-0.0090	0.0178	-0.0056	0.0053	-0.0085
	Y	0.0075	0.0051	-0.0151	0.0140	-0.0043	0.0100
	Z	0.0115	-0.0021	-0.0001	0.0058	-0.0002	0.0106
AT. 40	O X	-0.0029	0.0090	-0.0178	-0.0056	-0.0053	0.0085
	Y	0.0075	-0.0051	0.0151	0.0140	0.0043	-0.0100
	Z	-0.0115	-0.0021	-0.0001	-0.0058	-0.0002	0.0106
AT. 41	O X	0.0029	-0.0090	-0.0178	0.0056	-0.0053	-0.0085
	Y	0.0075	-0.0051	-0.0151	0.0140	-0.0043	-0.0100
	Z	0.0115	0.0021	-0.0001	0.0058	-0.0002	-0.0106
AT. 42	O X	0.0029	0.0090	0.0178	0.0056	0.0053	0.0085
	Y	0.0075	0.0051	0.0151	0.0140	0.0043	0.0100
	Z	-0.0115	0.0021	-0.0001	-0.0058	-0.0002	-0.0106
AT. 43	O X	-0.0029	-0.0090	0.0178	-0.0056	-0.0053	0.0085
	Y	0.0075	0.0051	-0.0151	0.0140	0.0043	-0.0100
	Z	0.0115	-0.0021	-0.0001	0.0058	0.0002	-0.0106
AT. 44	O X	-0.0029	0.0090	-0.0178	-0.0056	0.0053	-0.0085
	Y	0.0075	-0.0051	0.0151	0.0140	-0.0043	0.0100
	Z	-0.0115	-0.0021	-0.0001	-0.0058	0.0002	-0.0106
AT. 45	O X	0.0029	-0.0090	-0.0178	0.0056	0.0053	0.0085
	Y	0.0075	-0.0051	-0.0151	0.0140	0.0043	0.0100
	Z	0.0115	0.0021	-0.0001	0.0058	0.0002	0.0106
AT. 46	O X	0.0029	0.0090	0.0178	0.0056	-0.0053	-0.0085
	Y	0.0075	0.0051	0.0151	0.0140	-0.0043	-0.0100
	Z	-0.0115	0.0021	-0.0001	-0.0058	0.0002	0.0106
AT. 47	O X	0.0019	0.0000	0.0000	0.0041	-0.0045	-0.0053
	Y	-0.0046	0.0000	0.0000	0.0006	0.0057	-0.0098
	Z	0.0000	-0.0083	-0.0072	0.0000	0.0000	0.0000
AT. 48	O X	0.0019	0.0000	0.0000	0.0041	0.0045	0.0053
	Y	-0.0046	0.0000	0.0000	0.0006	-0.0057	0.0098
	Z	0.0000	-0.0083	-0.0072	0.0000	0.0000	0.0000
AT. 49	O X	-0.0019	0.0000	0.0000	-0.0041	0.0045	-0.0053
	Y	-0.0046	0.0000	0.0000	0.0006	0.0057	0.0098
	Z	0.0000	0.0083	-0.0072	0.0000	0.0000	0.0000
AT. 50	O X	-0.0019	0.0000	0.0000	-0.0041	-0.0045	0.0053
	Y	-0.0046	0.0000	0.0000	0.0006	-0.0057	-0.0098
	Z	0.0000	0.0083	-0.0072	0.0000	0.0000	0.0000
AT. 51	O X	0.0104	0.0000	0.0000	-0.0004	-0.0077	0.0005
	Y	0.0030	0.0000	0.0000	0.0009	-0.0009	0.0025
	Z	0.0000	0.0027	-0.0015	0.0000	0.0000	0.0000
AT. 52	O X	0.0104	0.0000	0.0000	-0.0004	0.0077	-0.0005
	Y	0.0030	0.0000	0.0000	0.0009	0.0009	-0.0025
	Z	0.0000	0.0027	-0.0015	0.0000	0.0000	0.0000
AT. 53	O X	-0.0104	0.0000	0.0000	0.0004	0.0077	0.0005
	Y	0.0030	0.0000	0.0000	0.0009	-0.0009	-0.0025
	Z	0.0000	-0.0027	-0.0015	0.0000	0.0000	0.0000
AT. 54	O X	-0.0104	0.0000	0.0000	0.0004	-0.0077	-0.0005
	Y	0.0030	0.0000	0.0000	0.0009	0.0009	0.0025
	Z	0.0000	-0.0027	-0.0015	0.0000	0.0000	0.0000
AT. 55	O X	0.0071	0.0000	0.0000	0.0014	0.0023	0.0092
	Y	-0.0054	0.0000	0.0000	-0.0101	-0.0031	-0.0054
	Z	0.0000	-0.0065	0.0086	0.0000	0.0000	0.0000
AT. 56	O X	0.0071	0.0000	0.0000	0.0014	-0.0023	-0.0092

	Y	-0.0054	0.0000	0.0000	-0.0101	0.0031	0.0054
	Z	0.0000	-0.0065	0.0086	0.0000	0.0000	0.0000
AT. 57 O	X	-0.0071	0.0000	0.0000	-0.0014	-0.0023	0.0092
	Y	-0.0054	0.0000	0.0000	-0.0101	-0.0031	0.0054
	Z	0.0000	0.0065	0.0086	0.0000	0.0000	0.0000
AT. 58 O	X	-0.0071	0.0000	0.0000	-0.0014	0.0023	-0.0092
	Y	-0.0054	0.0000	0.0000	-0.0101	0.0031	-0.0054
	Z	0.0000	0.0065	0.0086	0.0000	0.0000	0.0000

FREQ(CM**-1) 607.30 615.26 632.01 633.23 666.36 668.01

AT. 1 FE	X	0.0000	0.0000	-0.0001	-0.0023	0.0000	0.0000
	Y	-0.0005	-0.0008	0.0000	0.0000	0.0004	-0.0008
	Z	0.0010	0.0010	0.0000	0.0000	0.0012	-0.0004
AT. 2 FE	X	0.0000	0.0000	0.0001	0.0023	0.0000	0.0000
	Y	0.0005	-0.0008	0.0000	0.0000	0.0004	-0.0008
	Z	0.0010	-0.0010	0.0000	0.0000	-0.0012	0.0004
AT. 3 FE	X	0.0000	0.0000	-0.0001	0.0023	0.0000	0.0000
	Y	-0.0005	0.0008	0.0000	0.0000	-0.0004	-0.0008
	Z	0.0010	-0.0010	0.0000	0.0000	-0.0012	-0.0004
AT. 4 FE	X	0.0000	0.0000	0.0001	-0.0023	0.0000	0.0000
	Y	0.0005	0.0008	0.0000	0.0000	-0.0004	-0.0008
	Z	0.0010	0.0010	0.0000	0.0000	0.0012	0.0004
AT. 5 AL	X	0.0000	0.0059	0.0000	0.0000	0.0156	-0.0118
	Y	0.0000	0.0001	0.0000	0.0000	0.0182	-0.0065
	Z	0.0008	0.0000	0.0015	-0.0171	0.0000	0.0000
AT. 6 AL	X	0.0000	-0.0059	0.0000	0.0000	-0.0156	0.0118
	Y	0.0000	0.0001	0.0000	0.0000	0.0182	-0.0065
	Z	0.0008	0.0000	-0.0015	0.0171	0.0000	0.0000
AT. 7 AL	X	0.0000	-0.0059	0.0000	0.0000	-0.0156	-0.0118
	Y	0.0000	-0.0001	0.0000	0.0000	-0.0182	-0.0065
	Z	0.0008	0.0000	0.0015	0.0171	0.0000	0.0000
AT. 8 AL	X	0.0000	0.0059	0.0000	0.0000	0.0156	0.0118
	Y	0.0000	-0.0001	0.0000	0.0000	-0.0182	-0.0065
	Z	0.0008	0.0000	-0.0015	-0.0171	0.0000	0.0000
AT. 9 AL	X	0.0000	0.0000	0.0000	0.0121	0.0000	0.0143
	Y	0.0000	0.0000	0.0000	0.0068	0.0000	0.0166
	Z	-0.0310	0.0303	-0.0117	0.0000	-0.0052	0.0000
AT. 10 AL	X	0.0000	0.0000	0.0000	-0.0121	0.0000	0.0143
	Y	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0166
	Z	-0.0310	-0.0303	-0.0117	0.0000	0.0052	0.0000
AT. 11 AL	X	0.0000	0.0000	0.0000	0.0121	0.0000	-0.0143
	Y	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0166
	Z	-0.0310	0.0303	0.0117	0.0000	-0.0052	0.0000
AT. 12 AL	X	0.0000	0.0000	0.0000	-0.0121	0.0000	-0.0143
	Y	0.0000	0.0000	0.0000	0.0068	0.0000	0.0166
	Z	-0.0310	-0.0303	0.0117	0.0000	0.0052	0.0000
AT. 13 SI	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	-0.0268	0.0000	0.0000	0.0043	-0.0080
	Z	0.0246	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14 SI	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0268	0.0000	0.0000	-0.0043	-0.0080
	Z	0.0246	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15 SI	X	0.0000	0.0000	0.0000	0.0125	0.0000	0.0115

	Y	0.0000	0.0000	0.0000	0.0149	0.0000	-0.0010
	Z	-0.0029	-0.0020	-0.0090	0.0000	-0.0185	0.0000
AT. 16 SI	X	0.0000	0.0000	0.0000	-0.0125	0.0000	0.0115
	Y	0.0000	0.0000	0.0000	-0.0149	0.0000	-0.0010
	Z	-0.0029	0.0020	-0.0090	0.0000	0.0185	0.0000
AT. 17 SI	X	0.0000	0.0000	0.0000	0.0125	0.0000	-0.0115
	Y	0.0000	0.0000	0.0000	-0.0149	0.0000	-0.0010
	Z	-0.0029	-0.0020	0.0090	0.0000	-0.0185	0.0000
AT. 18 SI	X	0.0000	0.0000	0.0000	-0.0125	0.0000	-0.0115
	Y	0.0000	0.0000	0.0000	0.0149	0.0000	-0.0010
	Z	-0.0029	0.0020	0.0090	0.0000	0.0185	0.0000
AT. 19 SI	X	0.0000	0.0000	0.0000	-0.0003	0.0000	-0.0180
	Y	0.0000	0.0000	0.0000	0.0019	0.0000	0.0027
	Z	0.0024	0.0049	-0.0085	0.0000	0.0115	0.0000
AT. 20 SI	X	0.0000	0.0000	0.0000	0.0003	0.0000	-0.0180
	Y	0.0000	0.0000	0.0000	-0.0019	0.0000	0.0027
	Z	0.0024	-0.0049	-0.0085	0.0000	-0.0115	0.0000
AT. 21 SI	X	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0180
	Y	0.0000	0.0000	0.0000	-0.0019	0.0000	0.0027
	Z	0.0024	0.0049	0.0085	0.0000	0.0115	0.0000
AT. 22 SI	X	0.0000	0.0000	0.0000	0.0003	0.0000	0.0180
	Y	0.0000	0.0000	0.0000	0.0019	0.0000	0.0027
	Z	0.0024	-0.0049	0.0085	0.0000	-0.0115	0.0000
AT. 23 O	X	-0.0008	-0.0007	0.0031	-0.0052	-0.0027	0.0068
	Y	-0.0038	-0.0026	0.0211	-0.0005	-0.0172	0.0109
	Z	-0.0011	-0.0008	0.0028	-0.0051	-0.0011	0.0013
AT. 24 O	X	0.0008	-0.0007	-0.0031	0.0052	-0.0027	0.0068
	Y	0.0038	-0.0026	-0.0211	0.0005	-0.0172	0.0109
	Z	-0.0011	0.0008	0.0028	-0.0051	0.0011	-0.0013
AT. 25 O	X	0.0008	0.0007	0.0031	-0.0052	0.0027	-0.0068
	Y	-0.0038	-0.0026	-0.0211	0.0005	-0.0172	0.0109
	Z	-0.0011	-0.0008	-0.0028	0.0051	-0.0011	0.0013
AT. 26 O	X	-0.0008	0.0007	-0.0031	0.0052	0.0027	-0.0068
	Y	0.0038	-0.0026	0.0211	-0.0005	-0.0172	0.0109
	Z	-0.0011	0.0008	-0.0028	0.0051	0.0011	-0.0013
AT. 27 O	X	-0.0008	0.0007	0.0031	0.0052	0.0027	0.0068
	Y	-0.0038	0.0026	0.0211	0.0005	0.0172	0.0109
	Z	-0.0011	0.0008	0.0028	0.0051	0.0011	0.0013
AT. 28 O	X	0.0008	0.0007	-0.0031	-0.0052	0.0027	0.0068
	Y	0.0038	0.0026	-0.0211	-0.0005	0.0172	0.0109
	Z	-0.0011	-0.0008	0.0028	0.0051	-0.0011	-0.0013
AT. 29 O	X	0.0008	-0.0007	0.0031	0.0052	-0.0027	-0.0068
	Y	-0.0038	0.0026	-0.0211	-0.0005	0.0172	0.0109
	Z	-0.0011	0.0008	-0.0028	-0.0051	0.0011	0.0013
AT. 30 O	X	-0.0008	-0.0007	-0.0031	-0.0052	-0.0027	-0.0068
	Y	0.0038	0.0026	0.0211	0.0005	0.0172	0.0109
	Z	-0.0011	-0.0008	-0.0028	-0.0051	-0.0011	-0.0013
AT. 31 O	X	-0.0114	0.0077	0.0194	-0.0150	0.0000	0.0070
	Y	0.0096	-0.0021	0.0013	0.0028	-0.0006	-0.0017
	Z	0.0135	-0.0167	-0.0045	0.0045	0.0037	-0.0032
AT. 32 O	X	0.0114	0.0077	-0.0194	0.0150	0.0000	0.0070
	Y	-0.0096	-0.0021	-0.0013	-0.0028	-0.0006	-0.0017
	Z	0.0135	0.0167	-0.0045	0.0045	-0.0037	0.0032
AT. 33 O	X	0.0114	-0.0077	0.0194	-0.0150	0.0000	-0.0070

	Y	0.0096	-0.0021	-0.0013	-0.0028	-0.0006	-0.0017
	Z	0.0135	-0.0167	0.0045	-0.0045	0.0037	-0.0032
AT. 34	O X	-0.0114	-0.0077	-0.0194	0.0150	0.0000	-0.0070
	Y	-0.0096	-0.0021	0.0013	0.0028	-0.0006	-0.0017
	Z	0.0135	0.0167	0.0045	-0.0045	-0.0037	0.0032
AT. 35	O X	-0.0114	-0.0077	0.0194	0.0150	0.0000	0.0070
	Y	0.0096	0.0021	0.0013	-0.0028	0.0006	-0.0017
	Z	0.0135	0.0167	-0.0045	-0.0045	-0.0037	-0.0032
AT. 36	O X	0.0114	-0.0077	-0.0194	-0.0150	0.0000	0.0070
	Y	-0.0096	0.0021	-0.0013	0.0028	0.0006	-0.0017
	Z	0.0135	-0.0167	-0.0045	-0.0045	0.0037	0.0032
AT. 37	O X	0.0114	0.0077	0.0194	0.0150	0.0000	-0.0070
	Y	0.0096	0.0021	-0.0013	0.0028	0.0006	-0.0017
	Z	0.0135	0.0167	0.0045	0.0045	-0.0037	-0.0032
AT. 38	O X	-0.0114	0.0077	-0.0194	-0.0150	0.0000	-0.0070
	Y	-0.0096	0.0021	0.0013	-0.0028	0.0006	-0.0017
	Z	0.0135	-0.0167	0.0045	0.0045	0.0037	0.0032
AT. 39	O X	0.0051	-0.0026	0.0151	0.0043	-0.0105	0.0044
	Y	-0.0022	0.0043	-0.0099	-0.0135	0.0044	-0.0054
	Z	-0.0004	-0.0006	0.0024	-0.0095	-0.0014	0.0059
AT. 40	O X	-0.0051	-0.0026	-0.0151	-0.0043	-0.0105	0.0044
	Y	0.0022	0.0043	0.0099	0.0135	0.0044	-0.0054
	Z	-0.0004	0.0006	0.0024	-0.0095	0.0014	-0.0059
AT. 41	O X	-0.0051	0.0026	0.0151	0.0043	0.0105	-0.0044
	Y	-0.0022	0.0043	0.0099	0.0135	0.0044	-0.0054
	Z	-0.0004	-0.0006	-0.0024	0.0095	-0.0014	0.0059
AT. 42	O X	0.0051	0.0026	-0.0151	-0.0043	0.0105	-0.0044
	Y	0.0022	0.0043	-0.0099	-0.0135	0.0044	-0.0054
	Z	-0.0004	0.0006	-0.0024	0.0095	0.0014	-0.0059
AT. 43	O X	0.0051	0.0026	0.0151	-0.0043	0.0105	0.0044
	Y	-0.0022	-0.0043	-0.0099	0.0135	-0.0044	-0.0054
	Z	-0.0004	0.0006	0.0024	0.0095	0.0014	0.0059
AT. 44	O X	-0.0051	0.0026	-0.0151	0.0043	0.0105	0.0044
	Y	0.0022	-0.0043	0.0099	-0.0135	-0.0044	-0.0054
	Z	-0.0004	-0.0006	0.0024	0.0095	-0.0014	-0.0059
AT. 45	O X	-0.0051	-0.0026	0.0151	-0.0043	-0.0105	-0.0044
	Y	-0.0022	-0.0043	0.0099	-0.0135	-0.0044	-0.0054
	Z	-0.0004	0.0006	-0.0024	-0.0095	0.0014	0.0059
AT. 46	O X	0.0051	-0.0026	-0.0151	0.0043	-0.0105	-0.0044
	Y	0.0022	-0.0043	-0.0099	0.0135	-0.0044	-0.0054
	Z	-0.0004	-0.0006	-0.0024	-0.0095	-0.0014	-0.0059
AT. 47	O X	0.0000	0.0000	0.0000	-0.0038	0.0000	-0.0071
	Y	0.0000	0.0000	0.0000	0.0004	0.0000	-0.0103
	Z	-0.0010	0.0023	0.0061	0.0000	-0.0057	0.0000
AT. 48	O X	0.0000	0.0000	0.0000	0.0038	0.0000	-0.0071
	Y	0.0000	0.0000	0.0000	-0.0004	0.0000	-0.0103
	Z	-0.0010	-0.0023	0.0061	0.0000	0.0057	0.0000
AT. 49	O X	0.0000	0.0000	0.0000	-0.0038	0.0000	0.0071
	Y	0.0000	0.0000	0.0000	-0.0004	0.0000	-0.0103
	Z	-0.0010	0.0023	-0.0061	0.0000	-0.0057	0.0000
AT. 50	O X	0.0000	0.0000	0.0000	0.0038	0.0000	0.0071
	Y	0.0000	0.0000	0.0000	0.0004	0.0000	-0.0103
	Z	-0.0010	-0.0023	-0.0061	0.0000	0.0057	0.0000
AT. 51	O X	0.0000	0.0000	0.0000	-0.0054	0.0000	0.0035

	Y	0.0000	0.0000	0.0000	-0.0087	0.0000	-0.0063
	Z	0.0032	-0.0028	0.0035	0.0000	0.0042	0.0000
AT. 52 O	X	0.0000	0.0000	0.0000	0.0054	0.0000	0.0035
	Y	0.0000	0.0000	0.0000	0.0087	0.0000	-0.0063
	Z	0.0032	0.0028	0.0035	0.0000	-0.0042	0.0000
AT. 53 O	X	0.0000	0.0000	0.0000	-0.0054	0.0000	-0.0035
	Y	0.0000	0.0000	0.0000	0.0087	0.0000	-0.0063
	Z	0.0032	-0.0028	-0.0035	0.0000	0.0042	0.0000
AT. 54 O	X	0.0000	0.0000	0.0000	0.0054	0.0000	-0.0035
	Y	0.0000	0.0000	0.0000	-0.0087	0.0000	-0.0063
	Z	0.0032	0.0028	-0.0035	0.0000	-0.0042	0.0000
AT. 55 O	X	0.0000	0.0000	0.0000	-0.0027	0.0000	0.0001
	Y	0.0000	0.0000	0.0000	0.0121	0.0000	-0.0013
	Z	0.0014	0.0008	0.0064	0.0000	0.0028	0.0000
AT. 56 O	X	0.0000	0.0000	0.0000	0.0027	0.0000	0.0001
	Y	0.0000	0.0000	0.0000	-0.0121	0.0000	-0.0013
	Z	0.0014	-0.0008	0.0064	0.0000	-0.0028	0.0000
AT. 57 O	X	0.0000	0.0000	0.0000	-0.0027	0.0000	-0.0001
	Y	0.0000	0.0000	0.0000	-0.0121	0.0000	-0.0013
	Z	0.0014	0.0008	-0.0064	0.0000	0.0028	0.0000
AT. 58 O	X	0.0000	0.0000	0.0000	0.0027	0.0000	-0.0001
	Y	0.0000	0.0000	0.0000	0.0121	0.0000	-0.0013
	Z	0.0014	-0.0008	-0.0064	0.0000	-0.0028	0.0000

