date Sun May 15 15:12:55 CEST 2011
master hostname n025.leo1
master system Linux n025.leo1 2.6.18-194.17.4.el5 #1 SMP Mon Oct 25 15:50:53 EDT 2010 x86_64 x86_64 x86_64 GNU/Linux
user c71460
output data in /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.out
mpirun executable in /usr/site/hpc/x86_64/glibc-2.5/italy/openmpi/1.3.3/intel-11.0/bin
Pcrystal executable in /usr/site/hpc/x86_64/glibc-2.5/italy/crystal/09/intel-11.0/bin/Linux-ifort-11.1_amd64/v1_0_1
input data in /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/tmp_p635_c71460/Kilchoanite-FREQ.d12
creating temporary directories /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/tmp_p635_c71460
copying input file to file INPUT
CRYSTAL data /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/tmp_p635_c71460/Kilchoanite-FREQ.f9 not found or empty
Kilchoanite Ca6Si4O14, PBE(n=6) optimized
CRYSTAL
1 0 0
 I 2 c m
   11.51157168   5.11889300   22.14018122
15
 20   0.01341400807606 0.00000000000000 0.00000000000000
 20   -0.18988564754360 0.49932888173250 -0.25000000000000
 20   0.03436291191189 0.00264016275672 0.16869678919570
 20   0.24164783639260 0.49581582745780 0.10443527971780
 14   0.12054386308280 0.42745058464320 0.25000000000000
 14   0.43243645957090 -0.05850746031668 0.10096369227420
 14   0.26626629474170 0.00000000000000 0.00000000000000
  8   0.18699756077950 0.29541675787570 0.19138789504950
  8   -0.01049268744451 0.29098828265610 0.25000000000000
  8   0.12106639939790 -0.25282524125600 0.25000000000000
  8   0.36991849441090 -0.20053804553820 0.15892549753910
  8   0.05951388770774 -0.30639179656580 0.09282489935314
  8   0.35598442766570 -0.18748314609190 0.04132384675531
  8   0.42753560979460 0.25735035238450 0.09697871540298
  8   0.18477669661110 0.17955547865860 0.04132421742051
FREQCALC
RESTART
ANALYSIS
ENDFREQ
END
20 7   ! Ca(2+) 86-511G(21), optimized in Ca6Si4O14 with PBE(n=6)
0 0 8 2.0 1.0
  191300.0   0.0002204
  26970.0   0.001925
   5696.0   0.01109
   1489.4   0.04995
    448.3   0.17014
    154.62   0.3685
     60.37   0.4034
     25.09   0.1452
0 1 6 8.0 1.0
    448.6   -0.00575 0.00847
    105.7   -0.0767   0.06027
     34.69   -0.1122   0.2124

```
   13.50    0.2537   0.3771
    5.820    0.688    0.401
    1.819    0.349    0.198
 0 1 5 8.0 1.0
   20.75    -0.0020  -0.0365
    8.40    -0.1255  -0.0685
    3.597   -0.6960   0.1570
    1.408    1.029    1.482
    0.726    0.944    1.025
 0 1 1 0.0 1.0
    0.463    1.0000   1.0000
 0 1 1 0.0 1.0
    0.279    1.0000   1.0000
 0 3 2 0.0 1.0
    3.922    0.139
    1.095    0.326
 0 3 1 0.0 1.0
    0.343    0.427
 14  6        ! Si(4+) 86-311G(1), optimized in Ca6Si4O14 with PBE(n=6)
 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 0.0 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
    0.333    1.0000     1.0000
 0 1 1 0.0 1.0
    0.13     1.0000     1.0000
 0 3 1 0.0 1.0
    0.682    1.0000
 8  5        ! O(2-) 84-11G(1), optimized in Ca6Si4O14 with PBE(n=6)
 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  8.0  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
   0.460    1.0000     1.0000
 0 1 1  0.0  1.0
   0.170    1.0000     1.0000
 0 3 1  0.0  1.0
   0.556    1.0000
99 0
ENDBASIS
DFT
XLGRID
EXCHANGE
PBE
CORRELAT
PBE
HYBRID
16.667
ENDDFT
SCFDIR
SHRINK
4 4
TOLINTEG
7 7 7 7 15
TOLDEE
10
FMIXING
80
BROYDEN
0.0001 50 2
MAXCYCLE
200
BIPOSIZE
6818200
EXCHSIZE
6992232
ENDRUN
END Sun May 15 15:12:55 CEST 2011
/bin/bash: module: line 1: syntax error: unexpected end of file
/bin/bash: error importing function definition for `module'
 PROCESS         9 OF        16 WORKING
 PROCESS        13 OF        16 WORKING
 PROCESS        12 OF        16 WORKING
 PROCESS         3 OF        16 WORKING
 PROCESS        15 OF        16 WORKING
 PROCESS         0 OF        16 WORKING
 PROCESS         2 OF        16 WORKING
 PROCESS         6 OF        16 WORKING
 PROCESS         1 OF        16 WORKING
 PROCESS         4 OF        16 WORKING
```

```
*******************************************************************************
*                                              *
*                CRYSTAL09                     *
*                public : 1.0                  *
*          March 5th, 2010 - parallel executable        *
*                                              *
*                                              *
*                                              *
*                MAIN AUTHORS                   *
*                                              *
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*******************************************************************************
```

EEEEEEEEEE STARTING DATE 15 05 2011 TIME 15:12:56.9
Kilchoanite Ca6Si4O14, PBE(n=6) optimized

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

SPACE GROUP (NONCENTROSYMMETRIC)   : I 2 C M

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - CONVENTIONAL CELL
    A   B   C   ALPHA   BETA   GAMMA
  11.51157   5.11889   22.14018   90.00000   90.00000   90.00000

NUMBER OF IRREDUCIBLE ATOMS IN THE CONVENTIONAL CELL: 15

INPUT COORDINATES

ATOM AT. N.   COORDINATES

```
 1  20   1.341400807606E-02  0.000000000000E+00  0.000000000000E+00
 2  20  -1.898856475436E-01  4.993288817325E-01 -2.500000000000E-01
 3  20   3.436291191189E-02  2.640162756720E-03  1.686967891957E-01
 4  20   2.416478363926E-01  4.958158274578E-01  1.044352797178E-01
 5  14   1.205438630828E-01  4.274505846432E-01  2.500000000000E-01
 6  14   4.324364595709E-01 -5.850746031668E-02  1.009636922742E-01
 7  14   2.662662947417E-01  0.000000000000E+00  0.000000000000E+00
 8   8   1.869975607795E-01  2.954167578757E-01  1.913878950495E-01
 9   8  -1.049268744451E-02  2.909882826561E-01  2.500000000000E-01
10   8   1.210663993979E-01 -2.528252412560E-01  2.500000000000E-01
11   8   3.699184944109E-01 -2.005380455382E-01  1.589254975391E-01
12   8   5.951388770774E-02 -3.063917965658E-01  9.282489935314E-02
13   8   3.559844276657E-01 -1.874831460919E-01  4.132384675531E-02
14   8   4.275356097946E-01  2.573503523845E-01  9.697871540298E-02
15   8   1.847766966111E-01  1.795554786586E-01  4. PROCESS        5  OF        16  WORKING
```

132421742051E-02

****

<< 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
12.73683	12.73683	12.73683	126.26856	156.81514	59.28219	652.321735

COORDINATES OF THE EQUIVALENT ATOMS (FRACTIONAL UNITS)

N.	ATOM	EQUIV	AT. N.		X	Y	Z
1	1	1	20	CA	0.00000000000E+00	1.34140080761E-02	1.34140080761E-02
2	1	2	20	CA	-5.00000000000E-01	-4.86585991924E-01	1.34140080761E-02
3	2	1	20	CA	2.49328881733E-01	-4.39885647544E-01	3.09443234189E-01
4	2	2	20	CA	-2.49328881733E-01	6.01143524564E-02	3.10785470724E-01
5	3	1	20	CA	1.71336951952E-01	2.03059701108E-01	3.70030746686E-02
6	3	2	20	CA	-1.71336951952E-01	-1.34333877284E-01	3.17227491552E-02
7	3	3	20	CA	-3.33943373561E-01	-2.96940298892E-01	3.17227491552E-02
8	3	4	20	CA	3.33943373561E-01	3.65666122716E-01	3.70030746686E-02
9	4	1	20	CA	-3.99748892824E-01	3.46083116110E-01	-2.62536336150E-01
10	4	2	20	CA	3.99748892824E-01	1.37212556675E-01	-2.54167991065E-01
11	4	3	20	CA	1.08619452260E-01	-1.53916883890E-01	-2.54167991065E-01
12	4	4	20	CA	-1.08619452260E-01	-3.62787443325E-01	-2.62536336150E-01
13	5	1	14	SI	-3.22549415357E-01	3.70543863083E-01	-4.52005552274E-01
14	5	2	14	SI	3.22549415357E-01	-1.29456136917E-01	-3.06906721560E-01
15	6	1	14	SI	4.24562319575E-02	-4.66599848155E-01	3.73928999254E-01
16	6	2	14	SI	-4.24562319575E-02	3.31472767297E-01	4.90943919888E-01
17	6	3	14	SI	-3.40528847409E-01	3.34001518451E-02	4.90943919888E-01

18	6	4	14 SI	3.40528847409E-01	-1.68527232703E-01	3.73928999254E-01
19	7	1	14 SI	0.00000000000E+00	2.66266294742E-01	2.66266294742E-01
20	7	2	14 SI	-5.00000000000E-01	-2.33733705258E-01	2.66266294742E-01
21	8	1	8 O	4.86804652925E-01	3.78385455829E-01	4.82414318655E-01
22	8	2	8 O	-4.86804652925E-01	-4.39033427000E-03	-1.08419197096E-01
23	8	3	8 O	3.95971137174E-01	-1.21614544171E-01	-1.08419197096E-01
24	8	4	8 O	-3.95971137174E-01	4.95609665730E-01	4.82414318655E-01
25	9	1	8 O	-4.59011717344E-01	2.39507312555E-01	2.80495595212E-01
26	9	2	8 O	4.59011717344E-01	-2.60492687445E-01	-3.01480970101E-01
27	10	1	8 O	-2.82524125600E-03	3.71066399398E-01	-1.31758841858E-01
28	10	2	8 O	2.82524125600E-03	-1.28933600602E-01	3.73891640654E-01
29	11	1	8 O	-4.16125479991E-02	-4.71156008050E-01	1.69380448873E-01
30	11	2	8 O	4.16125479991E-02	2.10992996872E-01	-4.29543460051E-01
31	11	3	8 O	-1.40536456923E-01	2.88439919500E-02	-4.29543460051E-01
32	11	4	8 O	1.40536456923E-01	-2.89007003128E-01	1.69380448873E-01
33	12	1	8 O	-2.13566897213E-01	1.52338787061E-01	-2.46877908858E-01
34	12	2	8 O	2.13566897213E-01	-3.33110116454E-02	3.65905684274E-01
35	12	3	8 O	-1.00783304081E-01	-3.47661212939E-01	3.65905684274E-01
36	12	4	8 O	1.00783304081E-01	4.66688988355E-01	-2.46877908858E-01
37	13	1	8 O	-1.46159299337E-01	3.97308274421E-01	1.68501281574E-01
38	13	2	8 O	1.46159299337E-01	3.14660580910E-01	-4.56532426242E-01
39	13	3	8 O	-2.71193007153E-01	-1.02691725579E-01	-4.56532426242E-01
40	13	4	8 O	2.71193007153E-01	-1.85339419090E-01	1.68501281574E-01
41	14	1	8 O	3.54329067787E-01	-4.75485674802E-01	-3.15114037821E-01
42	14	2	8 O	-3.54329067787E-01	3.30556894392E-01	1.70185257410E-01
43	14	3	8 O	3.39628363018E-01	2.45143251976E-02	1.70185257410E-01
44	14	4	8 O	-3.39628363018E-01	-1.69443105608E-01	-3.15114037821E-01
45	15	1	8 O	2.20879696079E-01	2.26100914032E-01	3.64332175270E-01
46	15	2	8 O	-2.20879696079E-01	1.43452479191E-01	5.22121795250E-03
47	15	3	8 O	3.61768738762E-01	-2.73899085968E-01	5.22121795250E-03
48	15	4	8 O	-3.61768738762E-01	-3.56547520809E-01	3.64332175270E-01

NUMBER OF SYMMETRY OPERATORS   :   4

****

* GEOMETRY EDITING - INPUT COORDINATES ARE GIVEN IN ANGSTROM

****

GEOMETRY NOW FULLY CONSISTENT WITH THE GROUP

FRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFRQFR
QFRQ

            FREQUENCY CALCULATION

INFORMATION **** INPFREQ **** FREQUENCY CALCULATION RESTART(DATA FROM

FREQINFO.DAT)
INFORMATION **** INPFREQ **** ANALYSIS OF THE VIBRATIONAL MODES

GCALCO - MAX INDICES DIRECT LATTICE VECTOR   18   9   19
NO.OF VECTORS CREATED 6999 STARS 1041 RMAX   197.35268 BOHR

GEOMETRY FOR WAVE FUNCTION - DIMENSIONALITY OF THE SYSTEM   3
(NON PERIODIC DIRECTION: LATTICE PARAMETER FORMALLY SET TO 500)
****
LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 6/0 VOLUME=   652.321735 - DENSITY 2.931 g/cm^3
     A   B   C   ALPHA   BETA   GAMMA
  12.73682626   12.73682626   12.73682626   126.268555 156.815136 59.282191
****
ATOMS IN THE ASYMMETRIC UNIT   15 - ATOMS IN THE UNIT CELL: 48
    ATOM   X/A   Y/B   Z/C
****
  1 T 20 CA   0.000000000000E+00 1.341400807606E-02 1.341400807606E-02
  2 F 20 CA   5.000000000000E-01 -4.865859919239E-01 1.341400807606E-02
  3 T 20 CA   2.493288817325E-01 -4.398856475436E-01 3.094432341889E-01
  4 F 20 CA   -2.493288817325E-01 6.011435245640E-02 3.107854707239E-01
  5 T 20 CA   1.713369519524E-01 2.030597011076E-01 3.700307466861E-02
  6 F 20 CA   -1.713369519524E-01 -1.343338772838E-01 3.172274915517E-02
  7 F 20 CA   -3.339433735610E-01 -2.969402988924E-01 3.172274915517E-02
  8 F 20 CA   3.339433735610E-01 3.656661227162E-01 3.700307466861E-02
  9 T 20 CA   -3.997488928244E-01 3.460831161104E-01 -2.625363361496E-01
 10 F 20 CA   3.997488928244E-01 1.372125566748E-01 -2.541679910652E-01
 11 F 20 CA   1.086194522600E-01 -1.539168838896E-01 -2.541679910652E-01
 12 F 20 CA   -1.086194522600E-01 -3.627874433252E-01 -2.625363361496E-01
 13 T 14 SI -3.225494153568E-01 3.705438630828E-01 -4.520055522740E-01
 14 F 14 SI   3.225494153568E-01 -1.294561369172E-01 -3.069067215604E-01
 15 T 14 SI   4.245623195752E-02 -4.665998481549E-01 3.739289992542E-01
 16 F 14 SI -4.245623195752E-02 3.314727672967E-01 4.909439198876E-01
 17 F 14 SI -3.405288474091E-01 3.340015184510E-02 4.909439198876E-01
 18 F 14 SI   3.405288474091E-01 -1.685272327033E-01 3.739289992542E-01
 19 T 14 SI   0.000000000000E+00 2.662662947417E-01 2.662662947417E-01
 20 F 14 SI   5.000000000000E-01 -2.337337052583E-01 2.662662947417E-01
 21 T   8 O   4.868046529252E-01 3.783854558290E-01 4.824143186552E-01
 22 F   8 O   -4.868046529252E-01 -4.390334270000E-03 -1.084191970962E-01
 23 F   8 O   3.959711371738E-01 -1.216145441710E-01 -1.084191970962E-01
 24 F   8 O   -3.959711371738E-01 4.956096657300E-01 4.824143186552E-01
 25 T   8 O   -4.590117173439E-01 2.395073125555E-01 2.804955952116E-01
 26 F   8 O   4.590117173439E-01 -2.604926874445E-01 -3.014809701006E-01
 27 T   8 O   -2.825241256000E-03 3.710663993979E-01 -1.317588418581E-01
 28 F   8 O   2.825241256000E-03 -1.289336006021E-01 3.738916406539E-01
 29 T   8 O   -4.161254799910E-02 -4.711560080500E-01 1.693804488727E-01
 30 F   8 O   4.161254799910E-02 2.109929968718E-01 -4.295434600509E-01
 31 F   8 O   -1.405364569227E-01 2.884399195000E-02 -4.295434600509E-01
 32 F   8 O   1.405364569227E-01 -2.890070031282E-01 1.693804488727E-01
 33 T   8 O   -2.135668972127E-01 1.523387870609E-01 -2.468779088581E-01
 34 F   8 O   2.135668972127E-01 -3.331101164540E-02 3.659056842735E-01
 35 F   8 O   -1.007833040811E-01 -3.476612129391E-01 3.659056842735E-01
 36 F   8 O   1.007833040811E-01 4.666889883546E-01 -2.468779088581E-01
 37 T   8 O   -1.461592993366E-01 3.973082744210E-01 1.685012815738E-01

```
38 F   8 O    1.461592993366E-01  3.146605809104E-01 -4.565324262424E-01
39 F   8 O   -2.711930071528E-01 -1.026917255790E-01 -4.565324262424E-01
40 F   8 O    2.711930071528E-01 -1.853394190896E-01  1.685012815738E-01
41 T   8 O    3.543290677875E-01 -4.754856748024E-01 -3.151140378209E-01
42 F   8 O   -3.543290677875E-01  3.305568943916E-01  1.701852574101E-01
43 F   8 O    3.396283630185E-01  2.451432519758E-02  1.701852574101E-01
44 F   8 O   -3.396283630185E-01 -1.694431056084E-01 -3.151140378209E-01
45 T   8 O    2.208796960791E-01  2.261009140316E-01  3.643321752697E-01
46 F   8 O   -2.208796960791E-01  1.434524791906E-01  5.221217952500E-03
47 F   8 O    3.617687387619E-01 -2.738990859684E-01  5.221217952500E-03
48 F   8 O   -3.617687387619E-01 -3.565475208094E-01  3.643321752697E-01
```