FREQ(CM**-1) 675.04 683.99 693.38 700.00 701.93 704.81

AT. 1 FE	X	-0.0013	0.0006	0.0002	0.0000	0.0008	0.0000
	Y	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0006
	Z	0.0000	0.0000	0.0000	0.0008	0.0000	-0.0015
AT. 2 FE	X	0.0013	0.0006	0.0002	0.0000	-0.0008	0.0000
	Y	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0006
	Z	0.0000	0.0000	0.0000	0.0008	0.0000	-0.0015
AT. 3 FE	X	0.0013	-0.0006	0.0002	0.0000	0.0008	0.0000
	Y	0.0000	0.0000	0.0000	-0.0001	0.0000	-0.0006
	Z	0.0000	0.0000	0.0000	-0.0008	0.0000	-0.0015
AT. 4 FE	X	-0.0013	-0.0006	0.0002	0.0000	-0.0008	0.0000
	Y	0.0000	0.0000	0.0000	0.0001	0.0000	0.0006
	Z	0.0000	0.0000	0.0000	-0.0008	0.0000	-0.0015
AT. 5 AL	X	0.0000	0.0221	0.0150	0.0000	0.0000	0.0000
	Y	0.0000	0.0077	0.0013	0.0000	0.0000	0.0000
	Z	-0.0057	0.0000	0.0000	0.0062	0.0244	-0.0248
AT. 6 AL	X	0.0000	0.0221	0.0150	0.0000	0.0000	0.0000
	Y	0.0000	-0.0077	-0.0013	0.0000	0.0000	0.0000
	Z	0.0057	0.0000	0.0000	0.0062	-0.0244	-0.0248
AT. 7 AL	X	0.0000	-0.0221	0.0150	0.0000	0.0000	0.0000
	Y	0.0000	-0.0077	0.0013	0.0000	0.0000	0.0000
	Z	0.0057	0.0000	0.0000	-0.0062	0.0244	-0.0248
AT. 8 AL	X	0.0000	-0.0221	0.0150	0.0000	0.0000	0.0000
	Y	0.0000	0.0077	-0.0013	0.0000	0.0000	0.0000
	Z	-0.0057	0.0000	0.0000	-0.0062	-0.0244	-0.0248
AT. 9 AL	X	-0.0018	0.0000	0.0191	-0.0242	0.0000	0.0000
	Y	-0.0144	0.0000	-0.0022	-0.0068	0.0000	0.0000
	Z	0.0000	0.0041	0.0000	0.0000	0.0015	0.0001
AT. 10 AL	X	0.0018	0.0000	0.0191	0.0242	0.0000	0.0000

	Y	0.0144	0.0000	-0.0022	0.0068	0.0000	0.0000
	Z	0.0000	-0.0041	0.0000	0.0000	0.0015	0.0001
AT. 11	AL X	-0.0018	0.0000	0.0191	0.0242	0.0000	0.0000
	Y	0.0144	0.0000	0.0022	-0.0068	0.0000	0.0000
	Z	0.0000	-0.0041	0.0000	0.0000	-0.0015	0.0001
AT. 12	AL X	0.0018	0.0000	0.0191	-0.0242	0.0000	0.0000
	Y	-0.0144	0.0000	0.0022	0.0068	0.0000	0.0000
	Z	0.0000	0.0041	0.0000	0.0000	-0.0015	0.0001
AT. 13	SI X	0.0000	0.0091	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	-0.0001	0.0000	-0.0003
AT. 14	SI X	0.0000	-0.0091	0.0000	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0003
AT. 15	SI X	-0.0117	0.0000	-0.0124	0.0042	0.0000	0.0000
	Y	0.0046	0.0000	0.0036	-0.0003	0.0000	0.0000
	Z	0.0000	-0.0118	0.0000	0.0000	-0.0148	0.0157
AT. 16	SI X	0.0117	0.0000	-0.0124	-0.0042	0.0000	0.0000
	Y	-0.0046	0.0000	0.0036	0.0003	0.0000	0.0000
	Z	0.0000	0.0118	0.0000	0.0000	-0.0148	0.0157
AT. 17	SI X	-0.0117	0.0000	-0.0124	-0.0042	0.0000	0.0000
	Y	-0.0046	0.0000	-0.0036	-0.0003	0.0000	0.0000
	Z	0.0000	0.0118	0.0000	0.0000	0.0148	0.0157
AT. 18	SI X	0.0117	0.0000	-0.0124	0.0042	0.0000	0.0000
	Y	0.0046	0.0000	-0.0036	0.0003	0.0000	0.0000
	Z	0.0000	-0.0118	0.0000	0.0000	0.0148	0.0157
AT. 19	SI X	-0.0084	0.0000	-0.0141	-0.0213	0.0000	0.0000
	Y	0.0130	0.0000	0.0121	-0.0051	0.0000	0.0000
	Z	0.0000	-0.0177	0.0000	0.0000	0.0164	0.0164
AT. 20	SI X	0.0084	0.0000	-0.0141	0.0213	0.0000	0.0000
	Y	-0.0130	0.0000	0.0121	0.0051	0.0000	0.0000
	Z	0.0000	0.0177	0.0000	0.0000	0.0164	0.0164
AT. 21	SI X	-0.0084	0.0000	-0.0141	0.0213	0.0000	0.0000
	Y	-0.0130	0.0000	-0.0121	-0.0051	0.0000	0.0000
	Z	0.0000	0.0177	0.0000	0.0000	-0.0164	0.0164
AT. 22	SI X	0.0084	0.0000	-0.0141	-0.0213	0.0000	0.0000
	Y	0.0130	0.0000	-0.0121	0.0051	0.0000	0.0000
	Z	0.0000	-0.0177	0.0000	0.0000	-0.0164	0.0164
AT. 23	O X	0.0028	-0.0029	0.0022	-0.0028	0.0027	0.0045
	Y	0.0140	0.0115	0.0083	0.0031	0.0134	0.0113
	Z	0.0082	0.0010	0.0064	0.0030	-0.0001	0.0000
AT. 24	O X	-0.0028	-0.0029	0.0022	0.0028	-0.0027	-0.0045
	Y	-0.0140	0.0115	0.0083	-0.0031	-0.0134	-0.0113
	Z	0.0082	-0.0010	-0.0064	0.0030	-0.0001	0.0000
AT. 25	O X	0.0028	-0.0029	0.0022	0.0028	0.0027	-0.0045
	Y	-0.0140	-0.0115	-0.0083	0.0031	-0.0134	0.0113
	Z	-0.0082	-0.0010	-0.0064	0.0030	0.0001	0.0000
AT. 26	O X	-0.0028	-0.0029	0.0022	-0.0028	-0.0027	0.0045
	Y	0.0140	-0.0115	-0.0083	-0.0031	0.0134	-0.0113
	Z	-0.0082	0.0010	0.0064	0.0030	0.0001	0.0000
AT. 27	O X	-0.0028	0.0029	0.0022	0.0028	0.0027	0.0045
	Y	-0.0140	-0.0115	0.0083	-0.0031	0.0134	0.0113
	Z	-0.0082	-0.0010	0.0064	-0.0030	-0.0001	0.0000
AT. 28	O X	0.0028	0.0029	0.0022	-0.0028	-0.0027	-0.0045

	Y	0.0140	-0.0115	0.0083	0.0031	-0.0134	-0.0113
	Z	-0.0082	0.0010	-0.0064	-0.0030	-0.0001	0.0000
AT. 29	O X	-0.0028	0.0029	0.0022	-0.0028	0.0027	-0.0045
	Y	0.0140	0.0115	-0.0083	-0.0031	-0.0134	0.0113
	Z	0.0082	0.0010	-0.0064	-0.0030	0.0001	0.0000
AT. 30	O X	0.0028	0.0029	0.0022	0.0028	-0.0027	0.0045
	Y	-0.0140	0.0115	-0.0083	0.0031	0.0134	-0.0113
	Z	0.0082	-0.0010	0.0064	-0.0030	0.0001	0.0000
AT. 31	O X	0.0057	-0.0037	-0.0016	-0.0080	-0.0023	-0.0009
	Y	0.0009	0.0034	0.0008	0.0002	-0.0013	-0.0012
	Z	0.0064	0.0036	0.0011	0.0038	0.0001	0.0007
AT. 32	O X	-0.0057	-0.0037	-0.0016	0.0080	0.0023	0.0009
	Y	-0.0009	0.0034	0.0008	-0.0002	0.0013	0.0012
	Z	0.0064	-0.0036	-0.0011	0.0038	0.0001	0.0007
AT. 33	O X	0.0057	-0.0037	-0.0016	0.0080	-0.0023	0.0009
	Y	-0.0009	-0.0034	-0.0008	0.0002	0.0013	-0.0012
	Z	-0.0064	-0.0036	-0.0011	0.0038	-0.0001	0.0007
AT. 34	O X	-0.0057	-0.0037	-0.0016	-0.0080	0.0023	-0.0009
	Y	0.0009	-0.0034	-0.0008	-0.0002	-0.0013	0.0012
	Z	-0.0064	0.0036	0.0011	0.0038	-0.0001	0.0007
AT. 35	O X	-0.0057	0.0037	-0.0016	0.0080	-0.0023	-0.0009
	Y	-0.0009	-0.0034	0.0008	-0.0002	-0.0013	-0.0012
	Z	-0.0064	-0.0036	0.0011	-0.0038	0.0001	0.0007
AT. 36	O X	0.0057	0.0037	-0.0016	-0.0080	0.0023	0.0009
	Y	0.0009	-0.0034	0.0008	0.0002	0.0013	0.0012
	Z	-0.0064	0.0036	-0.0011	-0.0038	0.0001	0.0007
AT. 37	O X	-0.0057	0.0037	-0.0016	-0.0080	-0.0023	0.0009
	Y	0.0009	0.0034	-0.0008	-0.0002	0.0013	-0.0012
	Z	0.0064	0.0036	-0.0011	-0.0038	-0.0001	0.0007
AT. 38	O X	0.0057	0.0037	-0.0016	0.0080	0.0023	-0.0009
	Y	-0.0009	0.0034	-0.0008	0.0002	-0.0013	0.0012
	Z	0.0064	-0.0036	0.0011	-0.0038	-0.0001	0.0007
AT. 39	O X	0.0090	-0.0135	-0.0079	0.0041	-0.0106	0.0103
	Y	-0.0159	0.0065	0.0117	-0.0042	0.0092	-0.0086
	Z	0.0059	0.0001	-0.0047	-0.0096	0.0006	0.0007
AT. 40	O X	-0.0090	-0.0135	-0.0079	-0.0041	0.0106	-0.0103
	Y	0.0159	0.0065	0.0117	0.0042	-0.0092	0.0086
	Z	0.0059	-0.0001	0.0047	-0.0096	0.0006	0.0007
AT. 41	O X	0.0090	-0.0135	-0.0079	-0.0041	-0.0106	-0.0103
	Y	0.0159	-0.0065	-0.0117	-0.0042	-0.0092	-0.0086
	Z	-0.0059	-0.0001	0.0047	-0.0096	-0.0006	0.0007
AT. 42	O X	-0.0090	-0.0135	-0.0079	0.0041	0.0106	0.0103
	Y	-0.0159	-0.0065	-0.0117	0.0042	0.0092	0.0086
	Z	-0.0059	0.0001	-0.0047	-0.0096	-0.0006	0.0007
AT. 43	O X	-0.0090	0.0135	-0.0079	-0.0041	-0.0106	0.0103
	Y	0.0159	-0.0065	0.0117	0.0042	0.0092	-0.0086
	Z	-0.0059	-0.0001	-0.0047	0.0096	0.0006	0.0007
AT. 44	O X	0.0090	0.0135	-0.0079	0.0041	0.0106	-0.0103
	Y	-0.0159	-0.0065	0.0117	-0.0042	-0.0092	0.0086
	Z	-0.0059	0.0001	0.0047	0.0096	0.0006	0.0007
AT. 45	O X	-0.0090	0.0135	-0.0079	0.0041	-0.0106	-0.0103
	Y	-0.0159	0.0065	-0.0117	0.0042	-0.0092	-0.0086
	Z	0.0059	0.0001	0.0047	0.0096	-0.0006	0.0007
AT. 46	O X	0.0090	0.0135	-0.0079	-0.0041	0.0106	0.0103

	Y	0.0159	0.0065	-0.0117	-0.0042	0.0092	0.0086
	Z	0.0059	-0.0001	-0.0047	0.0096	-0.0006	0.0007
AT. 47 O	X	-0.0006	0.0000	-0.0028	-0.0084	0.0000	0.0000
	Y	-0.0136	0.0000	-0.0087	-0.0078	0.0000	0.0000
	Z	0.0000	0.0057	0.0000	0.0000	-0.0051	-0.0050
AT. 48 O	X	0.0006	0.0000	-0.0028	0.0084	0.0000	0.0000
	Y	0.0136	0.0000	-0.0087	0.0078	0.0000	0.0000
	Z	0.0000	-0.0057	0.0000	0.0000	-0.0051	-0.0050
AT. 49 O	X	-0.0006	0.0000	-0.0028	0.0084	0.0000	0.0000
	Y	0.0136	0.0000	0.0087	-0.0078	0.0000	0.0000
	Z	0.0000	-0.0057	0.0000	0.0000	0.0051	-0.0050
AT. 50 O	X	0.0006	0.0000	-0.0028	-0.0084	0.0000	0.0000
	Y	-0.0136	0.0000	0.0087	0.0078	0.0000	0.0000
	Z	0.0000	0.0057	0.0000	0.0000	0.0051	-0.0050
AT. 51 O	X	-0.0009	0.0000	-0.0003	-0.0010	0.0000	0.0000
	Y	0.0043	0.0000	0.0023	0.0043	0.0000	0.0000
	Z	0.0000	0.0044	0.0000	0.0000	0.0016	-0.0018
AT. 52 O	X	0.0009	0.0000	-0.0003	0.0010	0.0000	0.0000
	Y	-0.0043	0.0000	0.0023	-0.0043	0.0000	0.0000
	Z	0.0000	-0.0044	0.0000	0.0000	0.0016	-0.0018
AT. 53 O	X	-0.0009	0.0000	-0.0003	0.0010	0.0000	0.0000
	Y	-0.0043	0.0000	-0.0023	0.0043	0.0000	0.0000
	Z	0.0000	-0.0044	0.0000	0.0000	-0.0016	-0.0018
AT. 54 O	X	0.0009	0.0000	-0.0003	-0.0010	0.0000	0.0000
	Y	0.0043	0.0000	-0.0023	-0.0043	0.0000	0.0000
	Z	0.0000	0.0044	0.0000	0.0000	-0.0016	-0.0018
AT. 55 O	X	0.0067	0.0000	0.0066	0.0037	0.0000	0.0000
	Y	0.0008	0.0000	-0.0004	-0.0075	0.0000	0.0000
	Z	0.0000	0.0083	0.0000	0.0000	0.0027	-0.0059
AT. 56 O	X	-0.0067	0.0000	0.0066	-0.0037	0.0000	0.0000
	Y	-0.0008	0.0000	-0.0004	0.0075	0.0000	0.0000
	Z	0.0000	-0.0083	0.0000	0.0000	0.0027	-0.0059
AT. 57 O	X	0.0067	0.0000	0.0066	-0.0037	0.0000	0.0000
	Y	-0.0008	0.0000	0.0004	-0.0075	0.0000	0.0000
	Z	0.0000	-0.0083	0.0000	0.0000	-0.0027	-0.0059
AT. 58 O	X	-0.0067	0.0000	0.0066	0.0037	0.0000	0.0000
	Y	0.0008	0.0000	0.0004	0.0075	0.0000	0.0000
	Z	0.0000	0.0083	0.0000	0.0000	-0.0027	-0.0059

FREQ(CM**-1) 708.42 714.87 732.63 743.93 744.18 751.15

AT. 1 FE	X	0.0007	0.0003	0.0000	0.0000	0.0000	0.0021
	Y	0.0000	0.0000	0.0010	0.0020	0.0000	0.0000
	Z	0.0000	0.0000	0.0012	0.0002	0.0000	0.0000
AT. 2 FE	X	0.0007	-0.0003	0.0000	0.0000	0.0000	0.0021
	Y	0.0000	0.0000	-0.0010	0.0020	0.0000	0.0000
	Z	0.0000	0.0000	0.0012	-0.0002	0.0000	0.0000
AT. 3 FE	X	0.0007	-0.0003	0.0000	0.0000	0.0000	-0.0021
	Y	0.0000	0.0000	-0.0010	-0.0020	0.0000	0.0000
	Z	0.0000	0.0000	-0.0012	-0.0002	0.0000	0.0000
AT. 4 FE	X	0.0007	0.0003	0.0000	0.0000	0.0000	-0.0021
	Y	0.0000	0.0000	0.0010	-0.0020	0.0000	0.0000
	Z	0.0000	0.0000	-0.0012	0.0002	0.0000	0.0000
AT. 5 AL	X	-0.0013	0.0000	0.0000	0.0184	0.0000	-0.0032

	Y	0.0153	0.0000	0.0000	-0.0200	0.0000	0.0179
	Z	0.0000	-0.0130	0.0108	0.0000	0.0069	0.0000
AT. 6	AL X	-0.0013	0.0000	0.0000	-0.0184	0.0000	-0.0032
	Y	-0.0153	0.0000	0.0000	-0.0200	0.0000	-0.0179
	Z	0.0000	0.0130	0.0108	0.0000	-0.0069	0.0000
AT. 7	AL X	-0.0013	0.0000	0.0000	-0.0184	0.0000	0.0032
	Y	0.0153	0.0000	0.0000	0.0200	0.0000	-0.0179
	Z	0.0000	0.0130	-0.0108	0.0000	-0.0069	0.0000
AT. 8	AL X	-0.0013	0.0000	0.0000	0.0184	0.0000	0.0032
	Y	-0.0153	0.0000	0.0000	0.0200	0.0000	0.0179
	Z	0.0000	-0.0130	-0.0108	0.0000	0.0069	0.0000
AT. 9	AL X	-0.0124	-0.0196	0.0075	0.0000	0.0094	0.0000
	Y	0.0020	-0.0052	-0.0153	0.0000	-0.0077	0.0000
	Z	0.0000	0.0000	0.0000	-0.0038	0.0000	-0.0124
AT. 10	AL X	-0.0124	0.0196	-0.0075	0.0000	-0.0094	0.0000
	Y	0.0020	0.0052	0.0153	0.0000	0.0077	0.0000
	Z	0.0000	0.0000	0.0000	0.0038	0.0000	0.0124
AT. 11	AL X	-0.0124	-0.0196	-0.0075	0.0000	0.0094	0.0000
	Y	-0.0020	0.0052	-0.0153	0.0000	0.0077	0.0000
	Z	0.0000	0.0000	0.0000	-0.0038	0.0000	0.0124
AT. 12	AL X	-0.0124	0.0196	0.0075	0.0000	-0.0094	0.0000
	Y	-0.0020	-0.0052	0.0153	0.0000	-0.0077	0.0000
	Z	0.0000	0.0000	0.0000	0.0038	0.0000	-0.0124
AT. 13	SI X	0.0058	0.0000	0.0000	0.0000	0.0000	-0.0221
	Y	0.0000	0.0000	0.0000	0.0012	0.0000	0.0000
	Z	0.0000	0.0000	0.0077	0.0000	0.0000	0.0000
AT. 14	SI X	0.0058	0.0000	0.0000	0.0000	0.0000	0.0221
	Y	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000
	Z	0.0000	0.0000	-0.0077	0.0000	0.0000	0.0000
AT. 15	SI X	-0.0094	0.0122	-0.0186	0.0000	-0.0079	0.0000
	Y	-0.0180	0.0080	0.0095	0.0000	0.0192	0.0000
	Z	0.0000	0.0000	0.0000	0.0080	0.0000	-0.0104
AT. 16	SI X	-0.0094	-0.0122	0.0186	0.0000	0.0079	0.0000
	Y	-0.0180	-0.0080	-0.0095	0.0000	-0.0192	0.0000
	Z	0.0000	0.0000	0.0000	-0.0080	0.0000	0.0104
AT. 17	SI X	-0.0094	0.0122	0.0186	0.0000	-0.0079	0.0000
	Y	0.0180	-0.0080	0.0095	0.0000	-0.0192	0.0000
	Z	0.0000	0.0000	0.0000	0.0080	0.0000	0.0104
AT. 18	SI X	-0.0094	-0.0122	-0.0186	0.0000	0.0079	0.0000
	Y	0.0180	0.0080	-0.0095	0.0000	0.0192	0.0000
	Z	0.0000	0.0000	0.0000	-0.0080	0.0000	-0.0104
AT. 19	SI X	0.0130	-0.0186	-0.0036	0.0000	0.0012	0.0000
	Y	0.0177	-0.0103	0.0031	0.0000	-0.0156	0.0000
	Z	0.0000	0.0000	0.0000	0.0149	0.0000	0.0031
AT. 20	SI X	0.0130	0.0186	0.0036	0.0000	-0.0012	0.0000
	Y	0.0177	0.0103	-0.0031	0.0000	0.0156	0.0000
	Z	0.0000	0.0000	0.0000	-0.0149	0.0000	-0.0031
AT. 21	SI X	0.0130	-0.0186	0.0036	0.0000	0.0012	0.0000
	Y	-0.0177	0.0103	0.0031	0.0000	0.0156	0.0000
	Z	0.0000	0.0000	0.0000	0.0149	0.0000	-0.0031
AT. 22	SI X	0.0130	0.0186	-0.0036	0.0000	-0.0012	0.0000
	Y	-0.0177	-0.0103	-0.0031	0.0000	-0.0156	0.0000
	Z	0.0000	0.0000	0.0000	-0.0149	0.0000	0.0031
AT. 23	O X	0.0051	-0.0020	-0.0102	0.0054	0.0085	0.0016