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

****
CRYSTALLOGRAPHIC CELL (VOLUME=   1304.64347040)
     A   B   C   ALPHA   BETA   GAMMA
  11.51157168   5.11889300   22.14018122   90.000000 90.000000 90.000000

COORDINATES IN THE CRYSTALLOGRAPHIC CELL
  ATOM   X/A   Y/B   Z/C
****
```
 1 T  20 CA    1.341400807606E-02  0.000000000000E+00  0.000000000000E+00
 2 F  20 CA    1.341400807606E-02  0.000000000000E+00  5.000000000000E-01
 3 T  20 CA   -1.898856475436E-01  4.993288817325E-01 -2.500000000000E-01
 4 F  20 CA   -1.898856475436E-01 -4.993288817325E-01  2.500000000000E-01
 5 T  20 CA    3.436291191189E-02  2.640162756720E-03  1.686967891957E-01
 6 F  20 CA    3.436291191189E-02 -2.640162756720E-03 -1.686967891957E-01
 7 F  20 CA   -4.656370880881E-01  4.973598372433E-01  1.686967891957E-01
 8 F  20 CA   -4.656370880881E-01 -4.973598372433E-01 -1.686967891957E-01
 9 T  20 CA    2.416478363926E-01  4.958158274578E-01  1.044352797178E-01
10 F  20 CA    2.416478363926E-01 -4.958158274578E-01 -1.044352797178E-01
11 F  20 CA   -2.583521636074E-01  4.184172542200E-03  1.044352797178E-01
12 F  20 CA   -2.583521636074E-01 -4.184172542200E-03 -1.044352797178E-01
13 T  14 SI   1.205438630828E-01  4.274505846432E-01  2.500000000000E-01
14 F  14 SI   1.205438630828E-01 -4.274505846432E-01 -2.500000000000E-01
15 T  14 SI   4.324364595709E-01 -5.850746031668E-02  1.009636922742E-01
16 F  14 SI   4.324364595709E-01  5.850746031668E-02 -1.009636922742E-01
17 F  14 SI  -6.756354042910E-02 -4.414925396833E-01  1.009636922742E-01
18 F  14 SI  -6.756354042910E-02  4.414925396833E-01 -1.009636922742E-01
19 T  14 SI   2.662662947417E-01  0.000000000000E+00  0.000000000000E+00
20 F  14 SI   2.662662947417E-01  4.590873227954E-17  5.000000000000E-01
21 T   8 O    1.869975607795E-01  2.954167578757E-01  1.913878950495E-01
22 F   8 O    1.869975607795E-01 -2.954167578757E-01 -1.913878950495E-01
23 F   8 O   -3.130024392205E-01  2.045832421243E-01  1.913878950495E-01
24 F   8 O   -3.130024392205E-01 -2.045832421243E-01 -1.913878950495E-01
25 T   8 O   -1.049268744451E-02  2.909882826561E-01  2.500000000000E-01
26 F   8 O   -1.049268744451E-02 -2.909882826561E-01 -2.500000000000E-01
27 T   8 O    1.210663993979E-01 -2.528252412560E-01  2.500000000000E-01
28 F   8 O    1.210663993979E-01  2.528252412560E-01 -2.500000000000E-01
29 T   8 O    3.699184944109E-01 -2.005380455382E-01  1.589254975391E-01
30 F   8 O    3.699184944109E-01  2.005380455382E-01 -1.589254975391E-01
31 F   8 O   -1.300815055891E-01 -2.994619544618E-01  1.589254975391E-01
```

```
32 F  8 O  -1.300815055891E-01  2.994619544618E-01 -1.589254975391E-01
33 T  8 O   5.951388770774E-02 -3.063917965658E-01  9.282489935314E-02
34 F  8 O   5.951388770774E-02  3.063917965658E-01 -9.282489935314E-02
35 F  8 O  -4.404861122923E-01 -1.936082034342E-01  9.282489935314E-02
36 F  8 O  -4.404861122923E-01  1.936082034342E-01 -9.282489935314E-02
37 T  8 O   3.559844276657E-01 -1.874831460919E-01  4.132384675531E-02
38 F  8 O   3.559844276657E-01  1.874831460919E-01 -4.132384675531E-02
39 F  8 O  -1.440155723343E-01 -3.125168539081E-01  4.132384675531E-02
40 F  8 O  -1.440155723343E-01  3.125168539081E-01 -4.132384675531E-02
41 T  8 O   4.275356097946E-01  2.573503523845E-01  9.697871540298E-02
42 F  8 O   4.275356097946E-01 -2.573503523845E-01 -9.697871540298E-02
43 F  8 O  -7.246439020540E-02  2.426496476155E-01  9.697871540298E-02
44 F  8 O  -7.246439020540E-02 -2.426496476155E-01 -9.697871540298E-02
45 T  8 O   1.847766966111E-01  1.795554786586E-01  4.132421742051E-02
46 F  8 O   1.847766966111E-01 -1.795554786586E-01 -4.132421742051E-02
47 F  8 O  -3.152233033889E-01  3.204445213414E-01  4.132421742051E-02
48 F  8 O  -3.152233033889E-01 -3.204445213414E-01 -4.132421742051E-02
```

T = ATOM BELONGING TO THE ASYMMETRIC UNIT

**** 4 SYMMOPS - TRANSLATORS IN FRACTIONAL 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 -1.00  0.00  1.00 -1.00  1.00  0.00   0.00  0.00  0.00
3 3  0.00  1.00 -1.00  0.00  1.00  0.00 -1.00  1.00  0.00   0.50  0.50  0.00
4 4  0.00 -1.00  1.00 -1.00  0.00  1.00  0.00  0.00  1.00   0.50  0.50  0.00
```

DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)

```
      X                Y              Z
-0.575578584000E+01  0.255944650000E+01  0.110700906100E+02
 0.575578584000E+01 -0.255944650000E+01  0.110700906100E+02
 0.575578584000E+01  0.255944650000E+01 -0.110700906100E+02
```

CARTESIAN COORDINATES - PRIMITIVE CELL
****
```
*   ATOM      X(ANGSTROM)      Y(ANGSTROM)      Z(ANGSTROM)
*****************************************************************************
  1   20 CA   1.544163154837E-01  0.000000000000E+00  0.000000000000E+00
  2   20 CA  -1.135715536452E+01  0.000000000000E+00  1.107009061000E+01
  3   20 CA  -2.185882242701E+00  2.556011117398E+00 -5.535045305000E+00
  4   20 CA  -2.185882242701E+00 -2.556011117398E+00  5.535045305000E+00
  5   20 CA   3.955711236072E-01  1.351471065423E-02  3.734977484025E+00
  6   20 CA   3.955711236072E-01 -1.351471065423E-02 -3.734977484025E+00
  7   20 CA  -5.360214716393E+00  2.545931789346E+00  3.734977484025E+00
  8   20 CA  -5.360214716393E+00 -2.545931789346E+00 -3.734977484025E+00
  9   20 CA   2.781746389950E+00  2.538028168463E+00  2.312216018713E+00
 10   20 CA   2.781746389950E+00 -2.538028168463E+00 -2.312216018713E+00
 11   20 CA  -2.974039450050E+00  2.141833153706E-02  2.312216018713E+00
 12   20 CA  -2.974039450050E+00 -2.141833153706E-02 -2.312216018713E+00
 13   14 SI   1.387649320462E+00  2.188073805576E+00  5.535045305000E+00
 14   14 SI   1.387649320462E+00 -2.188073805576E+00 -5.535045305000E+00
 15   14 SI   4.978023301396E+00 -2.994934290628E-01  2.235354443591E+00
 16   14 SI   4.978023301396E+00  2.994934290628E-01 -2.235354443591E+00
```

17	14 SI	-7.777625386042E-01	-2.259953070937E+00	2.235354443591E+00
18	14 SI	-7.777625386042E-01	2.259953070937E+00	-2.235354443591E+00
19	14 SI	3.065143537887E+00	0.000000000000E+00	0.000000000000E+00
20	14 SI	-8.446428142113E+00	2.350018883046E-16	1.107009061000E+01
21	8 O	2.152635824898E+00	1.512206773973E+00	4.237362679710E+00
22	8 O	2.152635824898E+00	-1.512206773973E+00	-4.237362679710E+00
23	8 O	-3.603150015102E+00	1.047239726027E+00	4.237362679710E+00
24	8 O	-3.603150015102E+00	-1.047239726027E+00	-4.237362679710E+00
25	8 O	-1.207873236333E-01	1.489537883170E+00	5.535045305000E+00
26	8 O	-1.207873236333E-01	-1.489537883170E+00	-5.535045305000E+00
27	8 O	1.393664534708E+00	-1.294185357689E+00	5.535045305000E+00
28	8 O	1.393664534708E+00	1.294185357689E+00	-5.535045305000E+00
29	8 O	4.258343264169E+00	-1.026532797539E+00	3.518639315994E+00
30	8 O	4.258343264169E+00	1.026532797539E+00	-3.518639315994E+00
31	8 O	-1.497442575831E+00	-1.532913702461E+00	3.518639315994E+00
32	8 O	-1.497442575831E+00	1.532913702461E+00	-3.518639315994E+00
33	8 O	6.850983843031E-01	-1.568386822698E+00	2.055160093407E+00
34	8 O	6.850983843031E-01	1.568386822698E+00	-2.055160093407E+00
35	8 O	-5.070687455697E+00	-9.910596773019E-01	2.055160093407E+00
36	8 O	-5.070687455697E+00	9.910596773019E-01	-2.055160093407E+00
37	8 O	4.097940256037E+00	-9.597061641478E-01	9.149174558701E-01
38	8 O	4.097940256037E+00	9.597061641478E-01	-9.149174558701E-01
39	8 O	-1.657845583963E+00	-1.599740335852E+00	9.149174558701E-01
40	8 O	-1.657845583963E+00	1.599740335852E+00	-9.149174558701E-01
41	8 O	4.921606817903E+00	1.317348917369E+00	2.147126333505E+00
42	8 O	4.921606817903E+00	-1.317348917369E+00	-2.147126333505E+00
43	8 O	-8.341790220970E-01	1.242097582631E+00	2.147126333505E+00
44	8 O	-8.341790220970E-01	-1.242097582631E+00	-2.147126333505E+00
45	8 O	2.127070187832E+00	9.191252828172E-01	9.149256624648E-01
46	8 O	2.127070187832E+00	-9.191252828172E-01	-9.149256624648E-01
47	8 O	-3.628715652168E+00	1.640321217183E+00	9.149256624648E-01
48	8 O	-3.628715652168E+00	-1.640321217183E+00	-9.149256624648E-01

```
*******************************************************************************
LOCAL ATOMIC FUNCTIONS BASIS SET
*******************************************************************************
 ATOM  X(AU)  Y(AU)  Z(AU)   NO. TYPE  EXPONENT  S COEF   P COEF   D/F/G COEF
*******************************************************************************
 1 CA  0.292  0.000  0.000
                       1 S
                         1.913E+05 2.204E-04 0.000E+00 0.000E+00
                         2.697E+04 1.925E-03 0.000E+00 0.000E+00
                         5.696E+03 1.109E-02 0.000E+00 0.000E+00
                         1.489E+03 4.995E-02 0.000E+00 0.000E+00
                         4.483E+02 1.701E-01 0.000E+00 0.000E+00
                         1.546E+02 3.685E-01 0.000E+00 0.000E+00
                         6.037E+01 4.034E-01 0.000E+00 0.000E+00
                         2.509E+01 1.452E-01 0.000E+00 0.000E+00
                    2-   5 SP
                         4.486E+02-5.750E-03 8.470E-03 0.000E+00
                         1.057E+02-7.670E-02 6.027E-02 0.000E+00
                         3.469E+01-1.122E-01 2.124E-01 0.000E+00
                         1.350E+01 2.537E-01 3.771E-01 0.000E+00
                         5.820E+00 6.880E-01 4.010E-01 0.000E+00
```

```
                      1.819E+00 3.490E-01 1.980E-01 0.000E+00
        6-  9 SP
                      2.075E+01-2.000E-03-3.650E-02 0.000E+00
                      8.400E+00-1.255E-01-6.850E-02 0.000E+00
                      3.597E+00-6.960E-01 1.570E-01 0.000E+00
                      1.408E+00 1.029E+00 1.482E+00 0.000E+00
                      7.260E-01 9.440E-01 1.025E+00 0.000E+00
       10- 13 SP
                      4.630E-01 1.000E+00 1.000E+00 0.000E+00
       14- 17 SP
                      2.790E-01 1.000E+00 1.000E+00 0.000E+00
       18- 22 D
                      3.922E+00 0.000E+00 0.000E+00 1.390E-01
                      1.095E+00 0.000E+00 0.000E+00 3.260E-01
       23- 27 D
                      3.430E-01 0.000E+00 0.000E+00 4.270E-01
  2 CA-21.462  0.000 20.919
  3 CA -4.131  4.830-10.460
  4 CA -4.131 -4.830 10.460
  5 CA  0.748  0.026  7.058
  6 CA  0.748 -0.026 -7.058
  7 CA-10.129  4.811  7.058
  8 CA-10.129 -4.811 -7.058
  9 CA  5.257  4.796  4.369
 10 CA  5.257 -4.796 -4.369
 11 CA -5.620  0.040  4.369
 12 CA -5.620 -0.040 -4.369
 13 SI  2.622  4.135 10.460
                   325 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
      326- 329 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
      330- 333 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
      334- 337 SP
                      3.330E-01 1.000E+00 1.000E+00 0.000E+00
      338- 341 SP
                      1.300E-01 1.000E+00 1.000E+00 0.000E+00
      342- 346 D
                      6.820E-01 0.000E+00 0.000E+00 1.000E+00
```

```
14 SI   2.622 -4.135-10.460
15 SI   9.407 -0.566  4.224
16 SI   9.407  0.566 -4.224
17 SI  -1.470 -4.271  4.224
18 SI  -1.470  4.271 -4.224
19 SI   5.792  0.000  0.000
20 SI-15.961  0.000 20.919
21 O    4.068  2.858  8.007
                    501 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
                  502- 505 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
                  506- 509 SP
                         4.600E-01 1.000E+00 1.000E+00 0.000E+00
                  510- 513 SP
                         1.700E-01 1.000E+00 1.000E+00 0.000E+00
                  514- 518 D
                         5.560E-01 0.000E+00 0.000E+00 1.000E+00
22 O    4.068 -2.858 -8.007
23 O   -6.809  1.979  8.007
24 O   -6.809 -1.979 -8.007
25 O   -0.228  2.815 10.460
26 O   -0.228 -2.815-10.460
27 O    2.634 -2.446 10.460
28 O    2.634  2.446-10.460
29 O    8.047 -1.940  6.649
30 O    8.047  1.940 -6.649
31 O   -2.830 -2.897  6.649
32 O   -2.830  2.897 -6.649
33 O    1.295 -2.964  3.884
34 O    1.295  2.964 -3.884
35 O   -9.582 -1.873  3.884
36 O   -9.582  1.873 -3.884
37 O    7.744 -1.814  1.729
38 O    7.744  1.814 -1.729
39 O   -3.133 -3.023  1.729
40 O   -3.133  3.023 -1.729
41 O    9.300  2.489  4.057
42 O    9.300 -2.489 -4.057
43 O   -1.576  2.347  4.057
44 O   -1.576 -2.347 -4.057
45 O    4.020  1.737  1.729
46 O    4.020 -1.737 -1.729
47 O   -6.857  3.100  1.729
```

48 O -6.857 -3.100 -1.729
INFORMATION **** READM2 **** FULL DIRECT SCF (MONO AND BIEL INT) SELECTED
INFORMATION **** TOLINTEG **** COULOMB AND EXCHANGE SERIES TOLERANCES MODIFIED
INFORMATION **** TOLDEE **** SCF TOL ON TOTAL ENERGY SET TO   10

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
INFORMATION **** MAXCYCLE **** MAX NUMBER OF SCF CYCLES SET TO   200
INFORMATION **** BIPOSIZE **** COULOMB BIPOLAR BUFFER SET TO   6818200
INFORMATION **** EXCHSIZE **** EXCHANGE BIPOLAR BUFFER SIZE SET TO   6992232
****
N. OF ATOMS PER CELL   48 COULOMB OVERLAP TOL   (T1) 10** -7
NUMBER OF SHELLS   272 COULOMB PENETRATION TOL   (T2) 10** -7
NUMBER OF AO   1004 EXCHANGE OVERLAP TOL   (T3) 10** -7
N. OF ELECTRONS PER CELL 576 EXCHANGE PSEUDO OVP (F(G)) (T4) 10** -7
CORE ELECTRONS PER CELL 352 EXCHANGE PSEUDO OVP (P(G)) (T5) 10**-15
N. OF SYMMETRY OPERATORS   4 POLE ORDER IN MONO ZONE   4
****
TYPE OF CALCULATION : RESTRICTED CLOSED SHELL
KOHN-SHAM HAMILTONIAN

(EXCHANGE)[CORRELATION] FUNCTIONAL:(PERDEW-BURKE-ERNZERHOF)[PERDEW-BURKE-ERNZERHOF]

HYBRID EXCHANGE - PERCENTAGE OF FOCK EXCHANGE   16.6670

CAPPA:IS1 4;IS2 4;IS3 4; K PTS MONK NET   18; SYMMOPS: K SPACE 8;G SPACE 4

****
MAX NUMBER OF SCF CYCLES   200 CONVERGENCE ON DELTAP   10**-20
WEIGHT OF F(I) IN F(I+1)   80% CONVERGENCE ON ENERGY   10**-10
SHRINK. FACT.(MONKH.) 4 4 4 NUMBER OF K POINTS IN THE IBZ   18
SHRINKING FACTOR(GILAT NET)   4 NUMBER OF K POINTS(GILAT NET)   18
****
*** 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(0 1 0)
 5-C(1 1 0) 6-C(2 1 0) 7-C(3 1 0) 8-R(0 2 0)
 9-C(1 2 0) 10-R(2 2 0) 11-C(1 1 1) 12-C(3 1 1)
 13-C(2 2 1) 14-C(3 2 1) 15-C(1 3 1) 16-C(2 3 1)
 17-C(3 3 1) 18-R(2 2 2)

DIRECT LATTICE VECTORS COMPON. (A.U.)   RECIP. LATTICE VECTORS COMPON. (A.U.)
    X   Y   Z   X   Y   Z
 -10.8768589 4.8366529 20.9194395   0.0000000 0.6495386 0.1501758
  10.8768589 -4.8366529 20.9194395   0.2888327 0.0000000 0.1501758
  10.8768589   4.8366529 -20.9194395   0.2888327 0.6495386 0.0000000

DISK SPACE FOR EIGENVECTORS (FTN 10)   31248496 REALS

SYMMETRY ADAPTION OF THE BLOCH FUNCTIONS ENABLED
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT gordsh1   TELAPSE   0.38 TCPU   0.11

DIMENSIONS P(G)= 2206952 F(G)= 353010 P(G),F(G) (IRR) 290516
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 135

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT   TELAPSE   0.43 TCPU   0.16

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 CA 2   2.3608   4.4612 45 O   0 0 0 46 O   0 0 0
 1 CA 2   2.5847   4.8843 39 O   0 0 0 40 O   0 0 0
 1 CA 2   2.6392   4.9873 33 O   0 0 0 34 O   0 0 0
 1 CA 2   2.6703   5.0461 43 O   0 0 0 44 O   0 0 0
 1 CA 1   2.9107   5.5005 19 SI 0 0 0
 1 CA 2   3.3126   6.2599 17 SI 0 0 0 18 SI   0 0 0

 3 CA 1   2.3274   4.3981 26 O   1 0 1
 3 CA 2   2.3636   4.4665 29 O   0-1 0 32 O   0 0 0
 3 CA 2   2.4474   4.6249 21 O   0-1 0 24 O   1 0 1
 3 CA 1   2.5302   4.7814 27 O   0-1 0
 3 CA 1   3.0927   5.8444 13 SI 0-1 0
 3 CA 1   3.5931   6.7900 14 SI 1 0 1

 5 CA 1   2.3255   4.3946 33 O   0 0 0
 5 CA 1   2.3544   4.4491 43 O   0 0 0
 5 CA 1   2.3634   4.4662 21 O   0 0 0
 5 CA 1   2.3844   4.5059 25 O   0 0 0
 5 CA 1   2.4385   4.6082 27 O   0 0 0
 5 CA 1   2.4539   4.6372 31 O   0 0 0

 9 CA 1   2.2365   4.2263 45 O   0 0 0
 9 CA 1   2.2703   4.2903 21 O   0 0 0
 9 CA 1   2.3425   4.4266 33 O   1 0 1
 9 CA 1   2.4600   4.6488 29 O   1 0 1
 9 CA 1   2.4691   4.6659 41 O   0 0 0
 9 CA 1   2.5126   4.7481 37 O   1 0 1

13 SI 1   1.6366   3.0928 27 O   1 0 1
13 SI 2   1.6511   3.1200 21 O   0 0 0 24 O   1 1 1
13 SI 1   1.6623   3.1413 25 O   0 0 0
13 SI 2   2.9922   5.6544   5 CA 0 0 0   8 CA   1 1 1
13 SI 1   3.0927   5.8444   3 CA 0 1 0
13 SI 1   3.4823   6.5805 27 O   0 0 0

15 SI 1   1.6202   3.0618 41 O   0 0 0
15 SI 1   1.6281   3.0767 35 O   0 1 1
15 SI 1   1.6411   3.1013 29 O   0 0 0
15 SI 1   1.7187   3.2479 37 O   0 0 0
15 SI 1   2.9573   5.5885 19 SI 0 0 0
15 SI 1   2.9655   5.6040   7 CA -1 1 0

19 SI 2   1.6006   3.0247 45 O   0 0 0 46 O   0 0 0
19 SI 2   1.6807   3.1761 37 O   0 0 0 38 O   0 0 0

```
19 SI  1   2.9107   5.5005  1 CA   0 0 0
19 SI  2   2.9573   5.5885  15 SI  0 0 0  16 SI  0 0 0
19 SI  2   3.1292   5.9134  41 O   0 0 0  42 O   0 0 0
19 SI  2   3.4450   6.5102  9 CA   0 0 0  10 CA  0 0 0

21 O   1   1.6511   3.1200  13 SI  0 0 0
21 O   1   2.2703   4.2903  9 CA   0 0 0
21 O   1   2.3634   4.4662  5 CA   0 0 0
21 O   1   2.4474   4.6249  3 CA   0 1 0
21 O   1   2.5954   4.9045  24 O   1 1 1
21 O   1   2.6178   4.9470  25 O   0 0 0

25 O   1   1.6623   3.1413  13 SI  0 0 0
25 O   1   2.3274   4.3981  4 CA   1 0 1
25 O   2   2.3844   4.5059  5 CA   0 0 0  8 CA   1 1 1
25 O   2   2.6178   4.9470  21 O   0 0 0  24 O   1 1 1
25 O   1   2.7833   5.2596  27 O   1 0 1
25 O   1   3.1690   5.9886  27 O   0 0 0

27 O   1   1.6366   3.0928  13 SI  -1 0 -1
27 O   2   2.4385   4.6082  5 CA   0 0 0  8 CA   1 1 1
27 O   1   2.5302   4.7814  3 CA   0 1 0
27 O   2   2.7582   5.2122  21 O   -1 0 -1  24 O   0 1 0
27 O   1   2.7833   5.2596  25 O   -1 0 -1
27 O   1   3.1690   5.9886  25 O   0 0 0

29 O   1   1.6411   3.1013  15 SI  0 0 0
29 O   1   2.3636   4.4665  3 CA   0 1 0
29 O   1   2.4539   4.6372  7 CA   -1 1 0
29 O   1   2.4600   4.6488  9 CA   -1 0 -1
29 O   1   2.6095   4.9313  37 O   0 0 0
29 O   1   2.6280   4.9662  35 O   0 1 1

33 O   1   1.6281   3.0767  17 SI  0 0 0
33 O   1   2.3255   4.3946  5 CA   0 0 0
33 O   1   2.3425   4.4266  9 CA   -1 0 -1
33 O   1   2.6059   4.9244  39 O   0 0 0
33 O   1   2.6280   4.9662  31 O   0 0 0
33 O   1   2.6392   4.9873  1 CA   0 0 0

37 O   1   1.6807   3.1761  19 SI  0 0 0
37 O   1   1.7187   3.2479  15 SI  0 0 0
37 O   1   2.5126   4.7481  9 CA   -1 0 -1
37 O   1   2.5847   4.8843  2 CA   -1 1 1
37 O   1   2.6059   4.9244  35 O   0 1 1
37 O   1   2.6095   4.9313  29 O   0 0 0

41 O   1   1.6202   3.0618  15 SI  0 0 0
41 O   1   2.3544   4.4491  7 CA   0 1 1
41 O   1   2.4691   4.6659  9 CA   0 0 0
41 O   1   2.6703   5.0461  2 CA   0 1 2
41 O   1   2.7169   5.1343  37 O   0 0 0
41 O   1   2.7650   5.2252  35 O   0 1 1
```

```
45 O   1   1.6006   3.0247 19 SI   0 0 0
45 O   1   2.2365   4.2263  9 CA   0 0 0
45 O   1   2.3608   4.4612  1 CA   0 0 0
45 O   1   2.5937   4.9015 46 O    0 0 0
45 O   1   2.6897   5.0827 38 O    0 0 0
45 O   1   2.7229   5.1456 37 O    0 0 0
```

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 36
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM   TELAPSE   1.27 TCPU   0.73
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE   1.41 TCPU   0.87


```
*******************************************************************************
*                                         *
*                                         *
*     FFFFF RRRR  EEEE  EEE  U  U EEEE N  N CCC  Y  Y       *
*     F    R  R E     E E U  U E    NN N C    Y Y      *
*     FFF  RRRR  EEEE E  E U  U EEEE N N N C     Y        *
*     F    R  R E     E EE U  U E    N NN C      Y       *
*     F    R  R EEEE  EE E UUU  EEEE N  N CCC    Y        *
*                                         *
*                                         *
* CALCULATION OF PHONON FREQUENCIES AT THE GAMMA POINT.              *
*                                         *
* SYMMETRY IS EXPLOITED TO BUILD THE TOTAL HESSIAN MATRIX.           *
* (F. PASCALE PHD THESIS TURIN-PARIS 2002)                *
*                                         *
*******************************************************************************
```

```
*                                         *
* REFERENCES TO BE QUOTED WHEN USING THIS MODULE:              *
*                                         *
* F. Pascale, C.M. Zicovich-Wilson, F. Lopez, B. Civalleri          *
* R. Orlando, R. Dovesi                           *
* The calculation of the vibration frequencies of crystalline         *
* compounds and its implementation in the CRYSTAL code            *
* J. Comput. Chem. 25 (2004) 888-897                    *
*                                         *
* C.M. Zicovich-Wilson, F. Pascale, C. Roetti, V.R. Saunders,         *
* R. Orlando, R. Dovesi                           *
* The calculation of the vibration frequencies of alpha-quartz:        *
* the effect of hamiltonian and basis set                 *
* J. Comput. Chem. 25 (2004) 1873-1881                  *
*******************************************************************************
```


ATOMS ISOTOPIC MASS (AMU) FOR FREQUENCY CALCULATION

```
  1 CA   39.9626   2 CA   39.9626   3 CA   39.9626   4 CA   39.9626
  5 CA   39.9626   6 CA   39.9626   7 CA   39.9626   8 CA   39.9626
  9 CA   39.9626  10 CA   39.9626  11 CA   39.9626  12 CA   39.9626
 13 SI   27.9769  14 SI   27.9769  15 SI   27.9769  16 SI   27.9769
```

17 SI	27.9769	18 SI	27.9769	19 SI	27.9769	20 SI	27.9769
21 O	15.9949	22 O	15.9949	23 O	15.9949	24 O	15.9949
25 O	15.9949	26 O	15.9949	27 O	15.9949	28 O	15.9949
29 O	15.9949	30 O	15.9949	31 O	15.9949	32 O	15.9949
33 O	15.9949	34 O	15.9949	35 O	15.9949	36 O	15.9949
37 O	15.9949	38 O	15.9949	39 O	15.9949	40 O	15.9949
41 O	15.9949	42 O	15.9949	43 O	15.9949	44 O	15.9949
45 O	15.9949	46 O	15.9949	47 O	15.9949	48 O	15.9949

STEP SIZE   0.0030 ANGSTROM

INFORMATION CONCERNING THE SCF+GRADIENT CALCULATIONS REQUIRED FOR
GENERATING FREQUENCIES. IN PRINCIPLE 3N+1 SCF + GRADIENT
CALCULATIONS ARE REQUIRED;
FOR EACH OF THEM THE REMAINING POINT SYMMETRY IS INDICATED.
POINT SYMMETRY PERMITS TO GENERATE GRADIENTS FOR DISPLACEMENT B
STARTING FROM THE GRADIENT GENERATED BY DISPLACEMENT A.

 N LABEL SYMBOL DISPLACEMENT   SYM.

 1   EQUILIBRIUM GEOMETRY   4

N	LABEL	SYMBOL	DISPLACEMENT	SYM.
2	1	CA	DX	2
3	1	CA	DY	1
4	1	CA	DZ	1
5	3	CA	DX	2
6	3	CA	DY	2
7	3	CA	DZ	1
8	5	CA	DX	1
9	5	CA	DY	1
10	5	CA	DZ	1
11	9	CA	DX	1
12	9	CA	DY	1
13	9	CA	DZ	1
14	13	SI	DX	2
15	13	SI	DY	2
16	13	SI	DZ	1
17	15	SI	DX	1
18	15	SI	DY	1
19	15	SI	DZ	1
20	19	SI	DX	2
21	19	SI	DY	1
22	19	SI	DZ	1
23	21	O	DX	1
24	21	O	DY	1
25	21	O	DZ	1
26	25	O	DX	2
27	25	O	DY	2
28	25	O	DZ	1
29	27	O	DX	2
30	27	O	DY	2
31	27	O	DZ	1
32	29	O	DX	1
33	29	O	DY	1

34	29	O	DZ	1
35	33	O	DX	1
36	33	O	DY	1
37	33	O	DZ	1
38	37	O	DX	1
39	37	O	DY	1
40	37	O	DZ	1
41	41	O	DX	1
42	41	O	DY	1
43	41	O	DZ	1
44	45	O	DX	1
45	45	O	DY	1
46	45	O	DZ	1

USE OF RESIDUAL SYMMETRY AFTER DISPLACEMENT

NUMERICAL GRADIENT COMPUTED WITH A SINGLE DISPLACEMENT (+dx) FOR EACH
CARTESIAN COORDINATE WITH RESPECT TO THE EQUILIBRIUM CONFIGURATION
dx= 0.003
NUMBER OF IRREDUCIBLE ATOMS   15
NUMBER OF SCF+GRADIENT CALCULATIONS   46

ATOM	SYMOP	ORDER
1	2	2
3	2	2
5	2	2
9	2	2
13	1	1
15	1	1
19	1	1
21	1	1
25	1	1
27	1	1
29	1	1
33	1	1
37	2	2
41	2	2
45	1	1

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   18   9   19
NO.OF VECTORS CREATED 6999 STARS 1041 RMAX   197.35268 BOHR

CAPPA:IS1 4;IS2 4;IS3 4; K PTS MONK NET   18; SYMMOPS: K SPACE 8;G SPACE 4

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT gordsh1   TELAPSE   1.52 TCPU   0.95

DIMENSIONS P(G)= 2206952 F(G)= 353010 P(G),F(G) (IRR) 290516
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 135

TTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT   TELAPSE   1.57 TCPU   1.00

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 36
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM   TELAPSE   2.07 TCPU   1.37
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE   2.13 TCPU   1.43

     THE FIRST POINT IS RESTORED FROM THE FREQINFO.DAT

 RESTART FROM AN INCOMPLETE HESSIAN MATRIX

 HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
HHHHHHHHHHHHHH
          FORCE CONSTANT MATRIX - NUMERICAL ESTIMATE
 HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
HHHHHHHHHHHHHH
 MAX ABS(DGRAD): MAXIMUM ABSOLUTE GRADIENT DIFFERENCE WITH RESPECT TO
          THE CENTRAL POINT
 DE: ENERGY DIFFERENCE WITH RESPECT TO THE CENTRAL POINT
          (DE IS EXPECTED TO BE POSITIVE FOR ALL DISPLACEMENTS)

ATOM	MAX ABS(DGRAD)	TOTAL ENERGY (AU)	N.CYC	DE	SYM
CENTRAL POINT		-1.255266345597E+04	21	0.0000E+00	4
1 CA DX	6.0307E-04	-1.255266345416E+04	9	1.8056E-06	2
1 CA DY	2.2149E-04	-1.255266345531E+04	10	6.6013E-07	1
1 CA DZ	3.2569E-04	-1.255266345501E+04	8	9.5852E-07	1
3 CA DX	5.7128E-04	-1.255266345468E+04	12	1.2892E-06	2
3 CA DY	3.5959E-04	-1.255266345486E+04	12	1.1028E-06	2
3 CA DZ	4.9728E-04	-1.255266345452E+04	10	1.4465E-06	1
5 CA DX	4.2746E-04	-1.255266345481E+04	11	1.1531E-06	1
5 CA DY	5.6444E-04	-1.255266345490E+04	12	1.0706E-06	1
5 CA DZ	6.0005E-04	-1.255266345398E+04	14	1.9827E-06	1
9 CA DX	5.6102E-04	-1.255266345412E+04	12	1.8485E-06	1
9 CA DY	5.2038E-04	-1.255266345428E+04	14	1.6855E-06	1
9 CA DZ	5.6398E-04	-1.255266345537E+04	12	5.9547E-07	1
13 SI DX	2.4226E-03	-1.255266344950E+04	11	6.4675E-06	2
13 SI DY	2.9962E-03	-1.255266344796E+04	13	8.0075E-06	2
13 SI DZ	2.5534E-03	-1.255266344870E+04	13	7.2693E-06	1
15 SI DX	2.6371E-03	-1.255266344731E+04	10	8.6582E-06	1
15 SI DY	3.1304E-03	-1.255266344795E+04	15	8.0151E-06	1
15 SI DZ	2.2737E-03	-1.255266345055E+04	13	5.4215E-06	1
19 SI DX	3.0159E-03	-1.255266344856E+04	14	7.4041E-06	2
19 SI DY	2.5989E-03	-1.255266344857E+04	13	7.4011E-06	1
19 SI DZ	2.7619E-03	-1.255266344811E+04	10	7.8577E-06	1
21 O DX	7.9436E-04	-1.255266345393E+04	13	2.0403E-06	1
21 O DY	6.4503E-04	-1.255266345401E+04	14	1.9534E-06	1
21 O DZ	1.5390E-03	-1.255266345105E+04	12	4.9133E-06	1
25 O DX	1.6990E-03	-1.255266345038E+04	12	5.5907E-06	2
25 O DY	6.3614E-04	-1.255266345420E+04	13	1.7621E-06	2
25 O DZ	5.1007E-04	-1.255266345449E+04	11	1.4783E-06	1
27 O DX	3.9745E-04	-1.255266345490E+04	11	1.0640E-06	2
27 O DY	1.9273E-03	-1.255266345035E+04	17	5.6200E-06	2