	Y	0.0091	-0.0039	-0.0165	0.0088	0.0143	0.0125
	Z	0.0030	-0.0053	-0.0009	-0.0009	-0.0058	-0.0001
AT. 24	O X	0.0051	0.0020	0.0102	0.0054	-0.0085	0.0016
	Y	0.0091	0.0039	0.0165	0.0088	-0.0143	0.0125
	Z	-0.0030	-0.0053	-0.0009	0.0009	-0.0058	0.0001
AT. 25	O X	0.0051	-0.0020	0.0102	-0.0054	0.0085	0.0016
	Y	-0.0091	0.0039	-0.0165	0.0088	-0.0143	-0.0125
	Z	-0.0030	0.0053	-0.0009	-0.0009	0.0058	0.0001
AT. 26	O X	0.0051	0.0020	-0.0102	-0.0054	-0.0085	0.0016
	Y	-0.0091	-0.0039	0.0165	0.0088	0.0143	-0.0125
	Z	0.0030	0.0053	-0.0009	0.0009	0.0058	-0.0001
AT. 27	O X	0.0051	0.0020	0.0102	-0.0054	-0.0085	-0.0016
	Y	0.0091	0.0039	0.0165	-0.0088	-0.0143	-0.0125
	Z	0.0030	0.0053	0.0009	0.0009	0.0058	0.0001
AT. 28	O X	0.0051	-0.0020	-0.0102	-0.0054	0.0085	-0.0016
	Y	0.0091	-0.0039	-0.0165	-0.0088	0.0143	-0.0125
	Z	-0.0030	0.0053	0.0009	-0.0009	0.0058	-0.0001
AT. 29	O X	0.0051	0.0020	-0.0102	0.0054	-0.0085	-0.0016
	Y	-0.0091	-0.0039	0.0165	-0.0088	0.0143	0.0125
	Z	-0.0030	-0.0053	0.0009	0.0009	-0.0058	-0.0001
AT. 30	O X	0.0051	-0.0020	0.0102	0.0054	0.0085	-0.0016
	Y	-0.0091	0.0039	-0.0165	-0.0088	-0.0143	0.0125
	Z	0.0030	-0.0053	0.0009	-0.0009	-0.0058	0.0001
AT. 31	O X	-0.0030	0.0076	0.0010	0.0000	-0.0006	0.0102
	Y	0.0028	-0.0015	0.0043	0.0003	-0.0006	-0.0087
	Z	0.0035	-0.0032	-0.0006	0.0038	0.0000	-0.0121
AT. 32	O X	-0.0030	-0.0076	-0.0010	0.0000	0.0006	0.0102
	Y	0.0028	0.0015	-0.0043	0.0003	0.0006	-0.0087
	Z	-0.0035	-0.0032	-0.0006	-0.0038	0.0000	0.0121
AT. 33	O X	-0.0030	0.0076	-0.0010	0.0000	-0.0006	0.0102
	Y	-0.0028	0.0015	0.0043	0.0003	0.0006	0.0087
	Z	-0.0035	0.0032	-0.0006	0.0038	0.0000	0.0121
AT. 34	O X	-0.0030	-0.0076	0.0010	0.0000	0.0006	0.0102
	Y	-0.0028	-0.0015	-0.0043	0.0003	-0.0006	0.0087
	Z	0.0035	0.0032	-0.0006	-0.0038	0.0000	-0.0121
AT. 35	O X	-0.0030	-0.0076	-0.0010	0.0000	0.0006	-0.0102
	Y	0.0028	0.0015	-0.0043	-0.0003	0.0006	0.0087
	Z	0.0035	0.0032	0.0006	-0.0038	0.0000	0.0121
AT. 36	O X	-0.0030	0.0076	0.0010	0.0000	-0.0006	-0.0102
	Y	0.0028	-0.0015	0.0043	-0.0003	-0.0006	0.0087
	Z	-0.0035	0.0032	0.0006	0.0038	0.0000	-0.0121
AT. 37	O X	-0.0030	-0.0076	0.0010	0.0000	0.0006	-0.0102
	Y	-0.0028	-0.0015	-0.0043	-0.0003	-0.0006	-0.0087
	Z	-0.0035	-0.0032	0.0006	-0.0038	0.0000	-0.0121
AT. 38	O X	-0.0030	0.0076	-0.0010	0.0000	-0.0006	-0.0102
	Y	-0.0028	0.0015	0.0043	-0.0003	0.0006	-0.0087
	Z	0.0035	-0.0032	0.0006	0.0038	0.0000	0.0121
AT. 39	O X	-0.0026	-0.0029	0.0006	-0.0113	-0.0077	0.0007
	Y	0.0008	0.0032	0.0032	0.0103	0.0070	-0.0048
	Z	-0.0005	0.0048	-0.0005	0.0014	-0.0029	-0.0007
AT. 40	O X	-0.0026	0.0029	-0.0006	-0.0113	0.0077	0.0007
	Y	0.0008	-0.0032	-0.0032	0.0103	-0.0070	-0.0048
	Z	0.0005	0.0048	-0.0005	-0.0014	-0.0029	0.0007
AT. 41	O X	-0.0026	-0.0029	-0.0006	0.0113	-0.0077	0.0007

	Y	-0.0008	-0.0032	0.0032	0.0103	-0.0070	0.0048
	Z	0.0005	-0.0048	-0.0005	0.0014	0.0029	0.0007
AT. 42	O X	-0.0026	0.0029	0.0006	0.0113	0.0077	0.0007
	Y	-0.0008	0.0032	-0.0032	0.0103	0.0070	0.0048
	Z	-0.0005	-0.0048	-0.0005	-0.0014	0.0029	-0.0007
AT. 43	O X	-0.0026	0.0029	-0.0006	0.0113	0.0077	-0.0007
	Y	0.0008	-0.0032	-0.0032	-0.0103	-0.0070	0.0048
	Z	-0.0005	-0.0048	0.0005	-0.0014	0.0029	0.0007
AT. 44	O X	-0.0026	-0.0029	0.0006	0.0113	-0.0077	-0.0007
	Y	0.0008	0.0032	0.0032	-0.0103	0.0070	0.0048
	Z	0.0005	-0.0048	0.0005	0.0014	0.0029	-0.0007
AT. 45	O X	-0.0026	0.0029	0.0006	-0.0113	0.0077	-0.0007
	Y	-0.0008	0.0032	-0.0032	-0.0103	0.0070	-0.0048
	Z	0.0005	0.0048	0.0005	-0.0014	-0.0029	-0.0007
AT. 46	O X	-0.0026	-0.0029	-0.0006	-0.0113	-0.0077	-0.0007
	Y	-0.0008	-0.0032	0.0032	-0.0103	-0.0070	-0.0048
	Z	-0.0005	0.0048	0.0005	0.0014	-0.0029	0.0007
AT. 47	O X	0.0083	-0.0110	-0.0047	0.0000	-0.0047	0.0000
	Y	0.0020	-0.0049	-0.0057	0.0000	0.0032	0.0000
	Z	0.0000	0.0000	0.0000	-0.0050	0.0000	0.0002
AT. 48	O X	0.0083	0.0110	0.0047	0.0000	0.0047	0.0000
	Y	0.0020	0.0049	0.0057	0.0000	-0.0032	0.0000
	Z	0.0000	0.0000	0.0000	0.0050	0.0000	-0.0002
AT. 49	O X	0.0083	-0.0110	0.0047	0.0000	-0.0047	0.0000
	Y	-0.0020	0.0049	-0.0057	0.0000	-0.0032	0.0000
	Z	0.0000	0.0000	0.0000	-0.0050	0.0000	-0.0002
AT. 50	O X	0.0083	0.0110	-0.0047	0.0000	0.0047	0.0000
	Y	-0.0020	-0.0049	0.0057	0.0000	0.0032	0.0000
	Z	0.0000	0.0000	0.0000	0.0050	0.0000	0.0002
AT. 51	O X	0.0023	-0.0037	-0.0054	0.0000	-0.0090	0.0000
	Y	0.0020	0.0010	0.0061	0.0000	0.0047	0.0000
	Z	0.0000	0.0000	0.0000	0.0014	0.0000	0.0023
AT. 52	O X	0.0023	0.0037	0.0054	0.0000	0.0090	0.0000
	Y	0.0020	-0.0010	-0.0061	0.0000	-0.0047	0.0000
	Z	0.0000	0.0000	0.0000	-0.0014	0.0000	-0.0023
AT. 53	O X	0.0023	-0.0037	0.0054	0.0000	-0.0090	0.0000
	Y	-0.0020	-0.0010	0.0061	0.0000	-0.0047	0.0000
	Z	0.0000	0.0000	0.0000	0.0014	0.0000	-0.0023
AT. 54	O X	0.0023	0.0037	-0.0054	0.0000	0.0090	0.0000
	Y	-0.0020	0.0010	-0.0061	0.0000	0.0047	0.0000
	Z	0.0000	0.0000	0.0000	-0.0014	0.0000	0.0023
AT. 55	O X	-0.0005	0.0029	0.0087	0.0000	0.0043	0.0000
	Y	-0.0029	-0.0015	0.0023	0.0000	0.0027	0.0000
	Z	0.0000	0.0000	0.0000	-0.0026	0.0000	0.0046
AT. 56	O X	-0.0005	-0.0029	-0.0087	0.0000	-0.0043	0.0000
	Y	-0.0029	0.0015	-0.0023	0.0000	-0.0027	0.0000
	Z	0.0000	0.0000	0.0000	0.0026	0.0000	-0.0046
AT. 57	O X	-0.0005	0.0029	-0.0087	0.0000	0.0043	0.0000
	Y	0.0029	0.0015	0.0023	0.0000	-0.0027	0.0000
	Z	0.0000	0.0000	0.0000	-0.0026	0.0000	-0.0046
AT. 58	O X	-0.0005	-0.0029	0.0087	0.0000	-0.0043	0.0000
	Y	0.0029	-0.0015	-0.0023	0.0000	0.0027	0.0000
	Z	0.0000	0.0000	0.0000	0.0026	0.0000	0.0046

FREQ(CM**-1) 755.45 756.31 764.09 768.55 812.21 853.77

AT. 1	FE X	0.0000	0.0000	0.0015	0.0000	0.0001	-0.0001
	Y	-0.0005	0.0005	0.0000	-0.0013	0.0000	0.0000
	Z	0.0004	-0.0012	0.0000	-0.0003	0.0000	0.0000
AT. 2	FE X	0.0000	0.0000	0.0015	0.0000	0.0001	-0.0001
	Y	-0.0005	-0.0005	0.0000	-0.0013	0.0000	0.0000
	Z	-0.0004	-0.0012	0.0000	0.0003	0.0000	0.0000
AT. 3	FE X	0.0000	0.0000	0.0015	0.0000	-0.0001	-0.0001
	Y	-0.0005	-0.0005	0.0000	-0.0013	0.0000	0.0000
	Z	0.0004	0.0012	0.0000	-0.0003	0.0000	0.0000
AT. 4	FE X	0.0000	0.0000	0.0015	0.0000	-0.0001	-0.0001
	Y	-0.0005	0.0005	0.0000	-0.0013	0.0000	0.0000
	Z	-0.0004	0.0012	0.0000	0.0003	0.0000	0.0000
AT. 5	AL X	-0.0068	0.0000	-0.0044	-0.0098	0.0112	0.0081
	Y	0.0108	0.0000	0.0094	0.0164	-0.0174	-0.0130
	Z	0.0000	-0.0126	0.0000	0.0000	0.0000	0.0000
AT. 6	AL X	0.0068	0.0000	-0.0044	0.0098	0.0112	0.0081
	Y	0.0108	0.0000	-0.0094	0.0164	0.0174	0.0130
	Z	0.0000	-0.0126	0.0000	0.0000	0.0000	0.0000
AT. 7	AL X	-0.0068	0.0000	-0.0044	-0.0098	-0.0112	0.0081
	Y	0.0108	0.0000	0.0094	0.0164	0.0174	-0.0130
	Z	0.0000	0.0126	0.0000	0.0000	0.0000	0.0000
AT. 8	AL X	0.0068	0.0000	-0.0044	0.0098	-0.0112	0.0081
	Y	0.0108	0.0000	-0.0094	0.0164	-0.0174	0.0130
	Z	0.0000	0.0126	0.0000	0.0000	0.0000	0.0000
AT. 9	AL X	0.0189	0.0046	-0.0012	-0.0034	0.0000	-0.0093
	Y	-0.0054	-0.0026	-0.0159	0.0011	0.0000	-0.0027
	Z	0.0000	0.0000	0.0000	0.0000	-0.0101	0.0000
AT. 10	AL X	0.0189	-0.0046	-0.0012	-0.0034	0.0000	-0.0093
	Y	-0.0054	0.0026	-0.0159	0.0011	0.0000	-0.0027
	Z	0.0000	0.0000	0.0000	0.0000	0.0101	0.0000
AT. 11	AL X	-0.0189	-0.0046	-0.0012	0.0034	0.0000	-0.0093
	Y	-0.0054	-0.0026	0.0159	0.0011	0.0000	0.0027
	Z	0.0000	0.0000	0.0000	0.0000	0.0101	0.0000
AT. 12	AL X	-0.0189	0.0046	-0.0012	0.0034	0.0000	-0.0093
	Y	-0.0054	0.0026	0.0159	0.0011	0.0000	0.0027
	Z	0.0000	0.0000	0.0000	0.0000	-0.0101	0.0000
AT. 13	SI X	0.0000	0.0000	-0.0244	0.0000	-0.0149	-0.0077
	Y	0.0047	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	0.0000	0.0022	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	-0.0244	0.0000	0.0149	-0.0077
	Y	0.0047	0.0000	0.0000	0.0002	0.0000	0.0000
	Z	0.0000	-0.0022	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	-0.0126	0.0054	-0.0090	-0.0064	0.0000	0.0045
	Y	0.0144	0.0184	0.0060	-0.0126	0.0000	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000
AT. 16	SI X	-0.0126	-0.0054	-0.0090	-0.0064	0.0000	0.0045
	Y	0.0144	-0.0184	0.0060	-0.0126	0.0000	-0.0081
	Z	0.0000	0.0000	0.0000	0.0000	-0.0045	0.0000
AT. 17	SI X	0.0126	-0.0054	-0.0090	0.0064	0.0000	0.0045
	Y	0.0144	0.0184	-0.0060	-0.0126	0.0000	0.0081
	Z	0.0000	0.0000	0.0000	0.0000	-0.0045	0.0000
AT. 18	SI X	0.0126	0.0054	-0.0090	0.0064	0.0000	0.0045

	Y	0.0144	-0.0184	-0.0060	-0.0126	0.0000	0.0081
	Z	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000
AT. 19	SI X	-0.0113	0.0012	0.0027	0.0011	0.0000	0.0029
	Y	-0.0062	-0.0229	-0.0032	0.0220	0.0000	0.0108
	Z	0.0000	0.0000	0.0000	0.0000	-0.0067	0.0000
AT. 20	SI X	-0.0113	-0.0012	0.0027	0.0011	0.0000	0.0029
	Y	-0.0062	0.0229	-0.0032	0.0220	0.0000	0.0108
	Z	0.0000	0.0000	0.0000	0.0000	0.0067	0.0000
AT. 21	SI X	0.0113	-0.0012	0.0027	-0.0011	0.0000	0.0029
	Y	-0.0062	-0.0229	0.0032	0.0220	0.0000	-0.0108
	Z	0.0000	0.0000	0.0000	0.0000	0.0067	0.0000
AT. 22	SI X	0.0113	0.0012	0.0027	-0.0011	0.0000	0.0029
	Y	-0.0062	0.0229	0.0032	0.0220	0.0000	-0.0108
	Z	0.0000	0.0000	0.0000	0.0000	-0.0067	0.0000
AT. 23	O X	-0.0095	-0.0010	0.0056	-0.0020	-0.0024	-0.0086
	Y	-0.0119	-0.0040	0.0080	-0.0048	-0.0114	-0.0095
	Z	-0.0008	0.0065	-0.0015	-0.0043	-0.0021	0.0030
AT. 24	O X	-0.0095	0.0010	0.0056	-0.0020	-0.0024	-0.0086
	Y	-0.0119	0.0040	0.0080	-0.0048	-0.0114	-0.0095
	Z	0.0008	0.0065	0.0015	0.0043	0.0021	-0.0030
AT. 25	O X	0.0095	0.0010	0.0056	0.0020	-0.0024	-0.0086
	Y	-0.0119	-0.0040	-0.0080	-0.0048	0.0114	0.0095
	Z	-0.0008	0.0065	0.0015	-0.0043	0.0021	-0.0030
AT. 26	O X	0.0095	-0.0010	0.0056	0.0020	-0.0024	-0.0086
	Y	-0.0119	0.0040	-0.0080	-0.0048	0.0114	0.0095
	Z	0.0008	0.0065	-0.0015	0.0043	-0.0021	0.0030
AT. 27	O X	-0.0095	0.0010	0.0056	-0.0020	0.0024	-0.0086
	Y	-0.0119	0.0040	0.0080	-0.0048	0.0114	-0.0095
	Z	-0.0008	-0.0065	-0.0015	-0.0043	0.0021	0.0030
AT. 28	O X	-0.0095	-0.0010	0.0056	-0.0020	0.0024	-0.0086
	Y	-0.0119	-0.0040	0.0080	-0.0048	0.0114	-0.0095
	Z	0.0008	-0.0065	0.0015	0.0043	-0.0021	-0.0030
AT. 29	O X	0.0095	-0.0010	0.0056	0.0020	0.0024	-0.0086
	Y	-0.0119	0.0040	-0.0080	-0.0048	-0.0114	0.0095
	Z	-0.0008	-0.0065	0.0015	-0.0043	-0.0021	-0.0030
AT. 30	O X	0.0095	0.0010	0.0056	0.0020	0.0024	-0.0086
	Y	-0.0119	-0.0040	-0.0080	-0.0048	-0.0114	0.0095
	Z	0.0008	-0.0065	-0.0015	0.0043	0.0021	0.0030
AT. 31	O X	0.0023	-0.0004	0.0123	-0.0012	0.0091	0.0074
	Y	-0.0017	-0.0014	-0.0106	0.0002	-0.0080	-0.0078
	Z	-0.0009	-0.0001	-0.0124	-0.0023	-0.0112	-0.0091
AT. 32	O X	0.0023	0.0004	0.0123	-0.0012	0.0091	0.0074
	Y	-0.0017	0.0014	-0.0106	0.0002	-0.0080	-0.0078
	Z	0.0009	-0.0001	0.0124	0.0023	0.0112	0.0091
AT. 33	O X	-0.0023	0.0004	0.0123	0.0012	0.0091	0.0074
	Y	-0.0017	-0.0014	0.0106	0.0002	0.0080	0.0078
	Z	-0.0009	-0.0001	0.0124	-0.0023	0.0112	0.0091
AT. 34	O X	-0.0023	-0.0004	0.0123	0.0012	0.0091	0.0074
	Y	-0.0017	0.0014	0.0106	0.0002	0.0080	0.0078
	Z	0.0009	-0.0001	-0.0124	0.0023	-0.0112	-0.0091
AT. 35	O X	0.0023	0.0004	0.0123	-0.0012	-0.0091	0.0074
	Y	-0.0017	0.0014	-0.0106	0.0002	0.0080	-0.0078
	Z	-0.0009	0.0001	-0.0124	-0.0023	0.0112	-0.0091
AT. 36	O X	0.0023	-0.0004	0.0123	-0.0012	-0.0091	0.0074