```
27 O  DZ  4.3938E-04   -1.255266345468E+04  11  1.2822E-06  1
29 O  DX  7.4551E-04   -1.255266345357E+04  11  2.3947E-06  1
29 O  DY  6.6398E-04   -1.255266345413E+04  14  1.8413E-06  1
29 O  DZ  1.4667E-03   -1.255266345181E+04  12  4.1538E-06  1
33 O  DX  1.8922E-03   -1.255266345148E+04  12  4.4892E-06  1
33 O  DY  7.0718E-04   -1.255266345426E+04  13  1.7054E-06  1
33 O  DZ  4.6581E-04   -1.255266345392E+04  12  2.0464E-06  1
37 O  DX  1.1996E-03   -1.255266345222E+04  11  3.7421E-06  1
37 O  DY  9.9020E-04   -1.255266345215E+04  13  3.8140E-06  1
37 O  DZ  1.4920E-03   -1.255266345155E+04  13  4.4137E-06  1
41 O  DX  4.6047E-04   -1.255266345504E+04  10  9.2581E-07  1
41 O  DY  2.0452E-03   -1.255266345061E+04  15  5.3618E-06  1
41 O  DZ  4.0181E-04   -1.255266345473E+04  12  1.2333E-06  1
45 O  DX  1.0791E-03   -1.255266345267E+04  17  3.3019E-06  1
45 O  DY  1.1244E-03   -1.255266345228E+04  12  3.6876E-06  1
45 O  DZ  1.0979E-03   -1.255266345246E+04  14  3.5037E-06  1
```

GCALCO - MAX INDICES DIRECT LATTICE VECTOR   18   9   19
NO.OF VECTORS CREATED 6999 STARS 1041 RMAX   197.35268 BOHR

CAPPA:IS1 4;IS2 4;IS3 4; K PTS MONK NET   18; SYMMOPS: K SPACE 8;G SPACE 4

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT gordsh1   TELAPSE   29309.72 TCPU   28862.18

DIMENSIONS P(G)= 2206952 F(G)= 353010 P(G),F(G) (IRR) 290516
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 135

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT   TELAPSE   29309.74 TCPU   28862.20

SYMMETRY ALLOWED INTERNAL DEGREE(S) OF FREEDOM: 36
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM   TELAPSE   29310.22 TCPU   28862.48
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN TELAPSE   29310.28 TCPU   28862.54

+++ 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.
IN CLASSES WRITTEN AS CX.Y OR SX.Y, X.Y IS A DECIMAL NUMBER THAT
APPROACHES THE OPERATION FRACTIONAL ORDER.]

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

K[1] (0 0 0)

CLASS | GROUP OPERATORS (SEE SYMMOPS KEYWORD)

C2 | 2;
SGV | 3;
SGV' | 4;

```
  IRREP/CLA  E   C2   SGV  SGV'
 -------------------------------
   A1 |  1.00  1.00  1.00  1.00
   A2 |  1.00  1.00 -1.00 -1.00
   B1 |  1.00 -1.00  1.00 -1.00
   B2 |  1.00 -1.00 -1.00  1.00


 A1 -(1,  37); A2 -(1,  33); B1 -(1,  35); B2 -(1,  39);



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

 CONVERSION FACTORS FOR FREQUENCIES:
    1 CM**(-1) =  0.2194746E+06 HARTREE
    1 THZ     =  0.2997925E-01 CM**(-1)


 HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
 HHHHHHHHHHHHH

  MODES      EIGV       FREQUENCIES   IRREP IR INTENS   RAMAN
          (HARTREE**2)  (CM**-1)  (THZ)        (KM/MOL)
  1-  1  -0.9357E-10   -2.1231  -0.0636  (B2 )  A (   0.00)  A
  2-  2  -0.7924E-10   -1.9537  -0.0586  (A1 )  A (   0.00)  A
  3-  3  -0.4747E-10   -1.5121  -0.0453  (B1 )  A (   0.00)  A
  4-  4   0.1722E-06   91.0697   2.7302  (B1 )  A (   0.00)  A
  5-  5   0.1847E-06   94.3196   2.8276  (B2 )  A (   0.00)  A
  6-  6   0.2065E-06   99.7380   2.9901  (A2 )  I (   0.00)  A
  7-  7   0.2544E-06  110.6899   3.3184  (A2 )  I (   0.00)  A
  8-  8   0.2670E-06  113.3979   3.3996  (B2 )  A (   0.00)  A
  9-  9   0.2764E-06  115.3911   3.4593  (B1 )  A (   0.00)  A
 10- 10   0.2830E-06  116.7560   3.5003  (A1 )  A (   0.00)  A
 11- 11   0.3288E-06  125.8407   3.7726  (B1 )  A (   0.00)  A
 12- 12   0.3370E-06  127.4036   3.8195  (A1 )  A (   0.00)  A
 13- 13   0.3446E-06  128.8419   3.8626  (A2 )  I (   0.00)  A
 14- 14   0.3507E-06  129.9695   3.8964  (B2 )  A (   0.00)  A
 15- 15   0.4242E-06  142.9400   4.2852  (B1 )  A (   0.00)  A
 16- 16   0.4388E-06  145.3886   4.3586  (B2 )  A (   0.00)  A
 17- 17   0.4488E-06  147.0363   4.4080  (A2 )  I (   0.00)  A
 18- 18   0.4687E-06  150.2503   4.5044  (A1 )  A (   0.00)  A
 19- 19   0.4849E-06  152.8327   4.5818  (B2 )  A (   0.00)  A
 20- 20   0.5136E-06  157.2901   4.7154  (A1 )  A (   0.00)  A
 21- 21   0.5493E-06  162.6691   4.8767  (B1 )  A (   0.00)  A
 22- 22   0.5640E-06  164.8255   4.9413  (A2 )  I (   0.00)  A
 23- 23   0.6014E-06  170.1968   5.1024  (B2 )  A (   0.00)  A
 24- 24   0.6349E-06  174.8759   5.2426  (B1 )  A (   0.00)  A
 25- 25   0.6723E-06  179.9611   5.3951  (B2 )  A (   0.00)  A
 26- 26   0.6871E-06  181.9315   5.4542  (B1 )  A (   0.00)  A
 27- 27   0.6892E-06  182.2053   5.4624  (A2 )  I (   0.00)  A
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28- 28   0.7110E-06  185.0618  5.5480  (A1 )   A (    0.00)   A
29- 29   0.7652E-06  191.9884  5.7557  (B2 )   A (    0.00)   A
30- 30   0.7831E-06  194.2170  5.8225  (B1 )   A (    0.00)   A
31- 31   0.8290E-06  199.8300  5.9908  (A2 )   I (    0.00)   A
32- 32   0.8339E-06  200.4158  6.0083  (A1 )   A (    0.00)   A
33- 33   0.8568E-06  203.1565  6.0905  (B1 )   A (    0.00)   A
34- 34   0.8950E-06  207.6353  6.2248  (B2 )   A (    0.00)   A
35- 35   0.8972E-06  207.8844  6.2322  (A1 )   A (    0.00)   A
36- 36   0.9032E-06  208.5762  6.2530  (B1 )   A (    0.00)   A
37- 37   0.1013E-05  220.8547  6.6211  (A2 )   I (    0.00)   A
38- 38   0.1021E-05  221.7700  6.6485  (A1 )   A (    0.00)   A
39- 39   0.1043E-05  224.1357  6.7194  (B2 )   A (    0.00)   A
40- 40   0.1117E-05  231.9249  6.9529  (A1 )   A (    0.00)   A
41- 41   0.1140E-05  234.3401  7.0253  (B1 )   A (    0.00)   A
42- 42   0.1212E-05  241.6047  7.2431  (A2 )   I (    0.00)   A
43- 43   0.1238E-05  244.1698  7.3200  (B2 )   A (    0.00)   A
44- 44   0.1257E-05  246.0481  7.3763  (A1 )   A (    0.00)   A
45- 45   0.1258E-05  246.1655  7.3799  (B2 )   A (    0.00)   A
46- 46   0.1272E-05  247.5394  7.4210  (A2 )   I (    0.00)   A
47- 47   0.1324E-05  252.5095  7.5700  (A1 )   A (    0.00)   A
48- 48   0.1336E-05  253.6715  7.6049  (A2 )   I (    0.00)   A
49- 49   0.1337E-05  253.7375  7.6069  (B2 )   A (    0.00)   A
50- 50   0.1349E-05  254.9143  7.6421  (B1 )   A (    0.00)   A
51- 51   0.1379E-05  257.7220  7.7263  (A1 )   A (    0.00)   A
52- 52   0.1390E-05  258.7681  7.7577  (A2 )   I (    0.00)   A
53- 53   0.1443E-05  263.6310  7.9035  (A2 )   I (    0.00)   A
54- 54   0.1518E-05  270.4015  8.1064  (B1 )   A (    0.00)   A
55- 55   0.1523E-05  270.8732  8.1206  (A1 )   A (    0.00)   A
56- 56   0.1546E-05  272.8705  8.1805  (B2 )   A (    0.00)   A
57- 57   0.1613E-05  278.7170  8.3557  (B1 )   A (    0.00)   A
58- 58   0.1637E-05  280.7980  8.4181  (A1 )   A (    0.00)   A
59- 59   0.1681E-05  284.5874  8.5317  (B1 )   A (    0.00)   A
60- 60   0.1685E-05  284.8589  8.5399  (A2 )   I (    0.00)   A
61- 61   0.1689E-05  285.2065  8.5503  (B2 )   A (    0.00)   A
62- 62   0.1826E-05  296.6131  8.8922  (B2 )   A (    0.00)   A
63- 63   0.1858E-05  299.1421  8.9681  (A2 )   I (    0.00)   A
64- 64   0.1859E-05  299.2529  8.9714  (A1 )   A (    0.00)   A
65- 65   0.1924E-05  304.4010  9.1257  (B2 )   A (    0.00)   A
66- 66   0.1979E-05  308.7303  9.2555  (B1 )   A (    0.00)   A
67- 67   0.2126E-05  319.9764  9.5927  (B2 )   A (    0.00)   A
68- 68   0.2130E-05  320.2946  9.6022  (A1 )   A (    0.00)   A
69- 69   0.2143E-05  321.2901  9.6320  (A2 )   I (    0.00)   A
70- 70   0.2241E-05  328.5874  9.8508  (A2 )   I (    0.00)   A
71- 71   0.2262E-05  330.0938  9.8960  (B1 )   A (    0.00)   A
72- 72   0.2353E-05  336.6607  10.0928  (B1 )   A (    0.00)   A
73- 73   0.2411E-05  340.8049  10.2171  (A1 )   A (    0.00)   A
74- 74   0.2457E-05  344.0006  10.3129  (B2 )   A (    0.00)   A
75- 75   0.2526E-05  348.7862  10.4563  (A1 )   A (    0.00)   A
76- 76   0.2574E-05  352.1279  10.5565  (B1 )   A (    0.00)   A
77- 77   0.2641E-05  356.6723  10.6928  (A2 )   I (    0.00)   A
78- 78   0.2707E-05  361.0981  10.8254  (B2 )   A (    0.00)   A
79- 79   0.2733E-05  362.8099  10.8768  (A1 )   A (    0.00)   A
80- 80   0.2905E-05  374.0982  11.2152  (A2 )   I (    0.00)   A
81- 81   0.3110E-05  387.0687  11.6040  (B1 )   A (    0.00)   A
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 82- 82   0.3111E-05   387.1074   11.6052 (B2 )   A (    0.00)   A
 83- 83   0.3272E-05   396.9978   11.9017 (B2 )   A (    0.00)   A
 84- 84   0.3289E-05   398.0133   11.9321 (B1 )   A (    0.00)   A
 85- 85   0.3312E-05   399.4262   11.9745 (A1 )   A (    0.00)   A
 86- 86   0.3539E-05   412.9093   12.3787 (A2 )   I (    0.00)   A
 87- 87   0.3540E-05   412.9170   12.3789 (B2 )   A (    0.00)   A
 88- 88   0.3675E-05   420.7202   12.6129 (B1 )   A (    0.00)   A
 89- 89   0.3748E-05   424.8696   12.7373 (A2 )   I (    0.00)   A
 90- 90   0.3854E-05   430.8824   12.9175 (B1 )   A (    0.00)   A
 91- 91   0.3883E-05   432.4979   12.9660 (A1 )   A (    0.00)   A
 92- 92   0.3983E-05   437.9924   13.1307 (B2 )   A (    0.00)   A
 93- 93   0.4631E-05   472.3075   14.1594 (B1 )   A (    0.00)   A
 94- 94   0.4718E-05   476.7066   14.2913 (A2 )   I (    0.00)   A
 95- 95   0.4804E-05   481.0517   14.4216 (B2 )   A (    0.00)   A
 96- 96   0.4836E-05   482.6387   14.4691 (A1 )   A (    0.00)   A
 97- 97   0.5157E-05   498.3860   14.9412 (A2 )   I (    0.00)   A
 98- 98   0.5397E-05   509.8604   15.2852 (A1 )   A (    0.00)   A
 99- 99   0.5431E-05   511.4612   15.3332 (B1 )   A (    0.00)   A
100- 100  0.5474E-05   513.5171   15.3949 (B2 )   A (    0.00)   A
101- 101  0.5664E-05   522.3506   15.6597 (A2 )   I (    0.00)   A
102- 102  0.5860E-05   531.2972   15.9279 (A1 )   A (    0.00)   A
103- 103  0.5917E-05   533.8844   16.0055 (B2 )   A (    0.00)   A
104- 104  0.6052E-05   539.9409   16.1870 (B1 )   A (    0.00)   A
105- 105  0.6247E-05   548.5565   16.4453 (A1 )   A (    0.00)   A
106- 106  0.6422E-05   556.1780   16.6738 (A2 )   I (    0.00)   A
107- 107  0.6644E-05   565.7138   16.9597 (A1 )   A (    0.00)   A
108- 108  0.6692E-05   567.7733   17.0214 (B2 )   A (    0.00)   A
109- 109  0.6705E-05   568.3015   17.0372 (B1 )   A (    0.00)   A
110- 110  0.6912E-05   577.0073   17.2982 (B2 )   A (    0.00)   A
111- 111  0.6952E-05   578.6851   17.3485 (A1 )   A (    0.00)   A
112- 112  0.7170E-05   587.6966   17.6187 (A2 )   I (    0.00)   A
113- 113  0.9279E-05   668.5653   20.0431 (A1 )   A (    0.00)   A
114- 114  0.9578E-05   679.2445   20.3632 (A2 )   I (    0.00)   A
115- 115  0.1041E-04   708.0469   21.2267 (B1 )   A (    0.00)   A
116- 116  0.1046E-04   709.8980   21.2822 (B2 )   A (    0.00)   A
117- 117  0.1398E-04   820.7474   24.6054 (B2 )   A (    0.00)   A
118- 118  0.1401E-04   821.3984   24.6249 (A1 )   A (    0.00)   A
119- 119  0.1411E-04   824.4722   24.7171 (B1 )   A (    0.00)   A
120- 120  0.1432E-04   830.5843   24.9003 (B2 )   A (    0.00)   A
121- 121  0.1494E-04   848.2964   25.4313 (A2 )   I (    0.00)   A
122- 122  0.1503E-04   850.9464   25.5107 (A1 )   A (    0.00)   A
123- 123  0.1550E-04   864.0546   25.9037 (A1 )   A (    0.00)   A
124- 124  0.1617E-04   882.4412   26.4549 (B2 )   A (    0.00)   A
125- 125  0.1624E-04   884.5126   26.5170 (A2 )   I (    0.00)   A
126- 126  0.1639E-04   888.4763   26.6359 (B1 )   A (    0.00)   A
127- 127  0.1667E-04   896.0043   26.8615 (B2 )   A (    0.00)   A
128- 128  0.1673E-04   897.6453   26.9107 (A1 )   A (    0.00)   A
129- 129  0.1696E-04   903.8423   27.0965 (A2 )   I (    0.00)   A
130- 130  0.1742E-04   915.9512   27.4595 (B1 )   A (    0.00)   A
131- 131  0.1768E-04   922.8638   27.6668 (B1 )   A (    0.00)   A
132- 132  0.1804E-04   932.3091   27.9499 (A1 )   A (    0.00)   A
133- 133  0.1814E-04   934.8533   28.0262 (B2 )   A (    0.00)   A
134- 134  0.1864E-04   947.5727   28.4075 (A1 )   A (    0.00)   A
135- 135  0.1869E-04   948.7198   28.4419 (A2 )   I (    0.00)   A
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136- 136   0.1913E-04   959.9044   28.7772  (B2 )   A (    0.00)   A
137- 137   0.1975E-04   975.3016   29.2388  (A1 )   A (    0.00)   A
138- 138   0.1984E-04   977.6905   29.3104  (B1 )   A (    0.00)   A
139- 139   0.2003E-04   982.2283   29.4465  (B2 )   A (    0.00)   A
140- 140   0.2055E-04   994.8184   29.8239  (A1 )   A (    0.00)   A
141- 141   0.2074E-04   999.4520   29.9628  (A2 )   I (    0.00)   A
142- 142   0.2144E-04   1016.1355  30.4630  (A2 )   I (    0.00)   A
143- 143   0.2244E-04   1039.6749  31.1687  (B2 )   A (    0.00)   A
144- 144   0.2262E-04   1043.9050  31.2955  (B1 )   A (    0.00)   A
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HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
HHHHHHHHHHHH
 VIBRATIONAL ANALYSIS:
 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 CONTAING A THIRD ATOM C (ANG) AND OUT OF THE PLANE (OUT).
 LONG+ANG+OUT=1.
 3) THE MODES ARE CLASSIFIED SO AS: LONG > 0.85 -> STRETCHING (S);
 ANG > 0.85 -> BENDING (B); OTHERWISE -> OTHER (O). TYPE (?) MEANS THE MODE IS
 LIKELY TO BE ROTATIONAL. THE POTENTIAL ENERGY CONTRIBUTION (PEC) IS IN KJ/MOL.
 HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
HHHHHHHHHHHH