	Y	-0.0017	-0.0014	-0.0106	0.0002	0.0080	-0.0078
	Z	0.0009	0.0001	0.0124	0.0023	-0.0112	0.0091
AT. 37	O X	-0.0023	-0.0004	0.0123	0.0012	-0.0091	0.0074
	Y	-0.0017	0.0014	0.0106	0.0002	-0.0080	0.0078
	Z	-0.0009	0.0001	0.0124	-0.0023	-0.0112	0.0091
AT. 38	O X	-0.0023	0.0004	0.0123	0.0012	-0.0091	0.0074
	Y	-0.0017	-0.0014	0.0106	0.0002	-0.0080	0.0078
	Z	0.0009	0.0001	-0.0124	0.0023	0.0112	-0.0091
AT. 39	O X	0.0006	0.0066	0.0009	0.0060	-0.0087	-0.0040
	Y	-0.0001	-0.0117	-0.0023	-0.0141	0.0079	0.0120
	Z	-0.0001	0.0016	0.0023	-0.0018	-0.0008	0.0029
AT. 40	O X	0.0006	-0.0066	0.0009	0.0060	-0.0087	-0.0040
	Y	-0.0001	0.0117	-0.0023	-0.0141	0.0079	0.0120
	Z	0.0001	0.0016	-0.0023	0.0018	0.0008	-0.0029
AT. 41	O X	-0.0006	-0.0066	0.0009	-0.0060	-0.0087	-0.0040
	Y	-0.0001	-0.0117	0.0023	-0.0141	-0.0079	-0.0120
	Z	-0.0001	0.0016	-0.0023	-0.0018	0.0008	-0.0029
AT. 42	O X	-0.0006	0.0066	0.0009	-0.0060	-0.0087	-0.0040
	Y	-0.0001	0.0117	0.0023	-0.0141	-0.0079	-0.0120
	Z	0.0001	0.0016	0.0023	0.0018	-0.0008	0.0029
AT. 43	O X	0.0006	-0.0066	0.0009	0.0060	0.0087	-0.0040
	Y	-0.0001	0.0117	-0.0023	-0.0141	-0.0079	0.0120
	Z	-0.0001	-0.0016	0.0023	-0.0018	0.0008	0.0029
AT. 44	O X	0.0006	0.0066	0.0009	0.0060	0.0087	-0.0040
	Y	-0.0001	-0.0117	-0.0023	-0.0141	-0.0079	0.0120
	Z	0.0001	-0.0016	-0.0023	0.0018	-0.0008	-0.0029
AT. 45	O X	-0.0006	0.0066	0.0009	-0.0060	0.0087	-0.0040
	Y	-0.0001	0.0117	0.0023	-0.0141	0.0079	-0.0120
	Z	-0.0001	-0.0016	-0.0023	-0.0018	-0.0008	-0.0029
AT. 46	O X	-0.0006	-0.0066	0.0009	-0.0060	0.0087	-0.0040
	Y	-0.0001	-0.0117	0.0023	-0.0141	0.0079	-0.0120
	Z	0.0001	-0.0016	0.0023	0.0018	0.0008	0.0029
AT. 47	O X	-0.0041	-0.0038	0.0010	0.0025	0.0000	-0.0009
	Y	-0.0023	0.0048	0.0014	-0.0035	0.0000	-0.0025
	Z	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000
AT. 48	O X	-0.0041	0.0038	0.0010	0.0025	0.0000	-0.0009
	Y	-0.0023	-0.0048	0.0014	-0.0035	0.0000	-0.0025
	Z	0.0000	0.0000	0.0000	0.0000	-0.0029	0.0000
AT. 49	O X	0.0041	0.0038	0.0010	-0.0025	0.0000	-0.0009
	Y	-0.0023	0.0048	-0.0014	-0.0035	0.0000	0.0025
	Z	0.0000	0.0000	0.0000	0.0000	-0.0029	0.0000
AT. 50	O X	0.0041	-0.0038	0.0010	-0.0025	0.0000	-0.0009
	Y	-0.0023	-0.0048	-0.0014	-0.0035	0.0000	0.0025
	Z	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000
AT. 51	O X	-0.0075	-0.0075	-0.0038	0.0034	0.0000	0.0087
	Y	0.0044	-0.0012	0.0040	-0.0001	0.0000	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
AT. 52	O X	-0.0075	0.0075	-0.0038	0.0034	0.0000	0.0087
	Y	0.0044	0.0012	0.0040	-0.0001	0.0000	-0.0048
	Z	0.0000	0.0000	0.0000	0.0000	-0.0008	0.0000
AT. 53	O X	0.0075	0.0075	-0.0038	-0.0034	0.0000	0.0087
	Y	0.0044	-0.0012	-0.0040	-0.0001	0.0000	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	-0.0008	0.0000
AT. 54	O X	0.0075	-0.0075	-0.0038	-0.0034	0.0000	0.0087

	Y	0.0044	0.0012	-0.0040	-0.0001	0.0000	0.0048
	Z	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
AT. 55 O	X	0.0056	0.0001	0.0023	0.0001	0.0000	-0.0014
	Y	-0.0006	0.0047	0.0010	0.0001	0.0000	0.0064
	Z	0.0000	0.0000	0.0000	0.0000	-0.0021	0.0000
AT. 56 O	X	0.0056	-0.0001	0.0023	0.0001	0.0000	-0.0014
	Y	-0.0006	-0.0047	0.0010	0.0001	0.0000	0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000
AT. 57 O	X	-0.0056	-0.0001	0.0023	-0.0001	0.0000	-0.0014
	Y	-0.0006	0.0047	-0.0010	0.0001	0.0000	-0.0064
	Z	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000
AT. 58 O	X	-0.0056	0.0001	0.0023	-0.0001	0.0000	-0.0014
	Y	-0.0006	-0.0047	-0.0010	0.0001	0.0000	-0.0064
	Z	0.0000	0.0000	0.0000	0.0000	-0.0021	0.0000

FREQ(CM**-1) 903.16 908.15 911.30 912.18 931.00 934.58

AT. 1 FE	X	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0001	0.0000	0.0001	0.0005
	Z	0.0000	0.0000	0.0001	0.0000	0.0006	-0.0004
AT. 2 FE	X	0.0000	0.0001	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	-0.0001	0.0000	0.0001	0.0005
	Z	0.0000	0.0000	0.0001	0.0000	-0.0006	0.0004
AT. 3 FE	X	0.0000	-0.0001	0.0000	0.0001	0.0000	0.0000
	Y	0.0000	0.0000	0.0001	0.0000	0.0001	-0.0005
	Z	0.0000	0.0000	0.0001	0.0000	0.0006	0.0004
AT. 4 FE	X	0.0000	-0.0001	0.0000	-0.0001	0.0000	0.0000
	Y	0.0000	0.0000	-0.0001	0.0000	0.0001	-0.0005
	Z	0.0000	0.0000	0.0001	0.0000	-0.0006	-0.0004
AT. 5 AL	X	0.0042	-0.0050	0.0000	0.0000	0.0070	0.0017
	Y	0.0042	-0.0019	0.0000	0.0000	0.0039	-0.0016
	Z	0.0000	0.0000	0.0085	-0.0082	0.0000	0.0000
AT. 6 AL	X	-0.0042	-0.0050	0.0000	0.0000	-0.0070	-0.0017
	Y	0.0042	0.0019	0.0000	0.0000	0.0039	-0.0016
	Z	0.0000	0.0000	0.0085	0.0082	0.0000	0.0000
AT. 7 AL	X	-0.0042	0.0050	0.0000	0.0000	0.0070	-0.0017
	Y	-0.0042	0.0019	0.0000	0.0000	0.0039	0.0016
	Z	0.0000	0.0000	0.0085	-0.0082	0.0000	0.0000
AT. 8 AL	X	0.0042	0.0050	0.0000	0.0000	-0.0070	0.0017
	Y	-0.0042	-0.0019	0.0000	0.0000	0.0039	0.0016
	Z	0.0000	0.0000	0.0085	0.0082	0.0000	0.0000
AT. 9 AL	X	0.0000	0.0000	0.0000	0.0000	0.0012	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
	Z	0.0001	0.0001	0.0000	0.0002	0.0000	0.0034
AT. 10 AL	X	0.0000	0.0000	0.0000	0.0000	0.0012	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
	Z	-0.0001	-0.0001	0.0000	0.0002	0.0000	-0.0034
AT. 11 AL	X	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
	Z	0.0001	-0.0001	0.0000	-0.0002	0.0000	0.0034
AT. 12 AL	X	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000
	Z	-0.0001	0.0001	0.0000	-0.0002	0.0000	-0.0034
AT. 13 SI	X	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000

	Y	0.0001	0.0000	0.0000	0.0000	-0.0061	0.0262
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000
	Y	-0.0001	0.0000	0.0000	0.0000	-0.0061	-0.0262
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0000	0.0000	0.0000	0.0000	0.0103	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000
	Z	0.0148	-0.0149	0.0135	-0.0133	0.0000	-0.0011
AT. 16	SI X	0.0000	0.0000	0.0000	0.0000	0.0103	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000
	Z	-0.0148	0.0149	0.0135	-0.0133	0.0000	0.0011
AT. 17	SI X	0.0000	0.0000	0.0000	0.0000	-0.0103	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000
	Z	0.0148	0.0149	0.0135	0.0133	0.0000	-0.0011
AT. 18	SI X	0.0000	0.0000	0.0000	0.0000	-0.0103	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000
	Z	-0.0148	-0.0149	0.0135	0.0133	0.0000	0.0011
AT. 19	SI X	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000
	Z	-0.0109	-0.0116	0.0102	0.0112	0.0000	-0.0010
AT. 20	SI X	0.0000	0.0000	0.0000	0.0000	-0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000
	Z	0.0109	0.0116	0.0102	0.0112	0.0000	0.0010
AT. 21	SI X	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000
	Z	-0.0109	0.0116	0.0102	-0.0112	0.0000	-0.0010
AT. 22	SI X	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000
	Z	0.0109	-0.0116	0.0102	-0.0112	0.0000	0.0010
AT. 23	O X	0.0102	0.0096	0.0097	0.0091	0.0091	-0.0007
	Y	-0.0085	-0.0064	-0.0094	-0.0079	-0.0080	0.0012
	Z	-0.0176	-0.0168	-0.0165	-0.0157	-0.0171	0.0019
AT. 24	O X	0.0102	0.0096	-0.0097	-0.0091	0.0091	-0.0007
	Y	-0.0085	-0.0064	0.0094	0.0079	-0.0080	0.0012
	Z	0.0176	0.0168	-0.0165	-0.0157	0.0171	-0.0019
AT. 25	O X	-0.0102	0.0096	-0.0097	0.0091	-0.0091	0.0007
	Y	-0.0085	0.0064	-0.0094	0.0079	-0.0080	0.0012
	Z	-0.0176	0.0168	-0.0165	0.0157	-0.0171	0.0019
AT. 26	O X	-0.0102	0.0096	0.0097	-0.0091	-0.0091	0.0007
	Y	-0.0085	0.0064	0.0094	-0.0079	-0.0080	0.0012
	Z	0.0176	-0.0168	-0.0165	0.0157	0.0171	-0.0019
AT. 27	O X	-0.0102	-0.0096	0.0097	0.0091	0.0091	0.0007
	Y	0.0085	0.0064	-0.0094	-0.0079	-0.0080	-0.0012
	Z	0.0176	0.0168	-0.0165	-0.0157	-0.0171	-0.0019
AT. 28	O X	-0.0102	-0.0096	-0.0097	-0.0091	0.0091	0.0007
	Y	0.0085	0.0064	0.0094	0.0079	-0.0080	-0.0012
	Z	-0.0176	-0.0168	-0.0165	-0.0157	0.0171	0.0019
AT. 29	O X	0.0102	-0.0096	-0.0097	0.0091	-0.0091	-0.0007
	Y	0.0085	-0.0064	-0.0094	0.0079	-0.0080	-0.0012
	Z	0.0176	-0.0168	-0.0165	0.0157	-0.0171	-0.0019
AT. 30	O X	0.0102	-0.0096	0.0097	-0.0091	-0.0091	-0.0007
	Y	0.0085	-0.0064	0.0094	-0.0079	-0.0080	-0.0012
	Z	-0.0176	0.0168	-0.0165	0.0157	0.0171	0.0019
AT. 31	O X	-0.0001	-0.0002	0.0001	0.0002	0.0035	-0.0117

	Y	-0.0001	0.0002	0.0000	0.0002	0.0032	-0.0163
	Z	-0.0003	0.0001	0.0000	0.0004	0.0047	-0.0164
AT. 32	O X	-0.0001	-0.0002	-0.0001	-0.0002	0.0035	-0.0117
	Y	-0.0001	0.0002	0.0000	-0.0002	0.0032	-0.0163
	Z	0.0003	-0.0001	0.0000	0.0004	-0.0047	0.0164
AT. 33	O X	0.0001	-0.0002	-0.0001	0.0002	-0.0035	0.0117
	Y	-0.0001	-0.0002	0.0000	-0.0002	0.0032	-0.0163
	Z	-0.0003	-0.0001	0.0000	-0.0004	0.0047	-0.0164
AT. 34	O X	0.0001	-0.0002	0.0001	-0.0002	-0.0035	0.0117
	Y	-0.0001	-0.0002	0.0000	0.0002	0.0032	-0.0163
	Z	0.0003	0.0001	0.0000	-0.0004	-0.0047	0.0164
AT. 35	O X	0.0001	0.0002	0.0001	0.0002	0.0035	0.0117
	Y	0.0001	-0.0002	0.0000	0.0002	0.0032	0.0163
	Z	0.0003	-0.0001	0.0000	0.0004	0.0047	0.0164
AT. 36	O X	0.0001	0.0002	-0.0001	-0.0002	0.0035	0.0117
	Y	0.0001	-0.0002	0.0000	-0.0002	0.0032	0.0163
	Z	-0.0003	0.0001	0.0000	0.0004	-0.0047	-0.0164
AT. 37	O X	-0.0001	0.0002	-0.0001	0.0002	-0.0035	-0.0117
	Y	0.0001	0.0002	0.0000	-0.0002	0.0032	0.0163
	Z	0.0003	0.0001	0.0000	-0.0004	0.0047	0.0164
AT. 38	O X	-0.0001	0.0002	0.0001	-0.0002	-0.0035	-0.0117
	Y	0.0001	0.0002	0.0000	0.0002	0.0032	0.0163
	Z	-0.0003	-0.0001	0.0000	-0.0004	-0.0047	-0.0164
AT. 39	O X	-0.0084	0.0096	-0.0100	0.0110	-0.0101	-0.0025
	Y	-0.0030	0.0030	-0.0031	0.0032	-0.0008	-0.0005
	Z	-0.0122	0.0135	-0.0125	0.0137	-0.0132	-0.0021
AT. 40	O X	-0.0084	0.0096	0.0100	-0.0110	-0.0101	-0.0025
	Y	-0.0030	0.0030	0.0031	-0.0032	-0.0008	-0.0005
	Z	0.0122	-0.0135	-0.0125	0.0137	0.0132	0.0021
AT. 41	O X	0.0084	0.0096	0.0100	0.0110	0.0101	0.0025
	Y	-0.0030	-0.0030	-0.0031	-0.0032	-0.0008	-0.0005
	Z	-0.0122	-0.0135	-0.0125	-0.0137	-0.0132	-0.0021
AT. 42	O X	0.0084	0.0096	-0.0100	-0.0110	0.0101	0.0025
	Y	-0.0030	-0.0030	0.0031	0.0032	-0.0008	-0.0005
	Z	0.0122	0.0135	-0.0125	-0.0137	0.0132	0.0021
AT. 43	O X	0.0084	-0.0096	-0.0100	0.0110	-0.0101	0.0025
	Y	0.0030	-0.0030	-0.0031	0.0032	-0.0008	0.0005
	Z	0.0122	-0.0135	-0.0125	0.0137	-0.0132	0.0021
AT. 44	O X	0.0084	-0.0096	0.0100	-0.0110	-0.0101	0.0025
	Y	0.0030	-0.0030	0.0031	-0.0032	-0.0008	0.0005
	Z	-0.0122	0.0135	-0.0125	0.0137	0.0132	-0.0021
AT. 45	O X	-0.0084	-0.0096	0.0100	0.0110	0.0101	-0.0025
	Y	0.0030	0.0030	-0.0031	-0.0032	-0.0008	0.0005
	Z	0.0122	0.0135	-0.0125	-0.0137	-0.0132	0.0021
AT. 46	O X	-0.0084	-0.0096	-0.0100	-0.0110	0.0101	-0.0025
	Y	0.0030	0.0030	0.0031	0.0032	-0.0008	0.0005
	Z	-0.0122	-0.0135	-0.0125	-0.0137	0.0132	-0.0021
AT. 47	O X	0.0000	0.0000	0.0000	0.0000	-0.0030	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	-0.0005	-0.0006	0.0008	0.0009	0.0000	-0.0016
AT. 48	O X	0.0000	0.0000	0.0000	0.0000	-0.0030	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	0.0005	0.0006	0.0008	0.0009	0.0000	0.0016
AT. 49	O X	0.0000	0.0000	0.0000	0.0000	0.0030	0.0000

	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	-0.0005	0.0006	0.0008	-0.0009	0.0000	-0.0016
AT. 50	O X	0.0000	0.0000	0.0000	0.0000	0.0030	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0002	0.0000
	Z	0.0005	-0.0006	0.0008	-0.0009	0.0000	0.0016
AT. 51	O X	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	0.0002	0.0000	0.0002	-0.0001	0.0000	0.0015
AT. 52	O X	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	-0.0002	0.0000	0.0002	-0.0001	0.0000	-0.0015
AT. 53	O X	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	0.0002	0.0000	0.0002	0.0001	0.0000	0.0015
AT. 54	O X	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
	Z	-0.0002	0.0000	0.0002	0.0001	0.0000	-0.0015
AT. 55	O X	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000
	Z	0.0007	-0.0004	0.0013	-0.0002	0.0000	-0.0003
AT. 56	O X	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000
	Z	-0.0007	0.0004	0.0013	-0.0002	0.0000	0.0003
AT. 57	O X	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000
	Z	0.0007	0.0004	0.0013	0.0002	0.0000	-0.0003
AT. 58	O X	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	-0.0064	0.0000
	Z	-0.0007	-0.0004	0.0013	0.0002	0.0000	0.0003

FREQ(CM**-1) 938.20 960.58 972.76 973.40 977.68 982.91

AT. 1	FE X	0.0003	0.0000	0.0000	0.0004	0.0000	0.0000
	Y	0.0000	-0.0002	-0.0003	0.0000	-0.0005	0.0006
	Z	0.0000	0.0005	0.0000	0.0000	-0.0001	-0.0003
AT. 2	FE X	-0.0003	0.0000	0.0000	0.0004	0.0000	0.0000
	Y	0.0000	0.0002	-0.0003	0.0000	0.0005	0.0006
	Z	0.0000	0.0005	0.0000	0.0000	-0.0001	0.0003
AT. 3	FE X	-0.0003	0.0000	0.0000	0.0004	0.0000	0.0000
	Y	0.0000	-0.0002	0.0003	0.0000	0.0005	0.0006
	Z	0.0000	0.0005	0.0000	0.0000	0.0001	-0.0003
AT. 4	FE X	0.0003	0.0000	0.0000	0.0004	0.0000	0.0000
	Y	0.0000	0.0002	0.0003	0.0000	-0.0005	0.0006
	Z	0.0000	0.0005	0.0000	0.0000	0.0001	0.0003
AT. 5	AL X	0.0000	0.0000	0.0045	0.0025	0.0000	0.0028
	Y	0.0000	0.0000	-0.0056	0.0080	0.0000	-0.0003
	Z	0.0099	0.0001	0.0000	0.0000	-0.0077	0.0000
AT. 6	AL X	0.0000	0.0000	-0.0045	0.0025	0.0000	-0.0028
	Y	0.0000	0.0000	-0.0056	-0.0080	0.0000	-0.0003
	Z	-0.0099	0.0001	0.0000	0.0000	-0.0077	0.0000
AT. 7	AL X	0.0000	0.0000	-0.0045	0.0025	0.0000	0.0028
	Y	0.0000	0.0000	0.0056	0.0080	0.0000	-0.0003
	Z	-0.0099	0.0001	0.0000	0.0000	0.0077	0.0000
AT. 8	AL X	0.0000	0.0000	0.0045	0.0025	0.0000	-0.0028