 MODE FRQ(CM**-1) IRREP TYP   A   B LONG   C ANG   PEC
  1   -2.1231 (B2)
  2   -1.9537 (A1)
  3   -1.5121 (B1)
  4   91.0697 (B1)
               (?)   5 CA   8 CA(0.0) 10 CA(1.0)   0.0
               (?)   7 CA   6 CA(0.0) 12 CA(1.0)   0.0
  5   94.3196 (B2)
               (?)   1 CA   5 CA(0.0) 17 SI(1.0)   0.0
               (?)   1 CA   6 CA(0.0) 18 SI(1.0)   0.0
               (?)   2 CA   7 CA(0.0) 15 SI(1.0)   0.0
               (?)   2 CA   8 CA(0.0) 16 SI(1.0)   0.0
  6   99.7380 (A2)
               (?)   3 CA   5 CA(0.0) 11 CA(1.0)   0.0
               (?)   3 CA   8 CA(0.0) 10 CA(1.0)   0.0
               (?)   4 CA   6 CA(0.0) 12 CA(1.0) -0.1
               (?)   4 CA   7 CA(0.0)   9 CA(1.0)   0.0
               (?)   8 CA   5 CA(0.0)   1 CA(1.0)   0.0
               (?) 11 CA   5 CA(0.1)   3 CA(0.9)   0.0
               (?)   6 CA   7 CA(0.0)   2 CA(1.0)   0.0
               (?) 12 CA   6 CA(0.1)   4 CA(0.9)   0.0
               (?)   9 CA   7 CA(0.1)   4 CA(0.9)   0.0
               (?) 10 CA   8 CA(0.1)   3 CA(0.9)   0.0
  7   110.6899 (A2)
               (S) 33 O   1 CA(0.7) 11 CA(0.3)   0.0
               (S) 34 O   1 CA(0.7) 12 CA(0.3)   0.0
               (S)   2 CA 35 O (0.7) 11 CA(0.3)   0.0
               (S)   2 CA 36 O (0.7) 12 CA(0.3)   0.0
               (B)   8 CA   5 CA(0.0)   4 CA(1.0)   0.0
               (B)   7 CA   6 CA(0.0)   3 CA(1.0)   0.0

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 8   113.3979  (B2 )
                (B)   45 O    1 CA(0.1)   5 CA(0.9)    0.0
                (B)   46 O    1 CA(0.1)   6 CA(0.9)    0.0
                (B)   47 O    2 CA(0.1)   7 CA(0.9)    0.0
                (B)   48 O    2 CA(0.1)   8 CA(0.9)    0.0
                (B)   45 O    9 CA(0.0)  21 O (0.9)    0.0
                (B)   46 O   10 CA(0.0)  22 O (0.9)    0.0
                (B)   47 O   11 CA(0.0)  23 O (0.9)    0.0
                (B)   48 O   12 CA(0.0)  24 O (0.9)    0.0
 9   115.3911  (B1 )
                (B)    1 CA  11 CA(0.0)   7 CA(1.0)    0.0
                (B)    1 CA  12 CA(0.0)   8 CA(1.0)    0.0
                (O)   19 SI   1 CA(0.0)  45 O (0.7)    0.0
                (O)    2 CA  20 SI(0.0)  48 O (0.7)    0.0
10   116.7560  (A1 )
                (B)    5 CA   1 CA(0.0)  46 O (0.9)    0.0
                (B)    6 CA   1 CA(0.0)  45 O (0.9)    0.0
                (B)    7 CA   2 CA(0.0)  48 O (0.9)    0.0
                (B)    8 CA   2 CA(0.0)  47 O (0.9)    0.0
11   125.8407  (B1 )
                (B)    1 CA  19 SI(0.0)  37 O (1.0)    0.0
                (B)   39 O    1 CA(0.0)  43 O (1.0)    0.0
                (B)   40 O    1 CA(0.0)  44 O (1.0)    0.0
                (S)   43 O    1 CA(1.0)              0.0
                (S)   44 O    1 CA(1.0)              0.0
                (B)   45 O    1 CA(0.0)  33 O (1.0)    0.0
                (B)   46 O    1 CA(0.0)  34 O (1.0)    0.0
                (B)    2 CA  20 SI(0.0)  40 O (1.0)    0.0
                (B)   47 O    2 CA(0.0)  35 O (1.0)    0.0
                (B)   48 O    2 CA(0.0)  36 O (1.0)    0.0
                (S)    9 CA   5 CA(0.6)   9 CA(0.4)    0.0
                (B)    9 CA   5 CA(0.3)   9 CA(0.7)    0.0
                (S)   10 CA   6 CA(0.6)  10 CA(0.4)    0.0
                (B)   10 CA   6 CA(0.3)  10 CA(0.7)    0.0
                (S)   11 CA   7 CA(0.6)  11 CA(0.4)    0.0
                (B)   11 CA   7 CA(0.3)  11 CA(0.7)    0.0
                (S)   12 CA   8 CA(0.6)  12 CA(0.4)    0.0
                (B)   12 CA   8 CA(0.3)  12 CA(0.7)    0.0
12   127.4036  (A1 )
                (B)   11 CA   5 CA(0.1)  21 O (0.9)    0.0
                (B)   12 CA   6 CA(0.1)  22 O (0.9)    0.0
                (B)    9 CA   7 CA(0.1)  23 O (0.9)    0.0
                (B)   10 CA   8 CA(0.1)  24 O (0.9)    0.0
13   128.8419  (A2 )
                (B)    8 CA   5 CA(0.0)   9 CA(1.0)    0.0
                (B)    7 CA   6 CA(0.0)  10 CA(1.0)    0.0
14   129.9695  (B2 )
                (B)   11 CA   1 CA(0.2)   6 CA(0.8)    0.0
                (B)   12 CA   1 CA(0.2)   5 CA(0.8)    0.0
15   142.9400  (B1 )
                (B)   11 CA   1 CA(0.3)   6 CA(0.7)    0.0
                (B)   12 CA   1 CA(0.3)   5 CA(0.7)    0.0
                (B)   19 SI   1 CA(0.0)  43 O (1.0)    0.0
                (B)   39 O    1 CA(0.4)  44 O (0.5)    0.0
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            (B)  40 O   1 CA(0.4)  43 O (0.5)    0.0
            (B)  20 SI  2 CA(0.0)  47 O (0.9)    0.0
16  145.3886  (B2 )
            (B)   1 CA   5 CA(0.2)  27 O (0.8)    0.0
            (B)   1 CA   6 CA(0.2)  28 O (0.8)   -0.1
            (B)  45 O   1 CA(0.0)  40 O (0.9)    0.0
            (B)  46 O   1 CA(0.0)  39 O (0.9)    0.0
            (B)   2 CA   7 CA(0.2)  28 O (0.8)    0.0
            (B)   2 CA   8 CA(0.2)  27 O (0.8)    0.0
            (O)  47 O   2 CA(0.0)  35 O (0.7)    0.0
            (O)  48 O   2 CA(0.0)  36 O (0.7)    0.0
17  147.0363  (A2 )
            (B)  11 CA   1 CA(0.1)  12 CA(0.9)    0.0
            (B)  12 CA   1 CA(0.1)  19 SI(0.9)    0.0
            (S)  39 O   1 CA(0.5)  19 SI(0.4)    0.0
            (S)  40 O   1 CA(0.5)  39 O (0.4)    0.0
            (B)   9 CA  33 O (0.0)   1 CA(0.9)    0.0
            (B)  10 CA  34 O (0.0)   1 CA(0.9)    0.0
            (B)  35 O  11 CA(0.0)   1 CA(0.9)    0.0
            (B)  36 O  12 CA(0.0)   1 CA(0.9)    0.0
18  150.2503  (A1 )
            (B)   5 CA   3 CA(0.0)   6 CA(1.0)    0.0
            (B)   8 CA   3 CA(0.0)   7 CA(1.0)    0.0
            (B)   6 CA   4 CA(0.0)   5 CA(1.0)    0.0
            (B)   7 CA   4 CA(0.0)   8 CA(1.0)   -0.1
19  152.8327  (B2 )
            (B)  19 SI  1 CA(0.0)  43 O (1.0)    0.0
            (B)  33 O   1 CA(0.3)   6 CA(0.7)    0.0
            (B)  34 O   1 CA(0.3)   5 CA(0.7)    0.0
            (S)  43 O   1 CA(1.0)            0.0
            (S)  44 O   1 CA(1.0)            0.0
            (B)  45 O   1 CA(0.2)  43 O (0.8)    0.0
            (B)  46 O   1 CA(0.2)  44 O (0.8)    0.0
            (B)  20 SI  2 CA(0.0)  47 O (1.0)    0.0
            (B)  35 O   2 CA(0.3)   8 CA(0.7)    0.0
            (B)  36 O   2 CA(0.3)   7 CA(0.7)    0.0
            (B)  47 O   2 CA(0.2)  20 SI(0.7)    0.0
            (B)  48 O   2 CA(0.2)  47 O (0.7)    0.0
20  157.2901  (A1 )
            (S)   8 CA   5 CA(1.0)            0.0
            (B)  13 SI  5 CA(0.0)  25 O (1.0)    0.0
            (S)   7 CA   6 CA(1.0)            0.0
            (B)  14 SI  6 CA(0.0)  26 O (1.0)    0.0
            (B)   7 CA  14 SI(0.0)  26 O (1.0)    0.0
            (B)   8 CA  13 SI(0.0)  25 O (1.0)    0.0
21  162.6691  (B1 )
            (S)   5 CA   1 CA(0.9)            0.0
            (S)   6 CA   1 CA(0.9)            0.0
            (B)   1 CA  11 CA(0.0)  35 O (1.0)    0.0
            (B)   1 CA  12 CA(0.0)  36 O (1.0)    0.0
            (S)   7 CA   2 CA(0.9)            0.0
            (S)   8 CA   2 CA(0.9)            0.0
            (B)   5 CA  11 CA(0.1)  35 O (0.9)    0.0
            (B)   6 CA  12 CA(0.1)  36 O (0.9)    0.0
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        (B)   7 CA   9 CA(0.1)  33 O (0.9)   0.0
        (B)   8 CA  10 CA(0.1)  34 O (0.9)   0.0
        (O)  45 O    9 CA(0.0)  21 O (0.5)   0.0
        (O)  46 O   10 CA(0.0)  22 O (0.5)   0.0
        (O)  47 O   11 CA(0.0)  23 O (0.5)   0.0
        (O)  48 O   12 CA(0.0)  24 O (0.5)   0.0
22  164.8255 (A2 )
        (B)   9 CA   5 CA(0.0)  27 O (1.0)   0.0
        (B)   9 CA   5 CA(0.2)   1 CA(0.8)   0.0
        (B)  10 CA   6 CA(0.0)  28 O (1.0)   0.0
        (B)  10 CA   6 CA(0.2)   1 CA(0.8)   0.0
        (B)  11 CA   7 CA(0.0)  28 O (1.0)   0.0
        (B)  11 CA   7 CA(0.2)   2 CA(0.8)   0.0
        (B)  12 CA   8 CA(0.0)  27 O (1.0)   0.0
        (B)  12 CA   8 CA(0.2)   2 CA(0.8)   0.0
23  170.1968 (B2 )
        (S)  33 O    1 CA(1.0)           0.0
        (S)  34 O    1 CA(1.0)           0.0
        (S)  35 O    2 CA(1.0)           0.0
        (S)  36 O    2 CA(1.0)           0.0
24  174.8759 (B1 )
        (S)  33 O    1 CA(0.9)           0.0
        (S)  34 O    1 CA(0.9)           0.0
        (S)  35 O    2 CA(0.9)           0.0
        (S)  36 O    2 CA(0.9)           0.0
25  179.9611 (B2 )
        (B)   1 CA   5 CA(0.3)  17 SI(0.7)   0.0
        (B)   1 CA   6 CA(0.3)  18 SI(0.7)   0.0
        (B)  11 CA   1 CA(0.0)  33 O (1.0)   0.0
        (B)  12 CA   1 CA(0.0)  34 O (1.0)   0.0
        (S)  39 O    1 CA(0.8)  45 O (0.2)   0.0
        (S)  40 O    1 CA(0.8)  46 O (0.2)   0.0
        (B)  45 O    1 CA(0.0)  12 CA(1.0)   0.0
        (B)  46 O    1 CA(0.0)  11 CA(1.0)   0.0
        (B)   2 CA   7 CA(0.3)  15 SI(0.7)   0.0
        (B)   2 CA   8 CA(0.3)  16 SI(0.7)   0.0
        (B)  47 O    2 CA(0.0)  35 O (0.9)   0.0
        (B)  48 O    2 CA(0.0)  36 O (0.9)   0.0
26  181.9315 (B1 )
        (B)   8 CA   5 CA(0.0)  27 O (1.0)   0.0
        (B)   7 CA   6 CA(0.0)  28 O (1.0)   0.0
27  182.2053 (A2 )
        (B)  45 O    1 CA(0.0)  33 O (1.0)   0.0
        (B)  46 O    1 CA(0.0)  34 O (1.0)   0.0
        (B)  47 O    2 CA(0.0)  35 O (1.0)   0.0
        (B)  48 O    2 CA(0.0)  36 O (1.0)   0.0
        (O)  45 O    9 CA(0.1)  21 O (0.7)   0.0
        (O)  46 O   10 CA(0.1)  22 O (0.7)   0.0
        (O)  47 O   11 CA(0.1)  23 O (0.7)   0.0
        (O)  48 O   12 CA(0.1)  24 O (0.7)   0.0
        (O)  45 O   19 SI(0.0)  37 O (0.7)   0.0
        (O)  46 O   19 SI(0.0)  38 O (0.7)   0.0
        (O)  47 O   20 SI(0.0)  39 O (0.7)   0.0
        (O)  48 O   20 SI(0.0)  40 O (0.7)   0.0
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28   185.0618  (A1 )
              (B)  29 O    3 CA(0.0)   7 CA(1.0)   0.0
              (B)  32 O    3 CA(0.0)   6 CA(1.0)   0.0
              (B)  30 O    4 CA(0.0)   8 CA(1.0)   0.0
              (B)  31 O    4 CA(0.0)   5 CA(1.0)   0.0
              (B)  43 O    5 CA(0.0)  27 O (0.9)   0.0
              (B)  44 O    6 CA(0.0)  28 O (0.9)   0.0
              (B)  41 O    7 CA(0.0)  28 O (0.9)   0.0
              (B)  42 O    8 CA(0.0)  27 O (0.9)   0.0
29   191.9884  (B2 )
              (B)   6 CA   3 CA(0.0)   7 CA(1.0)  -0.1
              (S)   6 CA   3 CA(0.6)  27 O (0.4)  -0.1
              (B)   7 CA   3 CA(0.0)   6 CA(1.0)  -0.1
              (S)   7 CA   3 CA(0.6)  27 O (0.4)  -0.1
              (B)   5 CA   4 CA(0.0)   8 CA(1.0)   0.0
              (S)   5 CA   4 CA(0.6)  28 O (0.4)   0.0
              (B)   8 CA   4 CA(0.0)   5 CA(1.0)   0.0
              (S)   8 CA   4 CA(0.6)  28 O (0.4)   0.0
30   194.2170  (B1 )
              (B)   9 CA  15 SI(0.0)  37 O (1.0)   0.0
              (B)  29 O    9 CA(0.2)  21 O (0.8)   0.0
              (B)  37 O    9 CA(0.5)  45 O (0.5)   0.0
              (O)  41 O    9 CA(0.0)  21 O (0.8)   0.0
              (B)  10 CA  16 SI(0.0)  38 O (1.0)   0.0
              (B)  30 O   10 CA(0.2)  22 O (0.8)   0.0
              (B)  38 O   10 CA(0.5)  46 O (0.5)   0.0
              (O)  42 O   10 CA(0.0)  22 O (0.8)   0.0
              (B)  11 CA  17 SI(0.0)  39 O (1.0)   0.0
              (B)  31 O   11 CA(0.2)  23 O (0.8)   0.0
              (B)  39 O   11 CA(0.5)  47 O (0.5)   0.0
              (O)  43 O   11 CA(0.0)  23 O (0.8)   0.0
              (B)  12 CA  18 SI(0.0)  40 O (1.0)   0.0
              (B)  32 O   12 CA(0.2)  24 O (0.8)   0.0
              (B)  40 O   12 CA(0.5)  48 O (0.5)   0.0
              (O)  44 O   12 CA(0.0)  24 O (0.8)   0.0
31   199.8300  (A2 )
              (B)   6 CA   3 CA(0.3)  21 O (0.7)   0.0
              (B)   3 CA   6 CA(0.0)  28 O (1.0)   0.0
              (B)   7 CA   3 CA(0.3)  24 O (0.7)   0.0
              (B)   3 CA   7 CA(0.0)  28 O (1.0)   0.0
              (B)   5 CA   4 CA(0.3)  22 O (0.7)   0.0
              (B)   4 CA   5 CA(0.0)  27 O (1.0)   0.0
              (B)   8 CA   4 CA(0.3)  23 O (0.7)   0.0
              (B)   4 CA   8 CA(0.0)  27 O (1.0)   0.0
              (B)  25 O    5 CA(0.2)   8 CA(0.8)   0.0
              (B)  31 O    5 CA(0.0)  11 CA(1.0)   0.0
              (B)  26 O    6 CA(0.2)   7 CA(0.8)   0.0
              (B)  32 O    6 CA(0.0)  12 CA(1.0)   0.0
              (B)  26 O    7 CA(0.2)   6 CA(0.8)   0.1
              (B)  29 O    7 CA(0.0)   9 CA(1.0)   0.1
              (B)  25 O    8 CA(0.2)   5 CA(0.8)   0.0
              (B)  30 O    8 CA(0.0)  10 CA(1.0)   0.0
32   200.4158  (A1 )
              (B)   3 CA   5 CA(0.4)  27 O (0.6)   0.0
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          (B)   3 CA   8 CA(0.4)  27 O (0.6)   0.0
          (S)  27 O    3 CA(0.9)             0.0
          (B)   4 CA   6 CA(0.4)  28 O (0.6)   0.0
          (B)   7 CA   4 CA(0.4)  28 O (0.6)   0.0
          (S)  28 O    4 CA(0.9)             0.0
33   203.1565  (B1 )
          (B)   5 CA   8 CA(0.0)  30 O (0.9)   0.0
          (S)  31 O    5 CA(0.8)  11 CA(0.2)   0.0
          (B)   6 CA   7 CA(0.0)  29 O (0.9)   0.0
          (S)  32 O    6 CA(0.8)  12 CA(0.2)   0.0
          (S)   7 CA  29 O (0.8)   9 CA(0.2)   0.0
          (S)  30 O    8 CA(0.8)  10 CA(0.2)   0.0
34   207.6353  (B2 )
          (B)   3 CA   5 CA(0.0)  17 SI(1.0)   0.0
          (B)   6 CA   3 CA(0.3)   6 CA(0.7)  -0.1
          (S)   6 CA   3 CA(0.5)   5 CA(0.5)  -0.1
          (B)   7 CA   3 CA(0.3)   7 CA(0.7)   0.0
          (S)   7 CA   3 CA(0.5)   8 CA(0.5)   0.0
          (B)   3 CA   8 CA(0.0)  16 SI(1.0)   0.0
          (B)  26 O    3 CA(0.1)  27 O (0.9)   0.0
          (B)   5 CA   4 CA(0.3)   5 CA(0.7)   0.0
          (S)   5 CA   4 CA(0.5)   6 CA(0.5)   0.0
          (B)   4 CA   6 CA(0.0)  18 SI(1.0)  -0.1
          (B)   4 CA   7 CA(0.0)  15 SI(1.0)  -0.1
          (B)   8 CA   4 CA(0.3)   8 CA(0.7)   0.0
          (S)   8 CA   4 CA(0.5)   7 CA(0.5)   0.0
          (B)  25 O    4 CA(0.1)  14 SI(0.9)   0.0
35   207.8844  (A1 )
          (B)  33 O    9 CA(0.3)   5 CA(0.7)   0.0
          (O)  45 O    9 CA(0.1)  33 O (0.7)   0.0
          (B)  34 O   10 CA(0.3)   6 CA(0.7)   0.0
          (O)  46 O   10 CA(0.1)  34 O (0.7)   0.0
          (B)  35 O   11 CA(0.3)   7 CA(0.7)   0.0
          (O)  47 O   11 CA(0.1)  35 O (0.7)   0.0
          (B)  36 O   12 CA(0.3)   8 CA(0.7)   0.0
          (O)  48 O   12 CA(0.1)  36 O (0.7)   0.0
36   208.5762  (B1 )
          (B)   3 CA   5 CA(0.4)  11 CA(0.5)   0.0
          (B)   6 CA   3 CA(0.1)  21 O (0.9)   0.0
          (B)   3 CA   6 CA(0.0)   1 CA(1.0)   0.0
          (B)   7 CA   3 CA(0.1)  24 O (0.9)  -0.1
          (B)   3 CA   7 CA(0.0)   2 CA(1.0)  -0.1
          (B)   3 CA   8 CA(0.4)  10 CA(0.5)   0.0
          (B)   5 CA   4 CA(0.1)  22 O (0.9)   0.0
          (B)   4 CA   5 CA(0.0)   1 CA(1.0)   0.0
          (B)   4 CA   6 CA(0.4)  12 CA(0.5)   0.0
          (B)   4 CA   7 CA(0.4)   9 CA(0.5)   0.0
          (B)   8 CA   4 CA(0.1)  23 O (0.9)   0.0
          (B)   4 CA   8 CA(0.0)   2 CA(1.0)   0.0
37   220.8547  (A2 )
          (B)   9 CA   5 CA(0.3)   9 CA(0.7)   0.0
          (S)   5 CA   9 CA(0.8)  15 SI(0.2)   0.0
          (B)  10 CA   6 CA(0.3)  10 CA(0.7)   0.0
          (S)   6 CA  10 CA(0.8)  16 SI(0.2)   0.0
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          (B)  11 CA   7 CA(0.3)  11 CA(0.7)   0.0
          (S)   7 CA  11 CA(0.8)  17 SI(0.2)    0.0
          (B)  12 CA   8 CA(0.3)  12 CA(0.7)   0.0
          (S)   8 CA  12 CA(0.8)  18 SI(0.2)    0.0
          (B)  21 O    9 CA(0.0)  41 O (1.0)    0.0
          (B)  29 O    9 CA(0.0)   5 CA(1.0)    0.0
          (B)  22 O   10 CA(0.0)  42 O (1.0)    0.1
          (B)  30 O   10 CA(0.0)   6 CA(1.0)    0.1
          (B)  23 O   11 CA(0.0)  43 O (1.0)    0.0
          (B)  31 O   11 CA(0.0)   7 CA(1.0)    0.0
          (B)  24 O   12 CA(0.0)  44 O (1.0)    0.0
          (B)  32 O   12 CA(0.0)   8 CA(1.0)    0.0
38   221.7700  (A1 )
          (B)  11 CA   5 CA(0.2)   4 CA(0.8)    0.0
          (B)  13 SI   5 CA(0.1)  31 O (0.9)    0.0
          (B)  25 O    5 CA(0.0)  33 O (1.0)    0.0
          (B)  27 O    5 CA(0.0)   4 CA(1.0)    0.0
          (B)  12 CA   6 CA(0.2)   3 CA(0.8)    0.0
          (B)  14 SI   6 CA(0.1)  32 O (0.9)    0.0
          (B)  26 O    6 CA(0.0)  34 O (1.0)    0.0
          (B)  28 O    6 CA(0.0)   3 CA(1.0)    0.0
          (B)   9 CA   7 CA(0.2)   3 CA(0.8)    0.0
          (B)  14 SI   7 CA(0.1)  29 O (0.9)    0.0
          (B)  26 O    7 CA(0.0)  35 O (1.0)    0.0
          (B)  28 O    7 CA(0.0)   3 CA(1.0)    0.0
          (B)  10 CA   8 CA(0.2)   4 CA(0.8)    0.0
          (B)  13 SI   8 CA(0.1)  30 O (0.9)    0.0
          (B)  25 O    8 CA(0.0)  36 O (1.0)    0.1
          (B)  27 O    8 CA(0.0)   4 CA(1.0)    0.1