	Y	0.0000	0.0000	0.0056	-0.0080	0.0000	-0.0003
	Z	0.0099	0.0001	0.0000	0.0000	0.0077	0.0000
AT. 9	AL X	-0.0025	0.0000	0.0000	-0.0009	-0.0005	0.0001
	Y	-0.0009	0.0000	0.0000	-0.0001	0.0013	0.0053
	Z	0.0000	0.0030	-0.0001	0.0000	0.0000	0.0000
AT. 10	AL X	0.0025	0.0000	0.0000	-0.0009	0.0005	0.0001
	Y	0.0009	0.0000	0.0000	-0.0001	-0.0013	0.0053
	Z	0.0000	0.0030	0.0001	0.0000	0.0000	0.0000
AT. 11	AL X	-0.0025	0.0000	0.0000	-0.0009	0.0005	-0.0001
	Y	0.0009	0.0000	0.0000	0.0001	0.0013	0.0053
	Z	0.0000	0.0030	-0.0001	0.0000	0.0000	0.0000
AT. 12	AL X	0.0025	0.0000	0.0000	-0.0009	-0.0005	-0.0001
	Y	-0.0009	0.0000	0.0000	0.0001	-0.0013	0.0053
	Z	0.0000	0.0030	0.0001	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	0.0039	0.0000	0.0000
	Y	0.0000	0.0000	-0.0038	0.0000	0.0000	0.0230
	Z	0.0000	0.0276	0.0000	0.0000	0.0169	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0039	0.0000	0.0000
	Y	0.0000	0.0000	0.0038	0.0000	0.0000	0.0230
	Z	0.0000	0.0276	0.0000	0.0000	-0.0169	0.0000
AT. 15	SI X	0.0107	0.0000	0.0000	0.0135	-0.0081	0.0005
	Y	0.0038	0.0000	0.0000	0.0041	-0.0012	0.0040
	Z	0.0000	0.0012	-0.0081	0.0000	0.0000	0.0000
AT. 16	SI X	-0.0107	0.0000	0.0000	0.0135	0.0081	0.0005
	Y	-0.0038	0.0000	0.0000	0.0041	0.0012	0.0040
	Z	0.0000	0.0012	0.0081	0.0000	0.0000	0.0000
AT. 17	SI X	0.0107	0.0000	0.0000	0.0135	0.0081	-0.0005
	Y	-0.0038	0.0000	0.0000	-0.0041	-0.0012	0.0040
	Z	0.0000	0.0012	-0.0081	0.0000	0.0000	0.0000
AT. 18	SI X	-0.0107	0.0000	0.0000	0.0135	-0.0081	-0.0005
	Y	0.0038	0.0000	0.0000	-0.0041	0.0012	0.0040
	Z	0.0000	0.0012	0.0081	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0050	0.0000	0.0000	0.0037	-0.0058	0.0008
	Y	0.0046	0.0000	0.0000	-0.0030	0.0053	0.0015
	Z	0.0000	-0.0020	-0.0129	0.0000	0.0000	0.0000
AT. 20	SI X	0.0050	0.0000	0.0000	0.0037	0.0058	0.0008
	Y	-0.0046	0.0000	0.0000	-0.0030	-0.0053	0.0015
	Z	0.0000	-0.0020	0.0129	0.0000	0.0000	0.0000
AT. 21	SI X	-0.0050	0.0000	0.0000	0.0037	0.0058	-0.0008
	Y	-0.0046	0.0000	0.0000	0.0030	0.0053	0.0015
	Z	0.0000	-0.0020	-0.0129	0.0000	0.0000	0.0000
AT. 22	SI X	0.0050	0.0000	0.0000	0.0037	-0.0058	-0.0008
	Y	0.0046	0.0000	0.0000	0.0030	-0.0053	0.0015
	Z	0.0000	-0.0020	0.0129	0.0000	0.0000	0.0000
AT. 23	O X	-0.0094	0.0008	-0.0075	-0.0121	-0.0062	0.0029
	Y	0.0078	-0.0011	0.0060	0.0097	0.0066	-0.0004
	Z	0.0177	-0.0018	0.0119	0.0202	0.0119	-0.0029
AT. 24	O X	0.0094	-0.0008	-0.0075	-0.0121	0.0062	0.0029
	Y	-0.0078	0.0011	0.0060	0.0097	-0.0066	-0.0004
	Z	0.0177	-0.0018	-0.0119	-0.0202	0.0119	0.0029
AT. 25	O X	-0.0094	-0.0008	0.0075	-0.0121	0.0062	-0.0029
	Y	-0.0078	-0.0011	0.0060	-0.0097	0.0066	-0.0004
	Z	-0.0177	-0.0018	0.0119	-0.0202	0.0119	-0.0029
AT. 26	O X	0.0094	0.0008	0.0075	-0.0121	-0.0062	-0.0029

	Y	0.0078	0.0011	0.0060	-0.0097	-0.0066	-0.0004
	Z	-0.0177	-0.0018	-0.0119	0.0202	0.0119	0.0029
AT. 27	O X	0.0094	0.0008	0.0075	-0.0121	0.0062	0.0029
	Y	-0.0078	-0.0011	-0.0060	0.0097	-0.0066	-0.0004
	Z	-0.0177	-0.0018	-0.0119	0.0202	-0.0119	-0.0029
AT. 28	O X	-0.0094	-0.0008	0.0075	-0.0121	-0.0062	0.0029
	Y	0.0078	0.0011	-0.0060	0.0097	0.0066	-0.0004
	Z	-0.0177	-0.0018	0.0119	-0.0202	-0.0119	0.0029
AT. 29	O X	0.0094	-0.0008	-0.0075	-0.0121	-0.0062	-0.0029
	Y	0.0078	-0.0011	-0.0060	-0.0097	-0.0066	-0.0004
	Z	0.0177	-0.0018	-0.0119	-0.0202	-0.0119	-0.0029
AT. 30	O X	-0.0094	0.0008	-0.0075	-0.0121	0.0062	-0.0029
	Y	-0.0078	0.0011	-0.0060	-0.0097	0.0066	-0.0004
	Z	0.0177	-0.0018	0.0119	0.0202	-0.0119	0.0029
AT. 31	O X	-0.0015	-0.0118	0.0020	-0.0007	-0.0075	-0.0099
	Y	-0.0029	-0.0144	0.0023	-0.0028	-0.0084	-0.0145
	Z	-0.0038	-0.0165	0.0019	-0.0037	-0.0109	-0.0162
AT. 32	O X	0.0015	0.0118	0.0020	-0.0007	0.0075	-0.0099
	Y	0.0029	0.0144	0.0023	-0.0028	0.0084	-0.0145
	Z	-0.0038	-0.0165	-0.0019	0.0037	-0.0109	0.0162
AT. 33	O X	-0.0015	0.0118	-0.0020	-0.0007	0.0075	0.0099
	Y	0.0029	-0.0144	0.0023	0.0028	-0.0084	-0.0145
	Z	0.0038	-0.0165	0.0019	0.0037	-0.0109	-0.0162
AT. 34	O X	0.0015	-0.0118	-0.0020	-0.0007	-0.0075	0.0099
	Y	-0.0029	0.0144	0.0023	0.0028	0.0084	-0.0145
	Z	0.0038	-0.0165	-0.0019	-0.0037	-0.0109	0.0162
AT. 35	O X	0.0015	-0.0118	-0.0020	-0.0007	0.0075	-0.0099
	Y	0.0029	-0.0144	-0.0023	-0.0028	0.0084	-0.0145
	Z	0.0038	-0.0165	-0.0019	-0.0037	0.0109	-0.0162
AT. 36	O X	-0.0015	0.0118	-0.0020	-0.0007	-0.0075	-0.0099
	Y	-0.0029	0.0144	-0.0023	-0.0028	-0.0084	-0.0145
	Z	0.0038	-0.0165	0.0019	0.0037	0.0109	0.0162
AT. 37	O X	0.0015	0.0118	0.0020	-0.0007	-0.0075	0.0099
	Y	-0.0029	-0.0144	-0.0023	0.0028	0.0084	-0.0145
	Z	-0.0038	-0.0165	-0.0019	0.0037	0.0109	-0.0162
AT. 38	O X	-0.0015	-0.0118	0.0020	-0.0007	0.0075	0.0099
	Y	0.0029	0.0144	-0.0023	0.0028	-0.0084	-0.0145
	Z	-0.0038	-0.0165	0.0019	-0.0037	0.0109	0.0162
AT. 39	O X	-0.0097	0.0018	-0.0119	-0.0016	0.0073	-0.0035
	Y	-0.0010	0.0006	-0.0054	-0.0020	0.0029	0.0002
	Z	-0.0121	0.0020	-0.0172	-0.0022	0.0109	-0.0028
AT. 40	O X	0.0097	-0.0018	-0.0119	-0.0016	-0.0073	-0.0035
	Y	0.0010	-0.0006	-0.0054	-0.0020	-0.0029	0.0002
	Z	-0.0121	0.0020	0.0172	0.0022	0.0109	0.0028
AT. 41	O X	-0.0097	-0.0018	0.0119	-0.0016	-0.0073	0.0035
	Y	0.0010	0.0006	-0.0054	0.0020	0.0029	0.0002
	Z	0.0121	0.0020	-0.0172	0.0022	0.0109	-0.0028
AT. 42	O X	0.0097	0.0018	0.0119	-0.0016	0.0073	0.0035
	Y	-0.0010	-0.0006	-0.0054	0.0020	-0.0029	0.0002
	Z	0.0121	0.0020	0.0172	-0.0022	0.0109	0.0028
AT. 43	O X	0.0097	0.0018	0.0119	-0.0016	-0.0073	-0.0035
	Y	0.0010	0.0006	0.0054	-0.0020	-0.0029	0.0002
	Z	0.0121	0.0020	0.0172	-0.0022	-0.0109	-0.0028
AT. 44	O X	-0.0097	-0.0018	0.0119	-0.0016	0.0073	-0.0035

	Y	-0.0010	-0.0006	0.0054	-0.0020	0.0029	0.0002
	Z	0.0121	0.0020	-0.0172	0.0022	-0.0109	0.0028
AT. 45 O	X	0.0097	-0.0018	-0.0119	-0.0016	0.0073	0.0035
	Y	-0.0010	0.0006	0.0054	0.0020	-0.0029	0.0002
	Z	-0.0121	0.0020	0.0172	0.0022	-0.0109	-0.0028
AT. 46 O	X	-0.0097	0.0018	-0.0119	-0.0016	-0.0073	0.0035
	Y	0.0010	-0.0006	0.0054	0.0020	0.0029	0.0002
	Z	-0.0121	0.0020	-0.0172	-0.0022	-0.0109	0.0028
AT. 47 O	X	-0.0025	0.0000	0.0000	-0.0043	0.0037	-0.0061
	Y	0.0006	0.0000	0.0000	-0.0002	-0.0003	-0.0003
	Z	0.0000	0.0008	-0.0003	0.0000	0.0000	0.0000
AT. 48 O	X	0.0025	0.0000	0.0000	-0.0043	-0.0037	-0.0061
	Y	-0.0006	0.0000	0.0000	-0.0002	0.0003	-0.0003
	Z	0.0000	0.0008	0.0003	0.0000	0.0000	0.0000
AT. 49 O	X	-0.0025	0.0000	0.0000	-0.0043	-0.0037	0.0061
	Y	-0.0006	0.0000	0.0000	0.0002	-0.0003	-0.0003
	Z	0.0000	0.0008	-0.0003	0.0000	0.0000	0.0000
AT. 50 O	X	0.0025	0.0000	0.0000	-0.0043	0.0037	0.0061
	Y	0.0006	0.0000	0.0000	0.0002	0.0003	-0.0003
	Z	0.0000	0.0008	0.0003	0.0000	0.0000	0.0000
AT. 51 O	X	-0.0005	0.0000	0.0000	-0.0031	0.0049	0.0072
	Y	0.0010	0.0000	0.0000	0.0023	-0.0027	-0.0052
	Z	0.0000	0.0013	-0.0006	0.0000	0.0000	0.0000
AT. 52 O	X	0.0005	0.0000	0.0000	-0.0031	-0.0049	0.0072
	Y	-0.0010	0.0000	0.0000	0.0023	0.0027	-0.0052
	Z	0.0000	0.0013	0.0006	0.0000	0.0000	0.0000
AT. 53 O	X	-0.0005	0.0000	0.0000	-0.0031	-0.0049	-0.0072
	Y	-0.0010	0.0000	0.0000	-0.0023	-0.0027	-0.0052
	Z	0.0000	0.0013	-0.0006	0.0000	0.0000	0.0000
AT. 54 O	X	0.0005	0.0000	0.0000	-0.0031	0.0049	-0.0072
	Y	0.0010	0.0000	0.0000	-0.0023	0.0027	-0.0052
	Z	0.0000	0.0013	0.0006	0.0000	0.0000	0.0000
AT. 55 O	X	-0.0017	0.0000	0.0000	-0.0008	-0.0009	-0.0016
	Y	-0.0069	0.0000	0.0000	-0.0033	-0.0010	-0.0050
	Z	0.0000	0.0001	-0.0008	0.0000	0.0000	0.0000
AT. 56 O	X	0.0017	0.0000	0.0000	-0.0008	0.0009	-0.0016
	Y	0.0069	0.0000	0.0000	-0.0033	0.0010	-0.0050
	Z	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000
AT. 57 O	X	-0.0017	0.0000	0.0000	-0.0008	0.0009	0.0016
	Y	0.0069	0.0000	0.0000	0.0033	-0.0010	-0.0050
	Z	0.0000	0.0001	-0.0008	0.0000	0.0000	0.0000
AT. 58 O	X	0.0017	0.0000	0.0000	-0.0008	-0.0009	0.0016
	Y	-0.0069	0.0000	0.0000	0.0033	0.0010	-0.0050
	Z	0.0000	0.0001	0.0008	0.0000	0.0000	0.0000

FREQ(CM**-1) 983.40 985.99 990.94 993.70 995.17 1011.15

AT. 1 FE	X	0.0003	0.0000	0.0002	0.0006	0.0008	0.0000
	Y	0.0000	-0.0005	0.0000	0.0000	0.0000	-0.0009
	Z	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0001
AT. 2 FE	X	0.0003	0.0000	0.0002	-0.0006	-0.0008	0.0000
	Y	0.0000	0.0005	0.0000	0.0000	0.0000	0.0009
	Z	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0001
AT. 3 FE	X	-0.0003	0.0000	0.0002	-0.0006	0.0008	0.0000

	Y	0.0000	0.0005	0.0000	0.0000	0.0000	-0.0009
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001
AT. 4	FE X	-0.0003	0.0000	0.0002	0.0006	-0.0008	0.0000
	Y	0.0000	-0.0005	0.0000	0.0000	0.0000	0.0009
	Z	0.0000	0.0002	0.0000	0.0000	0.0000	0.0001
AT. 5	AL X	0.0034	0.0000	0.0083	0.0000	0.0000	0.0000
	Y	-0.0033	0.0000	-0.0034	0.0000	0.0000	0.0000
	Z	0.0000	-0.0005	0.0000	0.0022	0.0007	0.0007
AT. 6	AL X	0.0034	0.0000	0.0083	0.0000	0.0000	0.0000
	Y	0.0033	0.0000	0.0034	0.0000	0.0000	0.0000
	Z	0.0000	-0.0005	0.0000	-0.0022	-0.0007	0.0007
AT. 7	AL X	-0.0034	0.0000	0.0083	0.0000	0.0000	0.0000
	Y	0.0033	0.0000	-0.0034	0.0000	0.0000	0.0000
	Z	0.0000	0.0005	0.0000	-0.0022	0.0007	0.0007
AT. 8	AL X	-0.0034	0.0000	0.0083	0.0000	0.0000	0.0000
	Y	-0.0033	0.0000	0.0034	0.0000	0.0000	0.0000
	Z	0.0000	0.0005	0.0000	0.0022	-0.0007	0.0007
AT. 9	AL X	0.0000	0.0028	-0.0020	-0.0010	0.0000	0.0000
	Y	0.0000	-0.0004	-0.0013	0.0063	0.0000	0.0000
	Z	0.0022	0.0000	0.0000	0.0000	0.0092	-0.0002
AT. 10	AL X	0.0000	-0.0028	-0.0020	0.0010	0.0000	0.0000
	Y	0.0000	0.0004	-0.0013	-0.0063	0.0000	0.0000
	Z	-0.0022	0.0000	0.0000	0.0000	0.0092	-0.0002
AT. 11	AL X	0.0000	-0.0028	-0.0020	-0.0010	0.0000	0.0000
	Y	0.0000	-0.0004	0.0013	-0.0063	0.0000	0.0000
	Z	-0.0022	0.0000	0.0000	0.0000	-0.0092	-0.0002
AT. 12	AL X	0.0000	0.0028	-0.0020	0.0010	0.0000	0.0000
	Y	0.0000	0.0004	0.0013	0.0063	0.0000	0.0000
	Z	0.0022	0.0000	0.0000	0.0000	-0.0092	-0.0002
AT. 13	SI X	-0.0055	0.0000	-0.0010	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	-0.0033	0.0000	0.0000	0.0000	0.0037
AT. 14	SI X	0.0055	0.0000	-0.0010	0.0000	0.0000	0.0000
	Y	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0033	0.0000	0.0000	0.0000	0.0037
AT. 15	SI X	0.0000	-0.0086	0.0001	-0.0004	0.0000	0.0000
	Y	0.0000	-0.0043	-0.0027	0.0000	0.0000	0.0000
	Z	-0.0102	0.0000	0.0000	0.0000	-0.0028	-0.0100
AT. 16	SI X	0.0000	0.0086	0.0001	0.0004	0.0000	0.0000
	Y	0.0000	0.0043	-0.0027	0.0000	0.0000	0.0000
	Z	0.0102	0.0000	0.0000	0.0000	-0.0028	-0.0100
AT. 17	SI X	0.0000	0.0086	0.0001	-0.0004	0.0000	0.0000
	Y	0.0000	-0.0043	0.0027	0.0000	0.0000	0.0000
	Z	0.0102	0.0000	0.0000	0.0000	0.0028	-0.0100
AT. 18	SI X	0.0000	-0.0086	0.0001	0.0004	0.0000	0.0000
	Y	0.0000	0.0043	0.0027	0.0000	0.0000	0.0000
	Z	-0.0102	0.0000	0.0000	0.0000	0.0028	-0.0100
AT. 19	SI X	0.0000	0.0055	0.0088	-0.0035	0.0000	0.0000
	Y	0.0000	-0.0045	-0.0085	0.0025	0.0000	0.0000
	Z	0.0120	0.0000	0.0000	0.0000	-0.0026	0.0135
AT. 20	SI X	0.0000	-0.0055	0.0088	0.0035	0.0000	0.0000
	Y	0.0000	0.0045	-0.0085	-0.0025	0.0000	0.0000
	Z	-0.0120	0.0000	0.0000	0.0000	-0.0026	0.0135
AT. 21	SI X	0.0000	-0.0055	0.0088	-0.0035	0.0000	0.0000