39   224.1357  (B2 )
          (O)  29 O    9 CA(0.1)  21 O (0.6)    0.0
          (B)   9 CA  33 O (0.0)   1 CA(1.0)    0.0
          (S)  37 O    9 CA(0.7)  45 O (0.3)    0.0
          (O)  30 O   10 CA(0.1)  22 O (0.6)    0.0
          (B)  10 CA  34 O (0.0)   1 CA(1.0)    0.0
          (S)  38 O   10 CA(0.7)  46 O (0.3)    0.0
          (O)  31 O   11 CA(0.1)  23 O (0.6)    0.1
          (B)  35 O   11 CA(0.0)   1 CA(1.0)    0.1
          (S)  39 O   11 CA(0.7)  47 O (0.3)    0.0
          (O)  32 O   12 CA(0.1)  24 O (0.6)    0.0
          (B)  36 O   12 CA(0.0)   1 CA(1.0)    0.0
          (S)  40 O   12 CA(0.7)  48 O (0.3)    0.0
40   231.9249  (A1 )
          (B)   9 CA   5 CA(0.0)  31 O (1.0)    0.0
          (B)   9 CA   5 CA(0.0)  25 O (1.0)    0.0
          (B)  11 CA   5 CA(0.5)   4 CA(0.5)    0.0
          (B)  31 O    5 CA(0.3)  11 CA(0.6)    0.0
          (B)  10 CA   6 CA(0.0)  32 O (1.0)    0.0
          (B)  10 CA   6 CA(0.0)  26 O (1.0)    0.0
          (B)  12 CA   6 CA(0.5)   3 CA(0.5)    0.0
          (B)  32 O    6 CA(0.3)  12 CA(0.6)    0.0
          (B)   9 CA   7 CA(0.5)   3 CA(0.5)    0.1
          (B)  11 CA   7 CA(0.0)  29 O (1.0)    0.0
          (B)  11 CA   7 CA(0.0)  26 O (1.0)    0.0
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      (B)   7 CA   29 O (0.3)   9 CA(0.6)   0.1
      (B)  10 CA    8 CA(0.5)   4 CA(0.5)   0.0
      (B)  12 CA    8 CA(0.0)  30 O (1.0)   0.0
      (B)  12 CA    8 CA(0.0)  25 O (1.0)   0.0
      (B)  30 O     8 CA(0.3)  10 CA(0.6)   0.0
      (B)  33 O     9 CA(0.0)  41 O (1.0)   0.0
      (B)  34 O    10 CA(0.0)  42 O (1.0)   0.0
      (B)  35 O    11 CA(0.0)  43 O (1.0)   0.0
      (B)  36 O    12 CA(0.0)  44 O (1.0)   0.0
41   234.3401  (B1 )
      (B)   8 CA    5 CA(0.0)  27 O (1.0)   0.0
      (B)   5 CA    9 CA(0.0)  41 O (1.0)   0.0
      (S)   9 CA    5 CA(0.9)              0.0
      (B)   7 CA    6 CA(0.0)  28 O (1.0)   0.0
      (B)   6 CA   10 CA(0.0)  42 O (1.0)   0.0
      (S)  10 CA    6 CA(0.9)              0.0
      (B)   7 CA   11 CA(0.0)  43 O (1.0)   0.0
      (S)  11 CA    7 CA(0.9)              0.0
      (B)   8 CA   12 CA(0.0)  44 O (1.0)   0.0
      (S)  12 CA    8 CA(0.9)              0.0
42   241.6047  (A2 )
      (O)  45 O     9 CA(0.1)  21 O (0.7)   0.0
      (O)  46 O    10 CA(0.1)  22 O (0.7)   0.0
      (O)  47 O    11 CA(0.1)  23 O (0.7)   0.0
      (O)  48 O    12 CA(0.1)  24 O (0.7)   0.0
43   244.1698  (B2 )
      (B)   3 CA    5 CA(0.2)  31 O (0.8)   0.0
      (B)   3 CA    8 CA(0.2)  30 O (0.8)   0.0
      (B)   4 CA    6 CA(0.2)  32 O (0.8)   0.0
      (B)   4 CA    7 CA(0.2)  29 O (0.8)   0.0
      (B)  27 O     5 CA(0.1)  43 O (0.9)   0.0
      (B)  28 O     6 CA(0.1)  44 O (0.9)   0.0
      (B)  28 O     7 CA(0.1)  41 O (0.9)   0.0
      (B)  27 O     8 CA(0.1)  42 O (0.9)   0.0
44   246.0481  (A1 )
      (S)  27 O     3 CA(0.8)  26 O (0.2)   0.0
      (S)  28 O     4 CA(0.8)  14 SI(0.2)   0.0
45   246.1655  (B2 )
      (S)   6 CA    3 CA(0.8)  26 O (0.2)   0.0
      (B)   6 CA    3 CA(0.3)   5 CA(0.7)   0.0
      (S)   7 CA    3 CA(0.8)  26 O (0.2)   0.0
      (B)   7 CA    3 CA(0.3)   8 CA(0.7)   0.0
      (B)   3 CA   13 SI(0.5)  25 O (0.5)   0.0
      (S)   5 CA    4 CA(0.8)  25 O (0.2)   0.0
      (B)   5 CA    4 CA(0.3)   6 CA(0.7)   0.0
      (S)   8 CA    4 CA(0.8)  25 O (0.2)   0.0
      (B)   8 CA    4 CA(0.3)   7 CA(0.7)   0.0
      (B)   4 CA   14 SI(0.5)  28 O (0.5)   0.0
46   247.5394  (A2 )
      (S)  31 O     5 CA(0.9)              0.0
      (S)  32 O     6 CA(0.9)              0.0
      (S)  29 O     7 CA(0.9)              0.0
      (S)  30 O     8 CA(0.9)              0.0
47   252.5095  (A1 )
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              (B)  43 O    1 CA(0.1) 44 O (0.9)   0.0
              (B)  44 O    1 CA(0.1) 19 SI(0.9)   0.0
48   253.6715  (A2 )
              (S)   9 CA   5 CA(0.8) 33 O (0.2)   0.0
              (B)   5 CA   9 CA(0.1) 15 SI(0.9)   0.0
              (B)  11 CA   5 CA(0.2) 21 O (0.8)   0.0
              (S)  10 CA   6 CA(0.8) 34 O (0.2)   0.0
              (B)   6 CA  10 CA(0.1) 16 SI(0.9)   0.0
              (B)  12 CA   6 CA(0.2) 22 O (0.8)   0.0
              (B)   9 CA   7 CA(0.2) 23 O (0.8)   0.0
              (S)  11 CA   7 CA(0.8) 35 O (0.2)   0.0
              (B)   7 CA  11 CA(0.1) 17 SI(0.9)   0.0
              (B)  10 CA   8 CA(0.2) 24 O (0.8)   0.0
              (S)  12 CA   8 CA(0.8) 36 O (0.2)   0.0
              (B)   8 CA  12 CA(0.1) 18 SI(0.9)   0.0
              (S)  29 O    9 CA(0.9)              0.1
              (S)  30 O   10 CA(0.9)              0.0
              (S)  31 O   11 CA(0.9)              0.0
              (S)  32 O   12 CA(0.9)              0.0
49   253.7375  (B2 )
              (S)   9 CA  29 O (0.7)  7 CA(0.2)   0.1
              (S)  10 CA  30 O (0.7)  8 CA(0.2)   0.0
              (S)  31 O   11 CA(0.7)  5 CA(0.2)   0.0
              (S)  12 CA  32 O (0.7)  6 CA(0.2)   0.0
50   254.9143  (B1 )
              (S)  21 O    3 CA(0.5)  6 CA(0.5)   0.0
              (S)  24 O    3 CA(0.5)  7 CA(0.5)   0.0
              (S)  22 O    4 CA(0.5)  5 CA(0.5)   0.0
              (S)  23 O    4 CA(0.5)  8 CA(0.5)   0.0
              (B)  21 O    9 CA(0.0)  7 CA(0.9)   0.1
              (B)  22 O   10 CA(0.0)  8 CA(0.9)   0.0
              (B)  23 O   11 CA(0.0)  5 CA(0.9)   0.1
              (B)  24 O   12 CA(0.0)  6 CA(0.9)   0.0
51   257.7220  (A1 )
              (B)  27 O    3 CA(0.3) 26 O (0.7)   0.0
              (B)  28 O    4 CA(0.3) 14 SI(0.7)   0.0
52   258.7681  (A2 )
              (S)  25 O    5 CA(0.7)  8 CA(0.3)   0.0
              (S)  26 O    6 CA(0.7)  7 CA(0.3)   0.1
              (S)  26 O    7 CA(0.7)  6 CA(0.3)   0.0
              (S)  25 O    8 CA(0.7)  5 CA(0.3)   0.0
              (B)  21 O    9 CA(0.0)  7 CA(0.9)   0.1
              (B)  22 O   10 CA(0.0)  8 CA(0.9)   0.0
              (B)  23 O   11 CA(0.0)  5 CA(0.9)   0.0
              (B)  24 O   12 CA(0.0)  6 CA(0.9)   0.0
53   263.6310  (A2 )
              (B)   5 CA   1 CA(0.0) 46 O (1.0)   0.0
              (B)   6 CA   1 CA(0.0) 45 O (1.0)   0.0
              (B)   7 CA   2 CA(0.0) 48 O (1.0)  -0.1
              (B)   8 CA   2 CA(0.0) 47 O (1.0)   0.0
54   270.4015  (B1 )
              (B)  13 SI   3 CA(0.0)  7 CA(1.0)   0.0
              (O)  26 O    3 CA(0.0)  6 CA(0.7)   0.0
              (O)  27 O    3 CA(0.0)  6 CA(0.8)   0.0
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          (B)   14 SI   4 CA(0.0)   8 CA(1.0)    0.0
          (O)    4 CA  25 O (0.0)   8 CA(0.7)    0.0
          (O)   28 O    4 CA(0.0)   8 CA(0.8)    0.0
55   270.8732  (A1 )
          (S)    9 CA  29 O (0.8)  15 SI(0.2)    0.1
          (S)   30 O   10 CA(0.8)  16 SI(0.2)    0.0
          (S)   11 CA  31 O (0.8)  17 SI(0.2)    0.0
          (S)   32 O   12 CA(0.8)  18 SI(0.2)    0.0
56   272.8705  (B2 )
          (S)   13 SI   3 CA(0.9)               0.0
          (S)   21 O    3 CA(0.6)  29 O (0.3)    0.0
          (S)   24 O    3 CA(0.6)  32 O (0.3)    0.0
          (B)   27 O    3 CA(0.0)  26 O (1.0)    0.0
          (S)   14 SI   4 CA(0.9)               0.0
          (S)   22 O    4 CA(0.6)  30 O (0.3)    0.0
          (S)   23 O    4 CA(0.6)  31 O (0.3)    0.0
          (B)    4 CA  28 O (0.0)  14 SI(1.0)    0.0
57   278.7170  (B1 )
          (S)   37 O    9 CA(0.7)   5 CA(0.3)    0.1
          (S)   41 O    9 CA(0.5)  29 O (0.5)    0.1
          (S)   38 O   10 CA(0.7)   6 CA(0.3)    0.0
          (S)   42 O   10 CA(0.5)  30 O (0.5)    0.0
          (S)   39 O   11 CA(0.7)   7 CA(0.3)    0.0
          (S)   43 O   11 CA(0.5)  31 O (0.5)    0.0
          (S)   40 O   12 CA(0.7)   8 CA(0.3)    0.0
          (S)   44 O   12 CA(0.5)  32 O (0.5)    0.0
58   280.7980  (A1 )
          (B)   31 O    5 CA(0.4)  27 O (0.5)    0.0
          (B)   33 O    5 CA(0.1)  27 O (0.8)    0.0
          (B)   32 O    6 CA(0.4)  28 O (0.5)    0.0
          (B)   34 O    6 CA(0.1)  28 O (0.8)    0.0
          (B)   29 O    7 CA(0.4)  28 O (0.5)    0.1
          (B)   35 O    7 CA(0.1)  28 O (0.8)    0.1
          (B)   30 O    8 CA(0.4)  27 O (0.5)    0.0
          (B)   36 O    8 CA(0.1)  27 O (0.8)    0.0
          (B)    9 CA  29 O (0.4)   7 CA(0.5)    0.0
          (B)   30 O   10 CA(0.4)   8 CA(0.5)    0.0
          (B)   31 O   11 CA(0.4)   5 CA(0.5)    0.1
          (B)   12 CA  32 O (0.4)   6 CA(0.5)    0.0
59   284.5874  (B1 )
          (S)   31 O    5 CA(1.0)               0.0
          (S)   32 O    6 CA(1.0)               0.0
          (S)   29 O    7 CA(1.0)               0.0
          (S)   30 O    8 CA(1.0)               0.0
60   284.8589  (A2 )
          (S)   27 O    5 CA(0.6)  33 O (0.4)    0.0
          (S)   28 O    6 CA(0.6)  34 O (0.4)    0.0
          (S)   28 O    7 CA(0.6)  35 O (0.4)    0.0
          (S)   27 O    8 CA(0.6)  36 O (0.4)    0.0
61   285.2065  (B2 )
          (S)   27 O    3 CA(0.8)  26 O (0.2)    0.0
          (S)   28 O    4 CA(0.8)  14 SI(0.2)    0.0
62   296.6131  (B2 )
          (S)   37 O    9 CA(0.9)               0.0
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            (S)  38 O   10 CA(0.9)           0.0
            (S)  39 O   11 CA(0.9)           0.0
            (S)  40 O   12 CA(0.9)           0.0
63  299.1421  (A2 )
            (B)  29 O    3 CA(0.4)   5 CA(0.6)   0.0
            (B)  32 O    3 CA(0.4)   8 CA(0.6)   0.0
            (B)  30 O    4 CA(0.4)   6 CA(0.6)   0.0
            (B)  31 O    4 CA(0.4)   7 CA(0.6)   0.0
64  299.2529  (A1 )
            (S)  26 O    3 CA(0.9)           0.0
            (S)  25 O    4 CA(0.9)           0.0
            (S)  25 O    5 CA(0.6)   8 CA(0.4)   0.0
            (S)  26 O    6 CA(0.6)   7 CA(0.4)   0.1
            (S)   7 CA  26 O (0.6)   6 CA(0.4)   0.1
            (S)   8 CA  25 O (0.6)   5 CA(0.4)   0.0
65  304.4010  (B2 )
            (S)  26 O    3 CA(0.9)           0.0
            (S)  25 O    4 CA(0.9)           0.0
            (B)  25 O    5 CA(0.3)  43 O (0.7)   0.0
            (B)  26 O    6 CA(0.3)  44 O (0.7)   0.1
            (B)  26 O    7 CA(0.3)  41 O (0.7)   0.1
            (B)  25 O    8 CA(0.3)  42 O (0.7)   0.0
            (B)  21 O    9 CA(0.1)   7 CA(0.9)   0.0
            (B)  22 O   10 CA(0.1)   8 CA(0.9)   0.0
            (B)  23 O   11 CA(0.1)   5 CA(0.9)   0.0
            (B)  24 O   12 CA(0.1)   6 CA(0.9)   0.0
            (B)  27 O   13 SI(0.0)  25 O (1.0)   0.0
            (B)  28 O   14 SI(0.0)   4 CA(1.0)   0.0
66  308.7303  (B1 )
            (B)  27 O    5 CA(0.4)  33 O (0.6)   0.1
            (B)  28 O    6 CA(0.4)  34 O (0.6)   0.1
            (B)  28 O    7 CA(0.4)  35 O (0.6)   0.0
            (B)  27 O    8 CA(0.4)  36 O (0.6)   0.0
67  319.9764  (B2 )
            (B)  33 O    5 CA(0.3)  43 O (0.7)   0.0
            (S)  43 O    5 CA(0.5)  17 SI(0.5)   0.0
            (B)  34 O    6 CA(0.3)  44 O (0.7)   0.0
            (S)  44 O    6 CA(0.5)  18 SI(0.5)   0.0
            (B)  35 O    7 CA(0.3)  41 O (0.7)   0.1
            (S)  41 O    7 CA(0.5)  15 SI(0.5)   0.0
            (B)  36 O    8 CA(0.3)  42 O (0.7)   0.0
            (S)  42 O    8 CA(0.5)  16 SI(0.5)   0.0
            (S)   9 CA  33 O (0.7)   1 CA(0.3)   0.0
            (S)  10 CA  34 O (0.7)   1 CA(0.3)   0.0
            (S)  35 O   11 CA(0.7)   1 CA(0.3)   0.1
            (S)  36 O   12 CA(0.7)   1 CA(0.3)   0.0
68  320.2946  (A1 )
            (B)  21 O    3 CA(0.2)  27 O (0.8)   0.0
            (B)  24 O    3 CA(0.2)  27 O (0.8)   0.0
            (B)  22 O    4 CA(0.2)  28 O (0.8)   0.0
            (B)  23 O    4 CA(0.2)  28 O (0.8)   0.0
69  321.2901  (A2 )
            (B)  27 O    5 CA(0.4)  33 O (0.6)   0.0
            (B)  28 O    6 CA(0.4)  34 O (0.6)   0.1
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       (B)   28 O    7 CA(0.4)  35 O (0.6)    0.0
       (B)   27 O    8 CA(0.4)  36 O (0.6)    0.0
       (O)   27 O   13 SI(0.0)   8 CA(0.8)    0.0
       (O)   28 O   14 SI(0.0)   7 CA(0.8)    0.0
70  328.5874  (A2 )
       (S)   43 O    5 CA(0.7)  17 SI(0.3)    0.0
       (S)   44 O    6 CA(0.7)  18 SI(0.3)    0.0
       (S)   41 O    7 CA(0.7)  15 SI(0.3)    0.1
       (S)   42 O    8 CA(0.7)  16 SI(0.3)    0.0
71  330.0938  (B1 )
       (S)   43 O    5 CA(0.9)             0.0
       (S)   44 O    6 CA(0.9)             0.0
       (S)   41 O    7 CA(0.9)             0.1
       (S)   42 O    8 CA(0.9)             0.0
72  336.6607  (B1 )
       (B)   45 O    9 CA(0.4)  15 SI(0.6)    0.0
       (B)   46 O   10 CA(0.4)  16 SI(0.6)    0.1
       (B)   47 O   11 CA(0.4)  17 SI(0.6)    0.0
       (B)   48 O   12 CA(0.4)  18 SI(0.6)    0.0
73  340.8049  (A1 )
       (S)   43 O    5 CA(1.0)             0.0
       (S)   44 O    6 CA(1.0)             0.0
       (S)   41 O    7 CA(1.0)             0.2
       (S)   42 O    8 CA(1.0)             0.0
       (B)   41 O    9 CA(0.0)   5 CA(1.0)    0.1
       (B)   42 O   10 CA(0.0)   6 CA(1.0)    0.0
       (B)   43 O   11 CA(0.0)   7 CA(1.0)    0.0
       (B)   44 O   12 CA(0.0)   8 CA(1.0)    0.0
74  344.0006  (B2 )
       (B)   43 O    1 CA(0.1)   5 CA(0.9)    0.0
       (B)    1 CA  44 O (0.1)   6 CA(0.9)    0.0
       (S)   43 O    5 CA(1.0)             0.0
       (S)   44 O    6 CA(1.0)             0.0
       (S)   41 O    7 CA(1.0)             0.1
       (S)   42 O    8 CA(1.0)             0.0
75  348.7862  (A1 )
       (S)    1 CA  45 O (0.8)   9 CA(0.2)    0.0
       (S)    1 CA  46 O (0.8)  10 CA(0.2)    0.0
       (S)    2 CA  47 O (0.8)  11 CA(0.2)    0.0
       (S)    2 CA  48 O (0.8)  12 CA(0.2)    0.0
76  352.1279  (B1 )
       (B)   33 O    5 CA(0.4)  43 O (0.6)    0.0
       (B)   34 O    6 CA(0.4)  44 O (0.6)    0.0
       (B)   35 O    7 CA(0.4)  41 O (0.6)    0.1
       (B)   36 O    8 CA(0.4)  42 O (0.6)    0.0
       (B)    9 CA  33 O (0.3)   1 CA(0.7)    0.0
       (B)   10 CA  34 O (0.3)   1 CA(0.7)    0.0
       (B)   35 O   11 CA(0.3)   1 CA(0.7)    0.1
       (B)   36 O   12 CA(0.3)   1 CA(0.7)    0.0
77  356.6723  (A2 )
       (S)   21 O    9 CA(0.8)  33 O (0.2)    0.0
       (O)   33 O    9 CA(0.1)  41 O (0.8)    0.0
       (B)   41 O    9 CA(0.0)  33 O (1.0)    0.0
       (S)   22 O   10 CA(0.8)  34 O (0.2)    0.0
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        (O)   34 O   10 CA(0.1)  42 O (0.8)   0.0
        (B)   42 O   10 CA(0.0)  34 O (1.0)   0.0
        (S)   23 O   11 CA(0.8)  35 O (0.2)   0.0
        (O)   35 O   11 CA(0.1)  43 O (0.8)   0.0
        (B)   43 O   11 CA(0.0)  35 O (1.0)   0.0
        (S)   24 O   12 CA(0.8)  36 O (0.2)   0.0
        (O)   36 O   12 CA(0.1)  44 O (0.8)   0.0
        (B)   44 O   12 CA(0.0)  36 O (1.0)   0.0
78  361.0981  (B2 )
        (B)   33 O    5 CA(0.1)   9 CA(0.9)   0.0
        (B)   43 O    5 CA(0.4)  21 O (0.6)   0.0
        (B)    6 CA  34 O (0.1)  10 CA(0.9)   0.0
        (B)   44 O    6 CA(0.4)  22 O (0.6)   0.0
        (B)   35 O    7 CA(0.1)  11 CA(0.9)   0.1
        (B)   41 O    7 CA(0.4)  23 O (0.6)   0.0
        (B)   36 O    8 CA(0.1)  12 CA(0.9)   0.0
        (B)   42 O    8 CA(0.4)  24 O (0.6)   0.0
        (S)   45 O    9 CA(0.6)   5 CA(0.4)   0.0