	Y	0.0000	-0.0045	0.0085	-0.0025	0.0000	0.0000
	Z	-0.0120	0.0000	0.0000	0.0000	0.0026	0.0135
AT. 22	SI X	0.0000	0.0055	0.0088	0.0035	0.0000	0.0000
	Y	0.0000	0.0045	0.0085	0.0025	0.0000	0.0000
	Z	0.0120	0.0000	0.0000	0.0000	0.0026	0.0135
AT. 23	O X	0.0085	-0.0089	0.0020	0.0021	0.0016	-0.0067
	Y	-0.0038	0.0088	-0.0008	-0.0021	-0.0014	0.0072
	Z	-0.0130	0.0161	-0.0040	-0.0038	-0.0031	0.0125
AT. 24	O X	0.0085	0.0089	0.0020	-0.0021	-0.0016	0.0067
	Y	-0.0038	-0.0088	-0.0008	0.0021	0.0014	-0.0072
	Z	0.0130	0.0161	0.0040	-0.0038	-0.0031	0.0125
AT. 25	O X	0.0085	0.0089	0.0020	0.0021	0.0016	0.0067
	Y	0.0038	0.0088	0.0008	0.0021	0.0014	0.0072
	Z	0.0130	0.0161	0.0040	0.0038	0.0031	0.0125
AT. 26	O X	0.0085	-0.0089	0.0020	-0.0021	-0.0016	-0.0067
	Y	0.0038	-0.0088	0.0008	-0.0021	-0.0014	-0.0072
	Z	-0.0130	0.0161	-0.0040	0.0038	0.0031	0.0125
AT. 27	O X	-0.0085	0.0089	0.0020	-0.0021	0.0016	-0.0067
	Y	0.0038	-0.0088	-0.0008	0.0021	-0.0014	0.0072
	Z	0.0130	-0.0161	-0.0040	0.0038	-0.0031	0.0125
AT. 28	O X	-0.0085	-0.0089	0.0020	0.0021	-0.0016	0.0067
	Y	0.0038	0.0088	-0.0008	-0.0021	0.0014	-0.0072
	Z	-0.0130	-0.0161	0.0040	0.0038	-0.0031	0.0125
AT. 29	O X	-0.0085	-0.0089	0.0020	-0.0021	0.0016	0.0067
	Y	-0.0038	-0.0088	0.0008	-0.0021	0.0014	0.0072
	Z	-0.0130	-0.0161	0.0040	-0.0038	0.0031	0.0125
AT. 30	O X	-0.0085	0.0089	0.0020	0.0021	-0.0016	-0.0067
	Y	-0.0038	0.0088	0.0008	0.0021	-0.0014	-0.0072
	Z	0.0130	-0.0161	-0.0040	-0.0038	0.0031	0.0125
AT. 31	O X	0.0013	0.0012	0.0008	0.0112	0.0109	-0.0020
	Y	0.0048	0.0019	-0.0004	0.0159	0.0172	-0.0020
	Z	0.0057	0.0025	-0.0002	0.0184	0.0201	-0.0018
AT. 32	O X	0.0013	-0.0012	0.0008	-0.0112	-0.0109	0.0020
	Y	0.0048	-0.0019	-0.0004	-0.0159	-0.0172	0.0020
	Z	-0.0057	0.0025	0.0002	0.0184	0.0201	-0.0018
AT. 33	O X	0.0013	-0.0012	0.0008	0.0112	0.0109	0.0020
	Y	-0.0048	0.0019	0.0004	-0.0159	-0.0172	-0.0020
	Z	-0.0057	0.0025	0.0002	-0.0184	-0.0201	-0.0018
AT. 34	O X	0.0013	0.0012	0.0008	-0.0112	-0.0109	-0.0020
	Y	-0.0048	-0.0019	0.0004	0.0159	0.0172	0.0020
	Z	0.0057	0.0025	-0.0002	-0.0184	-0.0201	-0.0018
AT. 35	O X	-0.0013	-0.0012	0.0008	-0.0112	0.0109	-0.0020
	Y	-0.0048	-0.0019	-0.0004	-0.0159	0.0172	-0.0020
	Z	-0.0057	-0.0025	-0.0002	-0.0184	0.0201	-0.0018
AT. 36	O X	-0.0013	0.0012	0.0008	0.0112	-0.0109	0.0020
	Y	-0.0048	0.0019	-0.0004	0.0159	-0.0172	0.0020
	Z	0.0057	-0.0025	0.0002	-0.0184	0.0201	-0.0018
AT. 37	O X	-0.0013	0.0012	0.0008	-0.0112	0.0109	0.0020
	Y	0.0048	-0.0019	0.0004	0.0159	-0.0172	-0.0020
	Z	0.0057	-0.0025	0.0002	0.0184	-0.0201	-0.0018
AT. 38	O X	-0.0013	-0.0012	0.0008	0.0112	-0.0109	-0.0020
	Y	0.0048	0.0019	0.0004	-0.0159	0.0172	0.0020
	Z	-0.0057	-0.0025	-0.0002	0.0184	-0.0201	-0.0018
AT. 39	O X	-0.0103	-0.0119	-0.0153	-0.0075	-0.0035	-0.0115

	Y	-0.0060	-0.0028	-0.0051	-0.0012	-0.0004	-0.0038
	Z	-0.0157	-0.0147	-0.0206	-0.0088	-0.0037	-0.0163
AT. 40	O X	-0.0103	0.0119	-0.0153	0.0075	0.0035	0.0115
	Y	-0.0060	0.0028	-0.0051	0.0012	0.0004	0.0038
	Z	0.0157	-0.0147	0.0206	-0.0088	-0.0037	-0.0163
AT. 41	O X	-0.0103	0.0119	-0.0153	-0.0075	-0.0035	0.0115
	Y	0.0060	-0.0028	0.0051	0.0012	0.0004	-0.0038
	Z	0.0157	-0.0147	0.0206	0.0088	0.0037	-0.0163
AT. 42	O X	-0.0103	-0.0119	-0.0153	0.0075	0.0035	-0.0115
	Y	0.0060	0.0028	0.0051	-0.0012	-0.0004	0.0038
	Z	-0.0157	-0.0147	-0.0206	0.0088	0.0037	-0.0163
AT. 43	O X	0.0103	0.0119	-0.0153	0.0075	-0.0035	-0.0115
	Y	0.0060	0.0028	-0.0051	0.0012	-0.0004	-0.0038
	Z	0.0157	0.0147	-0.0206	0.0088	-0.0037	-0.0163
AT. 44	O X	0.0103	-0.0119	-0.0153	-0.0075	0.0035	0.0115
	Y	0.0060	-0.0028	-0.0051	-0.0012	0.0004	0.0038
	Z	-0.0157	0.0147	0.0206	0.0088	-0.0037	-0.0163
AT. 45	O X	0.0103	-0.0119	-0.0153	0.0075	-0.0035	0.0115
	Y	-0.0060	0.0028	0.0051	-0.0012	0.0004	-0.0038
	Z	-0.0157	0.0147	0.0206	-0.0088	0.0037	-0.0163
AT. 46	O X	0.0103	0.0119	-0.0153	-0.0075	0.0035	-0.0115
	Y	-0.0060	-0.0028	0.0051	0.0012	-0.0004	0.0038
	Z	0.0157	0.0147	-0.0206	-0.0088	0.0037	-0.0163
AT. 47	O X	0.0000	0.0065	0.0013	-0.0006	0.0000	0.0000
	Y	0.0000	0.0010	-0.0002	0.0013	0.0000	0.0000
	Z	0.0002	0.0000	0.0000	0.0000	-0.0010	0.0000
AT. 48	O X	0.0000	-0.0065	0.0013	0.0006	0.0000	0.0000
	Y	0.0000	-0.0010	-0.0002	-0.0013	0.0000	0.0000
	Z	-0.0002	0.0000	0.0000	0.0000	-0.0010	0.0000
AT. 49	O X	0.0000	-0.0065	0.0013	-0.0006	0.0000	0.0000
	Y	0.0000	0.0010	0.0002	-0.0013	0.0000	0.0000
	Z	-0.0002	0.0000	0.0000	0.0000	0.0010	0.0000
AT. 50	O X	0.0000	0.0065	0.0013	0.0006	0.0000	0.0000
	Y	0.0000	-0.0010	0.0002	0.0013	0.0000	0.0000
	Z	0.0002	0.0000	0.0000	0.0000	0.0010	0.0000
AT. 51	O X	0.0000	-0.0006	-0.0038	-0.0008	0.0000	0.0000
	Y	0.0000	0.0015	0.0031	0.0015	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0005	0.0013
AT. 52	O X	0.0000	0.0006	-0.0038	0.0008	0.0000	0.0000
	Y	0.0000	-0.0015	0.0031	-0.0015	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	0.0005	0.0013
AT. 53	O X	0.0000	0.0006	-0.0038	-0.0008	0.0000	0.0000
	Y	0.0000	0.0015	-0.0031	-0.0015	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0013
AT. 54	O X	0.0000	-0.0006	-0.0038	0.0008	0.0000	0.0000
	Y	0.0000	-0.0015	-0.0031	0.0015	0.0000	0.0000
	Z	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0013
AT. 55	O X	0.0000	-0.0005	0.0015	-0.0014	0.0000	0.0000
	Y	0.0000	0.0019	0.0061	-0.0044	0.0000	0.0000
	Z	0.0003	0.0000	0.0000	0.0000	0.0001	-0.0009
AT. 56	O X	0.0000	0.0005	0.0015	0.0014	0.0000	0.0000
	Y	0.0000	-0.0019	0.0061	0.0044	0.0000	0.0000
	Z	-0.0003	0.0000	0.0000	0.0000	0.0001	-0.0009
AT. 57	O X	0.0000	0.0005	0.0015	-0.0014	0.0000	0.0000

	Y	0.0000	0.0019	-0.0061	0.0044	0.0000	0.0000
	Z	-0.0003	0.0000	0.0000	0.0000	-0.0001	-0.0009
AT. 58 O	X	0.0000	-0.0005	0.0015	0.0014	0.0000	0.0000
	Y	0.0000	-0.0019	-0.0061	-0.0044	0.0000	0.0000
	Z	0.0003	0.0000	0.0000	0.0000	-0.0001	-0.0009

FREQ(CM**-1) 1016.36 1021.26 1041.42 1051.53 1062.16 1062.67

AT. 1 FE	X	0.0000	-0.0006	0.0000	-0.0008	-0.0003	0.0004
	Y	0.0002	0.0000	-0.0002	0.0000	0.0000	0.0000
	Z	0.0001	0.0000	0.0012	0.0000	0.0000	0.0000
AT. 2 FE	X	0.0000	-0.0006	0.0000	-0.0008	0.0003	-0.0004
	Y	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000
	Z	-0.0001	0.0000	0.0012	0.0000	0.0000	0.0000
AT. 3 FE	X	0.0000	0.0006	0.0000	-0.0008	-0.0003	-0.0004
	Y	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000
	Z	0.0001	0.0000	-0.0012	0.0000	0.0000	0.0000
AT. 4 FE	X	0.0000	0.0006	0.0000	-0.0008	0.0003	0.0004
	Y	0.0002	0.0000	-0.0002	0.0000	0.0000	0.0000
	Z	-0.0001	0.0000	-0.0012	0.0000	0.0000	0.0000
AT. 5 AL	X	0.0053	0.0000	0.0000	-0.0011	0.0000	0.0000
	Y	-0.0066	0.0000	0.0000	-0.0008	0.0000	0.0000
	Z	0.0000	0.0000	0.0077	0.0000	-0.0007	-0.0002
AT. 6 AL	X	-0.0053	0.0000	0.0000	-0.0011	0.0000	0.0000
	Y	-0.0066	0.0000	0.0000	0.0008	0.0000	0.0000
	Z	0.0000	0.0000	0.0077	0.0000	0.0007	0.0002
AT. 7 AL	X	0.0053	0.0000	0.0000	-0.0011	0.0000	0.0000
	Y	-0.0066	0.0000	0.0000	-0.0008	0.0000	0.0000
	Z	0.0000	0.0000	-0.0077	0.0000	-0.0007	0.0002
AT. 8 AL	X	-0.0053	0.0000	0.0000	-0.0011	0.0000	0.0000
	Y	-0.0066	0.0000	0.0000	0.0008	0.0000	0.0000
	Z	0.0000	0.0000	-0.0077	0.0000	0.0007	-0.0002
AT. 9 AL	X	0.0013	0.0000	0.0008	0.0012	0.0000	0.0016
	Y	0.0002	0.0000	0.0036	-0.0042	0.0000	0.0053
	Z	0.0000	-0.0026	0.0000	0.0000	0.0036	0.0000
AT. 10 AL	X	0.0013	0.0000	-0.0008	0.0012	0.0000	-0.0016
	Y	0.0002	0.0000	-0.0036	-0.0042	0.0000	-0.0053
	Z	0.0000	0.0026	0.0000	0.0000	0.0036	0.0000
AT. 11 AL	X	-0.0013	0.0000	-0.0008	0.0012	0.0000	0.0016
	Y	0.0002	0.0000	0.0036	0.0042	0.0000	-0.0053
	Z	0.0000	0.0026	0.0000	0.0000	-0.0036	0.0000
AT. 12 AL	X	-0.0013	0.0000	0.0008	0.0012	0.0000	-0.0016
	Y	0.0002	0.0000	-0.0036	0.0042	0.0000	0.0053
	Z	0.0000	-0.0026	0.0000	0.0000	-0.0036	0.0000
AT. 13 SI	X	0.0000	0.0268	0.0000	0.0244	0.0000	0.0000
	Y	-0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	0.0191	0.0000	0.0000	0.0000
AT. 14 SI	X	0.0000	-0.0268	0.0000	0.0244	0.0000	0.0000
	Y	-0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
	Z	0.0000	0.0000	-0.0191	0.0000	0.0000	0.0000
AT. 15 SI	X	-0.0084	0.0000	0.0024	0.0004	0.0000	0.0074
	Y	-0.0010	0.0000	0.0029	-0.0032	0.0000	0.0051
	Z	0.0000	-0.0029	0.0000	0.0000	0.0119	0.0000
AT. 16 SI	X	-0.0084	0.0000	-0.0024	0.0004	0.0000	-0.0074

	Y	-0.0010	0.0000	-0.0029	-0.0032	0.0000	-0.0051
	Z	0.0000	0.0029	0.0000	0.0000	0.0119	0.0000
AT. 17 SI	X	0.0084	0.0000	-0.0024	0.0004	0.0000	0.0074
	Y	-0.0010	0.0000	0.0029	0.0032	0.0000	-0.0051
	Z	0.0000	0.0029	0.0000	0.0000	-0.0119	0.0000
AT. 18 SI	X	0.0084	0.0000	0.0024	0.0004	0.0000	-0.0074
	Y	-0.0010	0.0000	-0.0029	0.0032	0.0000	0.0051
	Z	0.0000	-0.0029	0.0000	0.0000	-0.0119	0.0000
AT. 19 SI	X	-0.0079	0.0000	0.0027	-0.0043	0.0000	0.0058
	Y	0.0068	0.0000	-0.0048	-0.0004	0.0000	-0.0093
	Z	0.0000	0.0038	0.0000	0.0000	0.0127	0.0000
AT. 20 SI	X	-0.0079	0.0000	-0.0027	-0.0043	0.0000	-0.0058
	Y	0.0068	0.0000	0.0048	-0.0004	0.0000	0.0093
	Z	0.0000	-0.0038	0.0000	0.0000	0.0127	0.0000
AT. 21 SI	X	0.0079	0.0000	-0.0027	-0.0043	0.0000	0.0058
	Y	0.0068	0.0000	-0.0048	0.0004	0.0000	0.0093
	Z	0.0000	-0.0038	0.0000	0.0000	-0.0127	0.0000
AT. 22 SI	X	0.0079	0.0000	0.0027	-0.0043	0.0000	-0.0058
	Y	0.0068	0.0000	0.0048	0.0004	0.0000	-0.0093
	Z	0.0000	0.0038	0.0000	0.0000	-0.0127	0.0000
AT. 23 O	X	-0.0076	0.0027	0.0040	0.0030	-0.0073	-0.0073
	Y	0.0068	-0.0005	-0.0033	-0.0008	0.0046	0.0056
	Z	0.0129	-0.0034	-0.0083	-0.0031	0.0132	0.0117
AT. 24 O	X	-0.0076	0.0027	-0.0040	0.0030	0.0073	0.0073
	Y	0.0068	-0.0005	0.0033	-0.0008	-0.0046	-0.0056
	Z	-0.0129	0.0034	-0.0083	0.0031	0.0132	0.0117
AT. 25 O	X	0.0076	0.0027	-0.0040	0.0030	-0.0073	-0.0073
	Y	0.0068	0.0005	-0.0033	0.0008	-0.0046	-0.0056
	Z	0.0129	0.0034	-0.0083	0.0031	-0.0132	-0.0117
AT. 26 O	X	0.0076	0.0027	0.0040	0.0030	0.0073	0.0073
	Y	0.0068	0.0005	0.0033	0.0008	0.0046	0.0056
	Z	-0.0129	-0.0034	-0.0083	-0.0031	-0.0132	-0.0117
AT. 27 O	X	-0.0076	-0.0027	-0.0040	0.0030	-0.0073	0.0073
	Y	0.0068	0.0005	0.0033	-0.0008	0.0046	-0.0056
	Z	0.0129	0.0034	0.0083	-0.0031	0.0132	-0.0117
AT. 28 O	X	-0.0076	-0.0027	0.0040	0.0030	0.0073	-0.0073
	Y	0.0068	0.0005	-0.0033	-0.0008	-0.0046	0.0056
	Z	-0.0129	-0.0034	0.0083	0.0031	0.0132	-0.0117
AT. 29 O	X	0.0076	-0.0027	0.0040	0.0030	-0.0073	0.0073
	Y	0.0068	-0.0005	0.0033	0.0008	-0.0046	0.0056
	Z	0.0129	-0.0034	0.0083	0.0031	-0.0132	0.0117
AT. 30 O	X	0.0076	-0.0027	-0.0040	0.0030	0.0073	-0.0073
	Y	0.0068	-0.0005	-0.0033	0.0008	0.0046	-0.0056
	Z	-0.0129	0.0034	0.0083	-0.0031	-0.0132	0.0117
AT. 31 O	X	0.0018	-0.0110	-0.0069	-0.0102	0.0007	0.0036
	Y	0.0007	-0.0138	-0.0094	-0.0122	0.0038	0.0070
	Z	0.0012	-0.0148	-0.0134	-0.0150	0.0052	0.0076
AT. 32 O	X	0.0018	-0.0110	0.0069	-0.0102	-0.0007	-0.0036
	Y	0.0007	-0.0138	0.0094	-0.0122	-0.0038	-0.0070
	Z	-0.0012	0.0148	-0.0134	0.0150	0.0052	0.0076
AT. 33 O	X	-0.0018	-0.0110	0.0069	-0.0102	0.0007	0.0036
	Y	0.0007	0.0138	-0.0094	0.0122	-0.0038	-0.0070
	Z	0.0012	0.0148	-0.0134	0.0150	-0.0052	-0.0076
AT. 34 O	X	-0.0018	-0.0110	-0.0069	-0.0102	-0.0007	-0.0036

	Y	0.0007	0.0138	0.0094	0.0122	0.0038	0.0070
	Z	-0.0012	-0.0148	-0.0134	-0.0150	-0.0052	-0.0076
AT. 35	O X	0.0018	0.0110	0.0069	-0.0102	0.0007	-0.0036
	Y	0.0007	0.0138	0.0094	-0.0122	0.0038	-0.0070
	Z	0.0012	0.0148	0.0134	-0.0150	0.0052	-0.0076
AT. 36	O X	0.0018	0.0110	-0.0069	-0.0102	-0.0007	0.0036
	Y	0.0007	0.0138	-0.0094	-0.0122	-0.0038	0.0070
	Z	-0.0012	-0.0148	0.0134	0.0150	0.0052	-0.0076
AT. 37	O X	-0.0018	0.0110	-0.0069	-0.0102	0.0007	-0.0036
	Y	0.0007	-0.0138	0.0094	0.0122	-0.0038	0.0070
	Z	0.0012	-0.0148	0.0134	0.0150	-0.0052	0.0076
AT. 38	O X	-0.0018	0.0110	0.0069	-0.0102	-0.0007	0.0036
	Y	0.0007	-0.0138	-0.0094	0.0122	0.0038	-0.0070
	Z	-0.0012	0.0148	0.0134	-0.0150	-0.0052	0.0076
AT. 39	O X	-0.0115	-0.0020	-0.0076	0.0008	0.0094	0.0091
	Y	-0.0048	-0.0021	-0.0026	-0.0001	0.0043	0.0060
	Z	-0.0161	-0.0043	-0.0119	0.0002	0.0145	0.0140
AT. 40	O X	-0.0115	-0.0020	0.0076	0.0008	-0.0094	-0.0091
	Y	-0.0048	-0.0021	0.0026	-0.0001	-0.0043	-0.0060
	Z	0.0161	0.0043	-0.0119	-0.0002	0.0145	0.0140
AT. 41	O X	0.0115	-0.0020	0.0076	0.0008	0.0094	0.0091
	Y	-0.0048	0.0021	-0.0026	0.0001	-0.0043	-0.0060
	Z	-0.0161	0.0043	-0.0119	-0.0002	-0.0145	-0.0140
AT. 42	O X	0.0115	-0.0020	-0.0076	0.0008	-0.0094	-0.0091
	Y	-0.0048	0.0021	0.0026	0.0001	0.0043	0.0060
	Z	0.0161	-0.0043	-0.0119	0.0002	-0.0145	-0.0140
AT. 43	O X	-0.0115	0.0020	0.0076	0.0008	0.0094	-0.0091
	Y	-0.0048	0.0021	0.0026	-0.0001	0.0043	-0.0060
	Z	-0.0161	0.0043	0.0119	0.0002	0.0145	-0.0140
AT. 44	O X	-0.0115	0.0020	-0.0076	0.0008	-0.0094	0.0091
	Y	-0.0048	0.0021	-0.0026	-0.0001	-0.0043	0.0060
	Z	0.0161	-0.0043	0.0119	-0.0002	0.0145	-0.0140
AT. 45	O X	0.0115	0.0020	-0.0076	0.0008	0.0094	-0.0091
	Y	-0.0048	-0.0021	0.0026	0.0001	-0.0043	0.0060
	Z	-0.0161	-0.0043	0.0119	-0.0002	-0.0145	0.0140
AT. 46	O X	0.0115	0.0020	0.0076	0.0008	-0.0094	0.0091
	Y	-0.0048	-0.0021	-0.0026	0.0001	0.0043	-0.0060
	Z	0.0161	0.0043	0.0119	0.0002	-0.0145	0.0140
AT. 47	O X	0.0020	0.0000	0.0047	0.0087	0.0000	0.0041
	Y	0.0003	0.0000	0.0006	0.0012	0.0000	0.0031
	Z	0.0000	0.0003	0.0000	0.0000	-0.0012	0.0000
AT. 48	O X	0.0020	0.0000	-0.0047	0.0087	0.0000	-0.0041
	Y	0.0003	0.0000	-0.0006	0.0012	0.0000	-0.0031
	Z	0.0000	-0.0003	0.0000	0.0000	-0.0012	0.0000
AT. 49	O X	-0.0020	0.0000	-0.0047	0.0087	0.0000	0.0041
	Y	0.0003	0.0000	0.0006	-0.0012	0.0000	-0.0031
	Z	0.0000	-0.0003	0.0000	0.0000	0.0012	0.0000
AT. 50	O X	-0.0020	0.0000	0.0047	0.0087	0.0000	-0.0041
	Y	0.0003	0.0000	-0.0006	-0.0012	0.0000	0.0031
	Z	0.0000	0.0003	0.0000	0.0000	0.0012	0.0000
AT. 51	O X	0.0038	0.0000	0.0042	-0.0082	0.0000	0.0025
	Y	-0.0033	0.0000	-0.0034	0.0063	0.0000	-0.0037
	Z	0.0000	-0.0012	0.0000	0.0000	-0.0020	0.0000
AT. 52	O X	0.0038	0.0000	-0.0042	-0.0082	0.0000	-0.0025

	Y	-0.0033	0.0000	0.0034	0.0063	0.0000	0.0037
	Z	0.0000	0.0012	0.0000	0.0000	-0.0020	0.0000
AT. 53 O	X	-0.0038	0.0000	-0.0042	-0.0082	0.0000	0.0025
	Y	-0.0033	0.0000	-0.0034	-0.0063	0.0000	0.0037
	Z	0.0000	0.0012	0.0000	0.0000	0.0020	0.0000
AT. 54 O	X	-0.0038	0.0000	0.0042	-0.0082	0.0000	-0.0025
	Y	-0.0033	0.0000	0.0034	-0.0063	0.0000	-0.0037
	Z	0.0000	-0.0012	0.0000	0.0000	0.0020	0.0000
AT. 55 O	X	-0.0007	0.0000	-0.0002	0.0005	0.0000	-0.0001
	Y	-0.0018	0.0000	0.0004	0.0009	0.0000	0.0028
	Z	0.0000	0.0000	0.0000	0.0000	-0.0020	0.0000
AT. 56 O	X	-0.0007	0.0000	0.0002	0.0005	0.0000	0.0001
	Y	-0.0018	0.0000	-0.0004	0.0009	0.0000	-0.0028
	Z	0.0000	0.0000	0.0000	0.0000	-0.0020	0.0000
AT. 57 O	X	0.0007	0.0000	0.0002	0.0005	0.0000	-0.0001
	Y	-0.0018	0.0000	0.0004	-0.0009	0.0000	-0.0028
	Z	0.0000	0.0000	0.0000	0.0000	0.0020	0.0000
AT. 58 O	X	0.0007	0.0000	-0.0002	0.0005	0.0000	0.0001
	Y	-0.0018	0.0000	-0.0004	-0.0009	0.0000	0.0028
	Z	0.0000	0.0000	0.0000	0.0000	0.0020	0.0000

FREQ(CM**-1) 1121.72 1123.22 1143.29 1152.92 1165.73 1168.81

AT. 1 FE	X	0.0000	0.0001	0.0000	0.0002	0.0000	0.0004
	Y	0.0001	0.0000	0.0003	0.0000	0.0002	0.0000
	Z	0.0000	0.0000	-0.0003	0.0000	0.0004	0.0000
AT. 2 FE	X	0.0000	-0.0001	0.0000	0.0002	0.0000	0.0004
	Y	-0.0001	0.0000	0.0003	0.0000	0.0002	0.0000
	Z	0.0000	0.0000	0.0003	0.0000	-0.0004	0.0000
AT. 3 FE	X	0.0000	-0.0001	0.0000	0.0002	0.0000	0.0004
	Y	-0.0001	0.0000	0.0003	0.0000	0.0002	0.0000
	Z	0.0000	0.0000	-0.0003	0.0000	0.0004	0.0000
AT. 4 FE	X	0.0000	0.0001	0.0000	0.0002	0.0000	0.0004
	Y	0.0001	0.0000	0.0003	0.0000	0.0002	0.0000
	Z	0.0000	0.0000	0.0003	0.0000	-0.0004	0.0000
AT. 5 AL	X	0.0000	0.0000	0.0006	0.0016	0.0023	-0.0007
	Y	0.0000	0.0000	-0.0022	0.0018	0.0002	0.0031
	Z	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000
AT. 6 AL	X	0.0000	0.0000	-0.0006	0.0016	-0.0023	-0.0007
	Y	0.0000	0.0000	-0.0022	-0.0018	0.0002	-0.0031
	Z	0.0002	-0.0002	0.0000	0.0000	0.0000	0.0000
AT. 7 AL	X	0.0000	0.0000	0.0006	0.0016	0.0023	-0.0007
	Y	0.0000	0.0000	-0.0022	0.0018	0.0002	0.0031
	Z	-0.0002	-0.0002	0.0000	0.0000	0.0000	0.0000
AT. 8 AL	X	0.0000	0.0000	-0.0006	0.0016	-0.0023	-0.0007
	Y	0.0000	0.0000	-0.0022	-0.0018	0.0002	-0.0031
	Z	-0.0002	0.0002	0.0000	0.0000	0.0000	0.0000
AT. 9 AL	X	0.0060	-0.0062	0.0059	-0.0066	0.0042	-0.0014
	Y	-0.0019	0.0020	-0.0028	0.0019	0.0021	0.0011
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10 AL	X	-0.0060	0.0062	0.0059	-0.0066	0.0042	-0.0014
	Y	0.0019	-0.0020	-0.0028	0.0019	0.0021	0.0011
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11 AL	X	-0.0060	-0.0062	-0.0059	-0.0066	-0.0042	-0.0014

	Y	-0.0019	-0.0020	-0.0028	-0.0019	0.0021	-0.0011
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	0.0060	0.0062	-0.0059	-0.0066	-0.0042	-0.0014
	Y	0.0019	0.0020	-0.0028	-0.0019	0.0021	-0.0011
	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	-0.0022
	Y	0.0000	0.0000	0.0023	0.0000	-0.0015	0.0000
	Z	0.0022	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 14	SI X	0.0000	0.0000	0.0000	0.0037	0.0000	-0.0022
	Y	0.0000	0.0000	0.0023	0.0000	-0.0015	0.0000
	Z	-0.0022	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 15	SI X	0.0069	-0.0071	0.0074	-0.0062	-0.0028	-0.0007
	Y	-0.0098	0.0096	-0.0053	0.0102	-0.0061	-0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	-0.0069	0.0071	0.0074	-0.0062	-0.0028	-0.0007
	Y	0.0098	-0.0096	-0.0053	0.0102	-0.0061	-0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	-0.0069	-0.0071	-0.0074	-0.0062	0.0028	-0.0007
	Y	-0.0098	-0.0096	-0.0053	-0.0102	-0.0061	0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	0.0069	0.0071	-0.0074	-0.0062	0.0028	-0.0007
	Y	0.0098	0.0096	-0.0053	-0.0102	-0.0061	0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0084	0.0079	0.0052	-0.0048	0.0076	-0.0080
	Y	-0.0022	0.0027	0.0053	-0.0025	-0.0029	-0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0084	-0.0079	0.0052	-0.0048	0.0076	-0.0080
	Y	0.0022	-0.0027	0.0053	-0.0025	-0.0029	-0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0084	0.0079	-0.0052	-0.0048	-0.0076	-0.0080
	Y	-0.0022	-0.0027	0.0053	0.0025	-0.0029	0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	-0.0084	-0.0079	-0.0052	-0.0048	-0.0076	-0.0080
	Y	0.0022	0.0027	0.0053	0.0025	-0.0029	0.0077
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0000	-0.0001	-0.0023	-0.0014	0.0006	-0.0024
	Y	-0.0010	-0.0007	0.0022	0.0016	-0.0007	0.0029
	Z	-0.0006	-0.0004	0.0039	0.0018	-0.0009	0.0036
AT. 24	O X	0.0000	0.0001	-0.0023	-0.0014	0.0006	-0.0024
	Y	0.0010	0.0007	0.0022	0.0016	-0.0007	0.0029
	Z	-0.0006	-0.0004	-0.0039	-0.0018	0.0009	-0.0036
AT. 25	O X	0.0000	-0.0001	0.0023	-0.0014	-0.0006	-0.0024
	Y	-0.0010	0.0007	0.0022	-0.0016	-0.0007	-0.0029
	Z	-0.0006	0.0004	0.0039	-0.0018	-0.0009	-0.0036
AT. 26	O X	0.0000	0.0001	0.0023	-0.0014	-0.0006	-0.0024
	Y	0.0010	-0.0007	0.0022	-0.0016	-0.0007	-0.0029
	Z	-0.0006	0.0004	-0.0039	0.0018	0.0009	0.0036
AT. 27	O X	0.0000	0.0001	-0.0023	-0.0014	0.0006	-0.0024
	Y	0.0010	0.0007	0.0022	0.0016	-0.0007	0.0029
	Z	0.0006	0.0004	0.0039	0.0018	-0.0009	0.0036
AT. 28	O X	0.0000	-0.0001	-0.0023	-0.0014	0.0006	-0.0024
	Y	-0.0010	-0.0007	0.0022	0.0016	-0.0007	0.0029
	Z	0.0006	0.0004	-0.0039	-0.0018	0.0009	-0.0036
AT. 29	O X	0.0000	0.0001	0.0023	-0.0014	-0.0006	-0.0024

	Y	0.0010	-0.0007	0.0022	-0.0016	-0.0007	-0.0029
	Z	0.0006	-0.0004	0.0039	-0.0018	-0.0009	-0.0036
AT. 30	O X	0.0000	-0.0001	0.0023	-0.0014	-0.0006	-0.0024
	Y	-0.0010	0.0007	0.0022	-0.0016	-0.0007	-0.0029
	Z	0.0006	-0.0004	-0.0039	0.0018	0.0009	0.0036
AT. 31	O X	-0.0015	-0.0007	-0.0013	-0.0019	0.0002	0.0004
	Y	-0.0013	-0.0003	-0.0016	-0.0020	0.0010	0.0023
	Z	-0.0016	-0.0002	-0.0015	-0.0022	0.0013	0.0023
AT. 32	O X	0.0015	0.0007	-0.0013	-0.0019	0.0002	0.0004
	Y	0.0013	0.0003	-0.0016	-0.0020	0.0010	0.0023
	Z	-0.0016	-0.0002	0.0015	0.0022	-0.0013	-0.0023
AT. 33	O X	0.0015	-0.0007	0.0013	-0.0019	-0.0002	0.0004
	Y	-0.0013	0.0003	-0.0016	0.0020	0.0010	-0.0023
	Z	-0.0016	0.0002	-0.0015	0.0022	0.0013	-0.0023
AT. 34	O X	-0.0015	0.0007	0.0013	-0.0019	-0.0002	0.0004
	Y	0.0013	-0.0003	-0.0016	0.0020	0.0010	-0.0023
	Z	-0.0016	0.0002	0.0015	-0.0022	-0.0013	0.0023
AT. 35	O X	0.0015	0.0007	-0.0013	-0.0019	0.0002	0.0004
	Y	0.0013	0.0003	-0.0016	-0.0020	0.0010	0.0023
	Z	0.0016	0.0002	-0.0015	-0.0022	0.0013	0.0023
AT. 36	O X	-0.0015	-0.0007	-0.0013	-0.0019	0.0002	0.0004
	Y	-0.0013	-0.0003	-0.0016	-0.0020	0.0010	0.0023
	Z	0.0016	0.0002	0.0015	0.0022	-0.0013	-0.0023
AT. 37	O X	-0.0015	0.0007	0.0013	-0.0019	-0.0002	0.0004
	Y	0.0013	-0.0003	-0.0016	0.0020	0.0010	-0.0023
	Z	0.0016	-0.0002	-0.0015	0.0022	0.0013	-0.0023
AT. 38	O X	0.0015	-0.0007	0.0013	-0.0019	-0.0002	0.0004
	Y	-0.0013	0.0003	-0.0016	0.0020	0.0010	-0.0023
	Z	0.0016	-0.0002	0.0015	-0.0022	-0.0013	0.0023
AT. 39	O X	0.0006	-0.0005	-0.0012	-0.0025	-0.0026	0.0017
	Y	0.0008	0.0005	-0.0004	-0.0023	-0.0014	0.0007
	Z	0.0012	-0.0002	-0.0010	-0.0033	-0.0032	0.0027
AT. 40	O X	-0.0006	0.0005	-0.0012	-0.0025	-0.0026	0.0017
	Y	-0.0008	-0.0005	-0.0004	-0.0023	-0.0014	0.0007
	Z	0.0012	-0.0002	0.0010	0.0033	0.0032	-0.0027
AT. 41	O X	-0.0006	-0.0005	0.0012	-0.0025	0.0026	0.0017
	Y	0.0008	-0.0005	-0.0004	0.0023	-0.0014	-0.0007
	Z	0.0012	0.0002	-0.0010	0.0033	-0.0032	-0.0027
AT. 42	O X	0.0006	0.0005	0.0012	-0.0025	0.0026	0.0017
	Y	-0.0008	0.0005	-0.0004	0.0023	-0.0014	-0.0007
	Z	0.0012	0.0002	0.0010	-0.0033	0.0032	0.0027
AT. 43	O X	-0.0006	0.0005	-0.0012	-0.0025	-0.0026	0.0017
	Y	-0.0008	-0.0005	-0.0004	-0.0023	-0.0014	0.0007
	Z	-0.0012	0.0002	-0.0010	-0.0033	-0.0032	0.0027
AT. 44	O X	0.0006	-0.0005	-0.0012	-0.0025	-0.0026	0.0017
	Y	0.0008	0.0005	-0.0004	-0.0023	-0.0014	0.0007
	Z	-0.0012	0.0002	0.0010	0.0033	0.0032	-0.0027
AT. 45	O X	0.0006	0.0005	0.0012	-0.0025	0.0026	0.0017
	Y	-0.0008	0.0005	-0.0004	0.0023	-0.0014	-0.0007
	Z	-0.0012	-0.0002	-0.0010	0.0033	-0.0032	-0.0027
AT. 46	O X	-0.0006	-0.0005	0.0012	-0.0025	0.0026	0.0017
	Y	0.0008	-0.0005	-0.0004	0.0023	-0.0014	-0.0007
	Z	-0.0012	-0.0002	0.0010	-0.0033	0.0032	0.0027
AT. 47	O X	0.0179	-0.0182	-0.0118	0.0169	-0.0272	0.0106

	Y	0.0032	-0.0034	-0.0026	0.0040	-0.0055	0.0014
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48 O	X	-0.0179	0.0182	-0.0118	0.0169	-0.0272	0.0106
	Y	-0.0032	0.0034	-0.0026	0.0040	-0.0055	0.0014
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49 O	X	-0.0179	-0.0182	0.0118	0.0169	0.0272	0.0106
	Y	0.0032	0.0034	-0.0026	-0.0040	-0.0055	-0.0014
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50 O	X	0.0179	0.0182	0.0118	0.0169	0.0272	0.0106
	Y	-0.0032	-0.0034	-0.0026	-0.0040	-0.0055	-0.0014
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51 O	X	-0.0203	0.0204	-0.0218	0.0208	0.0024	-0.0002
	Y	0.0184	-0.0185	0.0209	-0.0196	-0.0021	-0.0012
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52 O	X	0.0203	-0.0204	-0.0218	0.0208	0.0024	-0.0002
	Y	-0.0184	0.0185	0.0209	-0.0196	-0.0021	-0.0012
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53 O	X	0.0203	0.0204	0.0218	0.0208	-0.0024	-0.0002
	Y	0.0184	0.0185	0.0209	0.0196	-0.0021	0.0012
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54 O	X	-0.0203	-0.0204	0.0218	0.0208	-0.0024	-0.0002
	Y	-0.0184	-0.0185	0.0209	0.0196	-0.0021	0.0012
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55 O	X	0.0034	-0.0035	-0.0037	-0.0021	0.0073	0.0096
	Y	0.0106	-0.0107	-0.0134	-0.0050	0.0221	0.0309
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56 O	X	-0.0034	0.0035	-0.0037	-0.0021	0.0073	0.0096
	Y	-0.0106	0.0107	-0.0134	-0.0050	0.0221	0.0309
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57 O	X	-0.0034	-0.0035	0.0037	-0.0021	-0.0073	0.0096
	Y	0.0106	0.0107	-0.0134	0.0050	0.0221	-0.0309
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58 O	X	0.0034	0.0035	0.0037	-0.0021	-0.0073	0.0096
	Y	-0.0106	-0.0107	-0.0134	0.0050	0.0221	-0.0309
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

FREQ(CM**-1) 1170.77 1177.49 1181.45 1186.39 1197.66 1203.05

AT. 1 FE	X	0.0000	0.0005	0.0000	0.0002	0.0006	0.0000
	Y	-0.0003	0.0000	-0.0004	0.0000	0.0000	-0.0008
	Z	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
AT. 2 FE	X	0.0000	-0.0005	0.0000	0.0002	-0.0006	0.0000
	Y	0.0003	0.0000	-0.0004	0.0000	0.0000	0.0008
	Z	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000
AT. 3 FE	X	0.0000	-0.0005	0.0000	0.0002	-0.0006	0.0000
	Y	0.0003	0.0000	-0.0004	0.0000	0.0000	0.0008
	Z	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
AT. 4 FE	X	0.0000	0.0005	0.0000	0.0002	0.0006	0.0000
	Y	-0.0003	0.0000	-0.0004	0.0000	0.0000	-0.0008
	Z	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000
AT. 5 AL	X	0.0000	0.0000	-0.0018	0.0023	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	-0.0022	0.0000	0.0000
	Z	0.0012	0.0034	0.0000	0.0000	-0.0007	-0.0010
AT. 6 AL	X	0.0000	0.0000	0.0018	0.0023	0.0000	0.0000

	Y	0.0000	0.0000	-0.0002	0.0022	0.0000	0.0000
	Z	0.0012	-0.0034	0.0000	0.0000	0.0007	-0.0010
AT. 7	AL X	0.0000	0.0000	-0.0018	0.0023	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	-0.0022	0.0000	0.0000
	Z	-0.0012	-0.0034	0.0000	0.0000	0.0007	0.0010
AT. 8	AL X	0.0000	0.0000	0.0018	0.0023	0.0000	0.0000
	Y	0.0000	0.0000	-0.0002	0.0022	0.0000	0.0000
	Z	-0.0012	0.0034	0.0000	0.0000	-0.0007	0.0010
AT. 9	AL X	-0.0025	-0.0044	0.0002	-0.0030	0.0013	-0.0039
	Y	0.0027	0.0014	0.0008	-0.0028	0.0030	-0.0015
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 10	AL X	0.0025	0.0044	0.0002	-0.0030	-0.0013	0.0039
	Y	-0.0027	-0.0014	0.0008	-0.0028	-0.0030	0.0015
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 11	AL X	0.0025	-0.0044	-0.0002	-0.0030	0.0013	0.0039
	Y	0.0027	-0.0014	0.0008	0.0028	-0.0030	-0.0015
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 12	AL X	-0.0025	0.0044	-0.0002	-0.0030	-0.0013	-0.0039
	Y	-0.0027	0.0014	0.0008	0.0028	0.0030	0.0015
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 13	SI X	0.0000	0.0000	0.0000	-0.0084	0.0000	0.0000
	Y	0.0000	0.0000	-0.0058	0.0000	0.0000	0.0000
	Z	-0.0042	0.0000	0.0000	0.0000	0.0000	0.0042
AT. 14	SI X	0.0000	0.0000	0.0000	-0.0084	0.0000	0.0000
	Y	0.0000	0.0000	-0.0058	0.0000	0.0000	0.0000
	Z	0.0042	0.0000	0.0000	0.0000	0.0000	-0.0042
AT. 15	SI X	-0.0064	-0.0045	-0.0042	0.0069	-0.0054	0.0005
	Y	-0.0022	-0.0069	0.0100	-0.0009	0.0060	-0.0094
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 16	SI X	0.0064	0.0045	-0.0042	0.0069	0.0054	-0.0005
	Y	0.0022	0.0069	0.0100	-0.0009	-0.0060	0.0094
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 17	SI X	0.0064	-0.0045	0.0042	0.0069	-0.0054	-0.0005
	Y	-0.0022	0.0069	0.0100	0.0009	-0.0060	-0.0094
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 18	SI X	-0.0064	0.0045	0.0042	0.0069	0.0054	0.0005
	Y	0.0022	-0.0069	0.0100	0.0009	0.0060	0.0094
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 19	SI X	-0.0076	-0.0019	0.0100	-0.0089	-0.0127	0.0091
	Y	-0.0067	-0.0061	0.0047	0.0024	-0.0015	-0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 20	SI X	0.0076	0.0019	0.0100	-0.0089	0.0127	-0.0091
	Y	0.0067	0.0061	0.0047	0.0024	0.0015	0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 21	SI X	0.0076	-0.0019	-0.0100	-0.0089	-0.0127	-0.0091
	Y	-0.0067	0.0061	0.0047	-0.0024	0.0015	-0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 22	SI X	-0.0076	0.0019	-0.0100	-0.0089	0.0127	0.0091
	Y	0.0067	-0.0061	0.0047	-0.0024	-0.0015	0.0024
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 23	O X	0.0018	-0.0017	-0.0018	-0.0014	-0.0002	0.0000
	Y	-0.0008	0.0013	0.0010	-0.0013	-0.0002	0.0014
	Z	-0.0027	0.0030	0.0018	0.0002	-0.0006	0.0006
AT. 24	O X	-0.0018	0.0017	-0.0018	-0.0014	0.0002	0.0000

	Y	0.0008	-0.0013	0.0010	-0.0013	0.0002	-0.0014
	Z	-0.0027	0.0030	-0.0018	-0.0002	-0.0006	0.0006
AT. 25	O X	-0.0018	-0.0017	0.0018	-0.0014	-0.0002	0.0000
	Y	-0.0008	-0.0013	0.0010	0.0013	0.0002	0.0014
	Z	-0.0027	-0.0030	0.0018	-0.0002	0.0006	0.0006
AT. 26	O X	0.0018	0.0017	0.0018	-0.0014	0.0002	0.0000
	Y	0.0008	0.0013	0.0010	0.0013	-0.0002	-0.0014
	Z	-0.0027	-0.0030	-0.0018	0.0002	0.0006	0.0006
AT. 27	O X	-0.0018	0.0017	-0.0018	-0.0014	0.0002	0.0000
	Y	0.0008	-0.0013	0.0010	-0.0013	0.0002	-0.0014
	Z	0.0027	-0.0030	0.0018	0.0002	0.0006	-0.0006
AT. 28	O X	0.0018	-0.0017	-0.0018	-0.0014	-0.0002	0.0000
	Y	-0.0008	0.0013	0.0010	-0.0013	-0.0002	0.0014
	Z	0.0027	-0.0030	-0.0018	-0.0002	0.0006	-0.0006
AT. 29	O X	0.0018	0.0017	0.0018	-0.0014	0.0002	0.0000
	Y	0.0008	0.0013	0.0010	0.0013	-0.0002	-0.0014
	Z	0.0027	0.0030	0.0018	-0.0002	-0.0006	-0.0006
AT. 30	O X	-0.0018	-0.0017	0.0018	-0.0014	-0.0002	0.0000
	Y	-0.0008	-0.0013	0.0010	0.0013	0.0002	0.0014
	Z	0.0027	0.0030	-0.0018	0.0002	-0.0006	-0.0006
AT. 31	O X	0.0006	0.0010	0.0014	0.0037	0.0003	-0.0012
	Y	0.0019	0.0005	0.0045	0.0037	-0.0017	-0.0026
	Z	0.0029	0.0004	0.0038	0.0041	-0.0018	-0.0030
AT. 32	O X	-0.0006	-0.0010	0.0014	0.0037	-0.0003	0.0012
	Y	-0.0019	-0.0005	0.0045	0.0037	0.0017	0.0026
	Z	0.0029	0.0004	-0.0038	-0.0041	-0.0018	-0.0030
AT. 33	O X	-0.0006	0.0010	-0.0014	0.0037	0.0003	0.0012
	Y	0.0019	-0.0005	0.0045	-0.0037	0.0017	-0.0026
	Z	0.0029	-0.0004	0.0038	-0.0041	0.0018	-0.0030
AT. 34	O X	0.0006	-0.0010	-0.0014	0.0037	-0.0003	-0.0012
	Y	-0.0019	0.0005	0.0045	-0.0037	-0.0017	0.0026
	Z	0.0029	-0.0004	-0.0038	0.0041	0.0018	-0.0030
AT. 35	O X	-0.0006	-0.0010	0.0014	0.0037	-0.0003	0.0012
	Y	-0.0019	-0.0005	0.0045	0.0037	0.0017	0.0026
	Z	-0.0029	-0.0004	0.0038	0.0041	0.0018	0.0030
AT. 36	O X	0.0006	0.0010	0.0014	0.0037	0.0003	-0.0012
	Y	0.0019	0.0005	0.0045	0.0037	-0.0017	-0.0026
	Z	-0.0029	-0.0004	-0.0038	-0.0041	0.0018	0.0030
AT. 37	O X	0.0006	-0.0010	-0.0014	0.0037	-0.0003	-0.0012
	Y	-0.0019	0.0005	0.0045	-0.0037	-0.0017	0.0026
	Z	-0.0029	0.0004	0.0038	-0.0041	-0.0018	0.0030
AT. 38	O X	-0.0006	0.0010	-0.0014	0.0037	0.0003	0.0012
	Y	0.0019	-0.0005	0.0045	-0.0037	0.0017	-0.0026
	Z	-0.0029	0.0004	-0.0038	0.0041	-0.0018	0.0030
AT. 39	O X	0.0008	-0.0027	0.0023	-0.0016	-0.0018	-0.0001
	Y	0.0013	-0.0019	0.0014	0.0008	0.0002	0.0014
	Z	0.0013	-0.0044	0.0026	-0.0008	-0.0009	0.0009
AT. 40	O X	-0.0008	0.0027	0.0023	-0.0016	0.0018	0.0001
	Y	-0.0013	0.0019	0.0014	0.0008	-0.0002	-0.0014
	Z	0.0013	-0.0044	-0.0026	0.0008	-0.0009	0.0009
AT. 41	O X	-0.0008	-0.0027	-0.0023	-0.0016	-0.0018	0.0001
	Y	0.0013	0.0019	0.0014	-0.0008	-0.0002	0.0014
	Z	0.0013	0.0044	0.0026	0.0008	0.0009	0.0009
AT. 42	O X	0.0008	0.0027	-0.0023	-0.0016	0.0018	-0.0001

	Y	-0.0013	-0.0019	0.0014	-0.0008	0.0002	-0.0014
	Z	0.0013	0.0044	-0.0026	-0.0008	0.0009	0.0009
AT. 43	O X	-0.0008	0.0027	0.0023	-0.0016	0.0018	0.0001
	Y	-0.0013	0.0019	0.0014	0.0008	-0.0002	-0.0014
	Z	-0.0013	0.0044	0.0026	-0.0008	0.0009	-0.0009
AT. 44	O X	0.0008	-0.0027	0.0023	-0.0016	-0.0018	-0.0001
	Y	0.0013	-0.0019	0.0014	0.0008	0.0002	0.0014
	Z	-0.0013	0.0044	-0.0026	0.0008	0.0009	-0.0009
AT. 45	O X	0.0008	0.0027	-0.0023	-0.0016	0.0018	-0.0001
	Y	-0.0013	-0.0019	0.0014	-0.0008	0.0002	-0.0014
	Z	-0.0013	-0.0044	0.0026	0.0008	-0.0009	-0.0009
AT. 46	O X	-0.0008	-0.0027	-0.0023	-0.0016	-0.0018	0.0001
	Y	0.0013	0.0019	0.0014	-0.0008	-0.0002	0.0014
	Z	-0.0013	-0.0044	-0.0026	-0.0008	-0.0009	-0.0009
AT. 47	O X	0.0103	-0.0069	-0.0166	0.0264	0.0274	-0.0260
	Y	0.0015	-0.0017	-0.0023	0.0047	0.0050	-0.0051
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 48	O X	-0.0103	0.0069	-0.0166	0.0264	-0.0274	0.0260
	Y	-0.0015	0.0017	-0.0023	0.0047	-0.0050	0.0051
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 49	O X	-0.0103	-0.0069	0.0166	0.0264	0.0274	0.0260
	Y	0.0015	0.0017	-0.0023	-0.0047	-0.0050	-0.0051
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 50	O X	0.0103	0.0069	0.0166	0.0264	-0.0274	-0.0260
	Y	-0.0015	-0.0017	-0.0023	-0.0047	0.0050	0.0051
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 51	O X	0.0148	0.0083	0.0120	-0.0121	0.0140	-0.0061
	Y	-0.0134	-0.0073	-0.0100	0.0110	-0.0124	0.0056
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 52	O X	-0.0148	-0.0083	0.0120	-0.0121	-0.0140	0.0061
	Y	0.0134	0.0073	-0.0100	0.0110	0.0124	-0.0056
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 53	O X	-0.0148	0.0083	-0.0120	-0.0121	0.0140	0.0061
	Y	-0.0134	0.0073	-0.0100	-0.0110	0.0124	0.0056
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 54	O X	0.0148	-0.0083	-0.0120	-0.0121	-0.0140	-0.0061
	Y	0.0134	-0.0073	-0.0100	-0.0110	-0.0124	-0.0056
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 55	O X	0.0082	0.0099	-0.0066	-0.0042	0.0001	0.0054
	Y	0.0260	0.0315	-0.0213	-0.0118	-0.0014	0.0190
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 56	O X	-0.0082	-0.0099	-0.0066	-0.0042	-0.0001	-0.0054
	Y	-0.0260	-0.0315	-0.0213	-0.0118	0.0014	-0.0190
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 57	O X	-0.0082	0.0099	0.0066	-0.0042	0.0001	-0.0054
	Y	0.0260	-0.0315	-0.0213	0.0118	0.0014	0.0190
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AT. 58	O X	0.0082	-0.0099	0.0066	-0.0042	-0.0001	0.0054
	Y	-0.0260	0.0315	-0.0213	0.0118	-0.0014	-0.0190
	Z	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

VIBRATIONAL TEMPERATURES (K) [MODE NUMBER;IRREP]

TO MODES

101.4 [4;AG]	149.1 [5;B3G]	151.6 [6;B2G]	170.0 [7;B3G]
170.6 [8;B1U]	176.6 [9;AU]	191.5 [10;B1G]	192.6 [11;B3G]
195.0 [12;B2G]	195.7 [13;B3U]	207.2 [14;B3U]	207.7 [15;B1G]
220.2 [16;B1U]	221.2 [17;B2G]	227.6 [18;B3G]	233.8 [19;B3G]
237.8 [20;B2U]	238.4 [21;B3U]	239.8 [22;AG]	246.6 [23;B2U]
247.6 [24;B3U]	248.0 [25;B1G]	268.4 [26;B2U]	271.6 [27;B1U]
280.3 [28;AU]	281.5 [29;B1U]	290.1 [30;B2G]	291.2 [31;B3U]
297.0 [32;B3G]	300.1 [33;B2G]	305.0 [34;B1G]	307.3 [35;AU]
307.8 [36;B2G]	311.1 [37;B1U]	325.6 [38;B1G]	329.9 [39;AG]
334.7 [40;AU]	338.0 [41;B1U]	344.2 [42;B3G]	355.0 [43;AU]
357.3 [44;B3G]	368.1 [45;B1U]	371.5 [46;B2G]	371.7 [47;B1G]
372.9 [48;B2U]	382.6 [49;AG]	389.3 [50;AU]	389.7 [51;B3U]
395.4 [52;B2U]	399.7 [53;B3G]	419.1 [54;B3U]	420.0 [55;B1G]
426.0 [56;AG]	428.9 [57;B2G]	429.1 [58;B1G]	430.3 [59;AU]
436.5 [60;B2U]	441.0 [61;AG]	450.7 [62;B1G]	455.2 [63;B2U]
456.8 [64;B3G]	475.5 [65;B2G]	476.4 [66;B1U]	483.3 [67;AG]
487.3 [68;B3G]	491.5 [69;B3U]	494.8 [70;AG]	496.7 [71;B2U]
497.7 [72;B2G]	506.1 [73;B1G]	515.1 [74;B3U]	541.3 [75;AU]
542.4 [76;B2U]	542.6 [77;B3U]	545.0 [78;B1U]	548.6 [79;AG]
580.2 [80;B2G]	588.0 [81;B2U]	600.8 [82;B2U]	614.1 [83;B1G]
615.7 [84;B3U]	627.6 [85;B3U]	628.1 [86;AG]	664.1 [87;AU]
665.7 [88;B2U]	667.7 [89;B1G]	681.1 [90;B3G]	685.5 [91;B2G]
690.4 [92;AU]	703.1 [93;B3G]	705.0 [94;B1U]	707.4 [95;B3U]
711.2 [96;AG]	717.0 [97;B1G]	720.8 [98;B1U]	722.3 [99;B3G]
728.8 [100;B1U]	731.2 [101;B3U]	738.2 [102;B2G]	774.2 [103;B2U]
797.5 [104;AU]	811.4 [105;B1G]	815.5 [106;AG]	823.7 [107;B2U]
837.0 [108;B1G]	838.5 [109;B3U]	842.2 [110;AU]	844.4 [111;B1U]
858.0 [112;B3U]	864.7 [113;B1G]	868.1 [114;AG]	873.8 [115;B1U]
885.2 [116;B3G]	909.3 [117;AU]	911.1 [118;AG]	958.7 [119;B3G]
961.1 [120;B3U]	971.2 [121;AG]	984.1 [122;B2G]	997.6 [123;B2U]
1007.1 [124;B1G]	1009.9 [125;AU]	1014.1 [126;B1U]	1019.3 [127;B2U]
1028.5 [128;AG]	1054.1 [129;B1G]	1070.3 [130;B3G]	1070.7 [131;AG]
1080.7 [132;B2G]	1086.9 [133;B3U]	1088.2 [134;B1G]	1099.4 [135;B2U]
1105.8 [136;B3U]	1168.6 [137;B2G]	1228.4 [138;B2U]	1299.5 [139;B3G]
1306.6 [140;B2G]	1311.2 [141;B1U]	1312.4 [142;AU]	1339.5 [143;B3U]
1344.7 [144;B3G]	1349.9 [145;AG]	1382.1 [146;B1U]	1399.6 [147;B3G]
1400.5 [148;B2U]	1406.7 [149;B1G]	1414.2 [150;B3U]	1414.9 [151;B2G]
1418.6 [152;B1G]	1425.7 [153;B2U]	1429.7 [154;AG]	1431.8 [155;AU]
1454.8 [156;B1U]	1462.3 [157;B3U]	1469.4 [158;B2G]	1498.4 [159;B1G]
1512.9 [160;B2U]	1528.2 [161;AU]	1528.9 [162;AG]	1613.9 [163;B1G]
1616.1 [164;AG]	1644.9 [165;B3U]	1658.8 [166;B2U]	1677.2 [167;B3U]
1681.7 [168;B2U]	1684.5 [169;B1G]	1694.1 [170;AG]	1699.8 [171;B3U]
1706.9 [172;B2U]	1723.2 [173;AG]	1730.9 [174;B1G]	

HARMONIC VIBRATIONAL CONTRIBUTIONS TO THERMODYNAMIC FUNCTIONS AT GIVEN TEMPERATURE AND PRESSURE:

(EL = ELECTRONIC ENERGY

E0 = ZERO-POINT ENERGY

ET = THERMAL CONTRIBUTION TO THE VIBRATIONAL ENERGY

PV = PRESSURE * VOLUME
TS = TEMPERATURE * ENTROPY)

	AU/CELL	EV/CELL	KJ/MOL
EL	: -12600.775964630000	-342884.545911051740	-33083332.63284896
E0	: 0.206274826175	5.613023380822	541.57447980

THERMODYNAMIC FUNCTIONS WITH VIBRATIONAL CONTRIBUTIONS

AT (T = 298.15 K, P = 0.10132500E+00 MPA):

	AU/CELL	EV/CELL	KJ/MOL
ET :	0.050517185349	1.374642498833	132.63285144
PV :	0.000018793753	0.000511404014	0.04934299
TS :	0.085972170676	2.339421697995	225.71990230
ET+PV-TS :	-0.035436191574	-0.964267795148	-93.03770787
EL+E0+ET+PV-TS:	-12600.605125995398	-342879.897155466082	-33082884.09607702

OTHER THERMODYNAMIC FUNCTIONS:

	mHARTREE/(CELL*K)	mEV/(CELL*K)	J/(MOL*K)
ENTROPY :	0.288352073372	7.846458822723	757.06826195
HEAT CAPACITY :	0.333342712058	9.070716341412	875.19116717

```

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT END      TELAPSE 1736820.00 TCPU 1729001.88
EEEEEEEEEE TERMINATION  DATE 16 03 2010 TIME 10:54:37.3
Tue Mar 16 10:54:37 CET 2010
total 1575140

```

```
-rw-r--r-- 1 dtoebbens dtoebbens      0 Feb 24 08:27 ERROR
-rw-r--r-- 1 dtoebbens dtoebbens 7882378 Mar 16 10:54 FREQINFO.DAT
lrwxrwxrwx 1 dtoebbens dtoebbens      62 Feb 24 08:27 OPTHESS.DAT ->
/home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.opthess
lrwxrwxrwx 1 dtoebbens dtoebbens      62 Feb 24 08:27 OPTINFO.DAT ->
/home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP.optinfo
-rw-r--r-- 1 dtoebbens dtoebbens 552809 Mar 16 10:54 SCFOUT.LOG
-rw-r--r-- 1 dtoebbens dtoebbens 30992 Mar 16 10:54 fort.10
-rw-r--r-- 1 dtoebbens dtoebbens 39670456 Mar 16 01:34 fort.11
-rw-r--r-- 1 dtoebbens dtoebbens 89852 Mar 15 18:08 fort.12
-rw-r--r-- 1 dtoebbens dtoebbens 39532040 Feb 24 11:46 fort.13
-rw-r--r-- 1 dtoebbens dtoebbens 12552 Mar 16 10:54 fort.19
lrwxrwxrwx 1 dtoebbens dtoebbens      57 Feb 24 08:27 fort.20 -> /home/dtoebbens/CRYSTAL/test_cases/Fe-
Cordierite-B3LYP.f9
lrwxrwxrwx 1 dtoebbens dtoebbens      58 Feb 24 08:27 fort.34 -> /home/dtoebbens/CRYSTAL/test_cases/Fe-
Cordierite-B3LYP.gui
-rw-r--r-- 1 dtoebbens dtoebbens 39670416 Mar 16 01:34 fort.71
-rw-r--r-- 1 dtoebbens dtoebbens 39670416 Mar 16 01:34 fort.72
-rw-r--r-- 1 dtoebbens dtoebbens 1396965952 Mar 16 01:54 fort.8
-rw-r--r-- 1 dtoebbens dtoebbens 7444916 Feb 24 11:46 fort.9
-rw-r--r-- 1 dtoebbens dtoebbens 19910824 Mar 16 00:18 fort.95
-rw-r--r-- 1 dtoebbens dtoebbens 19835208 Mar 15 18:08 fort.96
```

wave function binary file /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.f9
Tue Mar 16 10:54:37 CET 2010
file SCFOUT.LOG saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.SCFLOG
file fort.20 saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.f20
geometry input file fort.34 saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.gui
file OPTHESS.DAT saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.opthess
file OPTINFO.DAT saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.optinfo
file FREQINFO.DAT saved as /home/dtoebbens/CRYSTAL/test_cases/Fe-Cordierite-B3LYP-FREQ.freqinfo
/home/dtoebbens/sr/tmp25028 removed