        (S)   46 O   10 CA(0.6)   6 CA(0.4)   0.0
        (S)   47 O   11 CA(0.6)   7 CA(0.4)   0.0
        (S)   48 O   12 CA(0.6)   8 CA(0.4)   0.0
        (B)   45 O   19 SI(0.0)  38 O (0.9)   0.0
        (B)   46 O   19 SI(0.0)  37 O (0.9)   0.0
        (B)   47 O   20 SI(0.0)  40 O (0.9)   0.0
        (B)   48 O   20 SI(0.0)  39 O (0.9)   0.0
79  362.8099  (A1 )
        (S)   31 O    5 CA(0.5)   9 CA(0.5)   0.0
        (B)   33 O    5 CA(0.5)  43 O (0.5)   0.0
        (B)   43 O    5 CA(0.2)   3 CA(0.8)   0.0
        (S)   32 O    6 CA(0.5)  10 CA(0.5)   0.0
        (B)   34 O    6 CA(0.5)  44 O (0.5)   0.0
        (B)   44 O    6 CA(0.2)   4 CA(0.8)   0.0
        (S)   29 O    7 CA(0.5)  11 CA(0.5)   0.0
        (B)   35 O    7 CA(0.5)  41 O (0.5)   0.0
        (B)   41 O    7 CA(0.2)   4 CA(0.8)   0.0
        (S)   30 O    8 CA(0.5)  12 CA(0.5)   0.0
        (B)   36 O    8 CA(0.5)  42 O (0.5)   0.0
        (B)   42 O    8 CA(0.2)   3 CA(0.8)   0.0
80  374.0982  (A2 )
        (S)   19 SI   1 CA(1.0)              0.0
        (B)   33 O    1 CA(0.5)  34 O (0.5)   0.0
        (B)   34 O    1 CA(0.5)  33 O (0.5)   0.0
        (B)   43 O    1 CA(0.1)  46 O (0.9)   0.0
        (B)   44 O    1 CA(0.1)  45 O (0.9)   0.0
        (S)   45 O    1 CA(0.6)  43 O (0.4)   0.0
        (S)   46 O    1 CA(0.6)  44 O (0.4)   0.0
        (S)   20 SI   2 CA(1.0)              0.0
        (B)   35 O    2 CA(0.5)  36 O (0.5)   0.0
        (B)   36 O    2 CA(0.5)  35 O (0.5)   0.0
        (S)    2 CA  47 O (0.6)  20 SI(0.3)   0.0
        (S)   48 O    2 CA(0.6)  47 O (0.3)   0.0
        (B)   15 SI  29 O (0.0)   3 CA(0.9)   0.0
        (B)   16 SI  30 O (0.0)   4 CA(0.9)   0.0
        (B)   17 SI  31 O (0.0)   4 CA(0.9)   0.0
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          (B)  18 SI  32 O (0.0)   3 CA(0.9)   0.0
81  387.0687  (B1 )
          (S)  45 O    9 CA(0.8)  29 O (0.2)   0.2
          (S)  46 O   10 CA(0.8)  30 O (0.2)   0.0
          (S)  47 O   11 CA(0.8)  31 O (0.2)   0.0
          (S)  48 O   12 CA(0.8)  32 O (0.2)   0.0
82  387.1074  (B2 )
          (S)   9 CA  45 O (0.8)   1 CA(0.2)   0.2
          (S)  10 CA  46 O (0.8)   1 CA(0.2)   0.0
          (S)  11 CA  47 O (0.8)   2 CA(0.2)   0.0
          (S)  12 CA  48 O (0.8)   2 CA(0.2)   0.0
83  396.9978  (B2 )
          (B)  31 O    5 CA(0.1)  27 O (0.8)   0.0
          (S)  33 O    5 CA(0.9)            0.0
          (B)  32 O    6 CA(0.1)  28 O (0.8)   0.0
          (S)  34 O    6 CA(0.9)            0.1
          (B)  29 O    7 CA(0.1)  28 O (0.8)   0.1
          (S)  35 O    7 CA(0.9)            0.0
          (B)  30 O    8 CA(0.1)  27 O (0.8)   0.0
          (S)  36 O    8 CA(0.9)            0.0
84  398.0133  (B1 )
          (S)  29 O    3 CA(0.5)   8 CA(0.4)   0.0
          (S)  32 O    3 CA(0.5)   5 CA(0.4)   0.0
          (S)  30 O    4 CA(0.5)   7 CA(0.4)   0.0
          (S)  31 O    4 CA(0.5)   6 CA(0.4)   0.0
          (S)  33 O    5 CA(0.9)            0.0
          (S)  34 O    6 CA(0.9)            0.1
          (S)  35 O    7 CA(0.9)            0.0
          (S)  36 O    8 CA(0.9)            0.0
85  399.4262  (A1 )
          (B)  26 O    3 CA(0.4)  27 O (0.6)   0.0
          (B)  25 O    4 CA(0.4)  14 SI(0.6)   0.0
86  412.9093  (A2 )
          (B)  21 O    3 CA(0.3)   5 CA(0.7)   0.0
          (B)  24 O    3 CA(0.3)   8 CA(0.7)   0.0
          (O)  27 O    3 CA(0.0)   6 CA(0.8)   0.0
          (B)   4 CA  22 O (0.3)   6 CA(0.7)   0.0
          (B)   4 CA  23 O (0.3)   7 CA(0.7)   0.0
          (O)  28 O    4 CA(0.0)   8 CA(0.8)   0.0
          (S)   5 CA  21 O (0.6)   3 CA(0.4)   0.0
          (B)  27 O    5 CA(0.5)   9 CA(0.5)   0.0
          (S)  22 O    6 CA(0.6)   4 CA(0.4)   0.0
          (B)  28 O    6 CA(0.5)  10 CA(0.5)   0.0
          (S)  23 O    7 CA(0.6)   4 CA(0.4)   0.0
          (B)  28 O    7 CA(0.5)  11 CA(0.5)   0.0
          (S)  24 O    8 CA(0.6)   3 CA(0.4)   0.0
          (B)  27 O    8 CA(0.5)  12 CA(0.5)   0.0
          (B)  21 O    9 CA(0.4)  45 O (0.6)   0.0
          (B)  22 O   10 CA(0.4)  46 O (0.6)   0.0
          (B)  23 O   11 CA(0.4)  47 O (0.6)   0.0
          (B)  24 O   12 CA(0.4)  48 O (0.6)   0.0
          (B)  21 O   13 SI(0.0)  27 O (1.0)   0.0
          (B)  24 O   13 SI(0.0)  27 O (1.0)   0.0
          (O)  27 O   13 SI(0.0)   8 CA(0.8)   0.0
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            (B)  22 O   14 SI(0.0)  28 O (1.0)    0.0
            (B)  23 O   14 SI(0.0)  28 O (1.0)    0.0
            (O)  28 O   14 SI(0.0)   7 CA(0.8)    0.0
87   412.9170  (B2 )
            (S)  26 O    3 CA(0.6)  27 O (0.4)    0.0
            (S)  25 O    4 CA(0.6)  14 SI(0.4)    0.0
            (B)  25 O    5 CA(0.4)   1 CA(0.6)    0.0
            (B)  26 O    6 CA(0.4)   1 CA(0.6)    0.1
            (B)  26 O    7 CA(0.4)   2 CA(0.6)    0.2
            (B)  25 O    8 CA(0.4)   2 CA(0.6)    0.0
            (B)  25 O   13 SI(0.0)  27 O (1.0)    0.0
            (B)  26 O   14 SI(0.0)   4 CA(1.0)    0.0
88   420.7202  (B1 )
            (B)  21 O    9 CA(0.4)  45 O (0.6)    0.1
            (B)  22 O   10 CA(0.4)  46 O (0.6)    0.0
            (B)  23 O   11 CA(0.4)  47 O (0.6)    0.0
            (B)  24 O   12 CA(0.4)  48 O (0.6)    0.0
89   424.8696  (A2 )
            (S)  21 O    5 CA(0.8)  11 CA(0.2)    0.0
            (S)  33 O    5 CA(1.0)               0.0
            (S)  22 O    6 CA(0.8)  12 CA(0.2)    0.0
            (S)  34 O    6 CA(1.0)               0.1
            (S)  23 O    7 CA(0.8)   9 CA(0.2)    0.0
            (S)  35 O    7 CA(1.0)               0.0
            (S)  24 O    8 CA(0.8)  10 CA(0.2)    0.0
            (S)  36 O    8 CA(1.0)               0.0
            (B)  21 O    9 CA(0.4)  45 O (0.6)    0.0
            (B)  22 O   10 CA(0.4)  46 O (0.6)    0.0
            (B)  23 O   11 CA(0.4)  47 O (0.6)    0.0
            (B)  24 O   12 CA(0.4)  48 O (0.6)    0.0
90   430.8824  (B1 )
            (B)  45 O   19 SI(0.0)  37 O (0.9)    0.0
            (B)  46 O   19 SI(0.0)  38 O (0.9)    0.0
            (B)  47 O   20 SI(0.0)  39 O (0.9)   -0.1
            (B)  48 O   20 SI(0.0)  40 O (0.9)    0.0
91   432.4979  (A1 )
            (B)  26 O    3 CA(0.4)  27 O (0.6)    0.0
            (B)  25 O    4 CA(0.4)  14 SI(0.6)    0.0
            (S)  25 O    5 CA(0.6)   8 CA(0.4)    0.0
            (S)  26 O    6 CA(0.6)   7 CA(0.4)    0.1
            (S)   7 CA  26 O (0.6)   6 CA(0.4)    0.1
            (S)   8 CA  25 O (0.6)   5 CA(0.4)    0.0
            (B)  25 O   13 SI(0.0)  27 O (1.0)    0.0
            (B)  14 SI  26 O (0.0)   3 CA(1.0)    0.0
92   437.9924  (B2 )
            (B)  29 O   15 SI(0.0)   7 CA(1.0)    0.0
            (B)  30 O   16 SI(0.0)   8 CA(1.0)    0.0
            (B)  31 O   17 SI(0.0)   5 CA(1.0)    0.0
            (B)  18 SI  32 O (0.0)   6 CA(1.0)    0.0
            (B)  45 O   19 SI(0.0)  37 O (1.0)    0.0
            (B)  46 O   19 SI(0.0)  38 O (1.0)    0.0
            (B)  47 O   20 SI(0.0)  39 O (1.0)   -0.1
            (B)  48 O   20 SI(0.0)  40 O (1.0)    0.0
93   472.3075  (B1 )
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         (B)   15 SI  29 O (0.0)   3 CA(1.0)    0.0
         (B)   35 O   15 SI(0.0) 37 O (1.0)     0.0
         (O)   41 O   15 SI(0.0) 37 O (0.7)     0.0
         (B)   16 SI  30 O (0.0)   4 CA(1.0)    0.0
         (B)   36 O   16 SI(0.0) 38 O (1.0)     0.0
         (O)   42 O   16 SI(0.0) 38 O (0.7)     0.0
         (B)   17 SI  31 O (0.0)   4 CA(1.0)    0.0
         (B)   33 O   17 SI(0.0) 39 O (1.0)     0.0
         (O)   17 SI  43 O (0.0)   1 CA(0.8)    0.0
         (B)   18 SI  32 O (0.0)   3 CA(1.0)    0.0
         (B)   34 O   18 SI(0.0) 40 O (1.0)     0.0
         (O)   18 SI  44 O (0.0)   1 CA(0.8)    0.0
94   476.7066  (A2 )
         (B)   15 SI  29 O (0.0)   3 CA(1.0)    0.0
         (B)   15 SI  35 O (0.0)   2 CA(1.0)    0.0
         (O)   41 O   15 SI(0.0) 37 O (0.8)     0.0
         (B)   16 SI  30 O (0.0)   4 CA(1.0)    0.0
         (B)   16 SI  36 O (0.0)   2 CA(1.0)    0.0
         (O)   42 O   16 SI(0.0) 38 O (0.8)     0.0
         (B)   17 SI  31 O (0.0)   4 CA(1.0)    0.0
         (B)   17 SI  33 O (0.0)   1 CA(1.0)    0.0
         (O)   43 O   17 SI(0.0) 39 O (0.8)     0.0
         (B)   18 SI  32 O (0.0)   3 CA(1.0)    0.0
         (B)   18 SI  34 O (0.0)   1 CA(1.0)    0.0
         (O)   44 O   18 SI(0.0) 40 O (0.8)     0.0
95   481.0517  (B2 )
         (B)   35 O   15 SI(0.0) 37 O (1.0)     0.0
         (B)   36 O   16 SI(0.0) 38 O (1.0)     0.0
         (B)   33 O   17 SI(0.0) 39 O (1.0)     0.0
         (B)   34 O   18 SI(0.0) 40 O (1.0)     0.0
96   482.6387  (A1 )
         (B)   29 O   15 SI(0.0) 41 O (1.0)     0.0
         (B)   30 O   16 SI(0.0) 42 O (1.0)     0.0
         (B)   31 O   17 SI(0.0) 43 O (1.0)     0.0
         (B)   32 O   18 SI(0.0) 44 O (1.0)     0.0
97   498.3860  (A2 )
         (O)   25 O   13 SI(0.0) 24 O (0.7)     0.0
         (O)   26 O   14 SI(0.0) 22 O (0.7)     0.0
98   509.8604  (A1 )
         (O)   29 O   15 SI(0.0) 37 O (0.7)     0.0
         (O)   37 O   15 SI(0.0) 35 O (0.7)     0.0
         (B)   41 O   15 SI(0.0)   9 CA(1.0)    0.0
         (O)   30 O   16 SI(0.0) 38 O (0.7)     0.0
         (O)   38 O   16 SI(0.0) 36 O (0.7)     0.0
         (B)   42 O   16 SI(0.0) 10 CA(1.0)     0.0
         (O)   31 O   17 SI(0.0) 39 O (0.7)     0.0
         (O)   39 O   17 SI(0.0) 33 O (0.7)     0.0
         (B)   43 O   17 SI(0.0) 11 CA(1.0)     0.0
         (O)   32 O   18 SI(0.0) 40 O (0.7)     0.0
         (O)   40 O   18 SI(0.0) 34 O (0.7)     0.0
         (B)   44 O   18 SI(0.0) 12 CA(1.0)     0.0
99   511.4612  (B1 )
         (B)   35 O   15 SI(0.0) 41 O (0.9)     0.0
         (B)   36 O   16 SI(0.0) 42 O (0.9)     0.0
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          (B)  33 O   17 SI(0.0)  43 O (0.9)   0.0
          (B)  34 O   18 SI(0.0)  44 O (0.9)   0.0
100  513.5171  (B2 )
          (B)  35 O   15 SI(0.0)   7 CA(0.9)   0.0
          (B)  36 O   16 SI(0.0)   8 CA(0.9)   0.0
          (B)  33 O   17 SI(0.0)   5 CA(0.9)   0.0
          (B)  34 O   18 SI(0.0)   6 CA(0.9)   0.0
101  522.3506  (A2 )
          (O)  37 O   15 SI(0.1)  35 O (0.7)   0.0
          (O)  38 O   16 SI(0.1)  36 O (0.7)   0.0
          (O)  39 O   17 SI(0.1)  33 O (0.7)   0.0
          (O)  40 O   18 SI(0.1)  34 O (0.7)   0.0
102  531.2972  (A1 )
          (O)  21 O   13 SI(0.0)  25 O (0.8)   0.1
          (O)  24 O   13 SI(0.0)  25 O (0.8)   0.0
          (O)  22 O   14 SI(0.0)  26 O (0.8)   0.0
          (O)  23 O   14 SI(0.0)  26 O (0.8)   0.1
103  533.8844  (B2 )
          (O)  21 O   13 SI(0.0)  25 O (0.8)   0.1
          (O)  24 O   13 SI(0.0)  25 O (0.8)   0.0
          (O)  22 O   14 SI(0.0)  26 O (0.8)   0.0
          (O)  23 O   14 SI(0.0)  26 O (0.8)   0.1
104  539.9409  (B1 )
          (O)  25 O   13 SI(0.0)  24 O (0.7)   0.0
          (O)  26 O   14 SI(0.0)  22 O (0.7)   0.0
105  548.5565  (A1 )
          (B)  35 O   15 SI(0.0)  29 O (0.9)   0.0
          (B)  36 O   16 SI(0.0)  30 O (0.9)   0.0
          (B)  33 O   17 SI(0.0)  31 O (0.9)   0.0
          (B)  34 O   18 SI(0.0)  32 O (0.9)   0.0
106  556.1780  (A2 )
          (O)  25 O   13 SI(0.0)  24 O (0.7)   0.0
          (O)  26 O   14 SI(0.0)  22 O (0.7)   0.0
107  565.7138  (A1 )
          (B)  21 O   13 SI(0.0)   8 CA(1.0)   0.0
          (B)  24 O   13 SI(0.0)   5 CA(1.0)   0.1
          (B)  25 O   13 SI(0.0)  27 O (1.0)   0.0
          (B)  22 O   14 SI(0.0)   7 CA(1.0)   0.0
          (B)  23 O   14 SI(0.0)   6 CA(1.0)   0.0
          (B)  26 O   14 SI(0.0)   4 CA(1.0)   0.0
108  567.7733  (B2 )
          (B)  13 SI  21 O (0.0)   9 CA(1.0)   0.0
          (B)  13 SI  24 O (0.0)  12 CA(1.0)   0.0
          (B)  25 O   13 SI(0.0)  27 O (1.0)   0.0
          (B)  14 SI  22 O (0.0)  10 CA(1.0)   0.0
          (B)  14 SI  23 O (0.0)  11 CA(1.0)   0.0
          (B)  26 O   14 SI(0.0)   4 CA(1.0)   0.0
109  568.3015  (B1 )
          (B)  29 O   15 SI(0.0)  35 O (0.9)   0.0
          (B)  15 SI  37 O (0.0)  19 SI(0.9)   0.0
          (B)  41 O   15 SI(0.0)   7 CA(1.0)   0.0
          (B)  30 O   16 SI(0.0)  36 O (0.9)   0.0
          (B)  16 SI  38 O (0.0)  19 SI(0.9)   0.0
          (B)  42 O   16 SI(0.0)   8 CA(1.0)   0.0
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      (B)  31 O   17 SI(0.0)  33 O  (0.9)   0.0
      (B)  17 SI  39 O  (0.0)  20 SI(0.9)    0.0
      (B)  43 O   17 SI(0.0)   5 CA(1.0)     0.0
      (B)  32 O   18 SI(0.0)  34 O  (0.9)    0.0
      (B)  18 SI  40 O  (0.0)  20 SI(0.9)    0.0
      (B)  44 O   18 SI(0.0)   6 CA(1.0)     0.0
      (B)  37 O   19 SI(0.0)  45 O  (0.9)    0.0
      (B)  38 O   19 SI(0.0)  46 O  (0.9)    0.0
      (B)  39 O   20 SI(0.0)  47 O  (0.9)    0.0
      (B)  40 O   20 SI(0.0)  48 O  (0.9)    0.0
110  577.0073  (B2 )
      (B)  21 O   13 SI(0.0)   5 CA(0.9)     0.0
      (B)  24 O   13 SI(0.0)   8 CA(0.9)     0.0
      (B)  22 O   14 SI(0.0)   6 CA(0.9)     0.0
      (B)  23 O   14 SI(0.0)   7 CA(0.9)     0.0
111  578.6851  (A1 )
      (B)  19 SI  45 O  (0.0)   1 CA(1.0)    0.0
      (B)  19 SI  46 O  (0.0)   1 CA(1.0)    0.0
      (B)  20 SI  47 O  (0.0)   2 CA(1.0)   -0.1
      (B)  48 O   20 SI(0.0)  47 O  (1.0)    0.0
112  587.6966  (A2 )
      (B)  37 O   15 SI(0.1)  41 O  (0.8)    0.0
      (B)  38 O   16 SI(0.1)  42 O  (0.8)    0.0
      (B)  39 O   17 SI(0.1)  43 O  (0.8)    0.0
      (B)  40 O   18 SI(0.1)  44 O  (0.8)    0.0
113  668.5653  (A1 )
      (S)  15 SI  37 O  (0.7)  19 SI(0.3)    0.0
      (S)  16 SI  38 O  (0.7)  19 SI(0.3)    0.0
      (S)  17 SI  39 O  (0.7)  20 SI(0.3)    0.0
      (S)  18 SI  40 O  (0.7)  20 SI(0.3)    0.0
114  679.2445  (A2 )
      (S)  15 SI  37 O  (0.7)  19 SI(0.2)    0.0
      (S)  16 SI  38 O  (0.7)  19 SI(0.2)    0.0
      (S)  17 SI  39 O  (0.7)  20 SI(0.2)    0.0
      (S)  18 SI  40 O  (0.7)  20 SI(0.2)    0.0
115  708.0469  (B1 )
      (S)  37 O   15 SI(0.8)   7 CA(0.2)     0.0
      (S)  38 O   16 SI(0.8)   8 CA(0.2)     0.0
      (S)  39 O   17 SI(0.8)   5 CA(0.2)     0.0
      (S)  40 O   18 SI(0.8)   6 CA(0.2)     0.0
      (B)  37 O   19 SI(0.3)  46 O  (0.7)    0.0
      (B)  38 O   19 SI(0.3)  45 O  (0.7)    0.0
      (B)  39 O   20 SI(0.3)  48 O  (0.7)    0.0
      (B)  40 O   20 SI(0.3)  47 O  (0.7)    0.0
116  709.8980  (B2 )
      (S)  15 SI  37 O  (0.8)  19 SI(0.2)    0.0
      (S)  16 SI  38 O  (0.8)  19 SI(0.2)    0.0
      (S)  17 SI  39 O  (0.8)  20 SI(0.2)    0.0
      (S)  18 SI  40 O  (0.8)  20 SI(0.2)    0.0
      (B)  37 O   19 SI(0.3)  46 O  (0.7)    0.0
      (B)  38 O   19 SI(0.3)  45 O  (0.7)    0.0
      (B)  39 O   20 SI(0.3)  48 O  (0.7)    0.0
      (B)  40 O   20 SI(0.3)  47 O  (0.7)    0.0
117  820.7474  (B2 )
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            (S)  25 O  13 SI(0.9)         0.0
            (S)  26 O  14 SI(0.9)         0.0
118  821.3984 (A1 )
            (S)  25 O  13 SI(1.0)         0.1
            (S)  26 O  14 SI(1.0)         0.1
119  824.4722 (B1 )
            (S)  29 O  15 SI(0.9)         0.0
            (S)  37 O  15 SI(0.8) 41 O (0.2)  0.0
            (S)  30 O  16 SI(0.9)         0.0
            (S)  38 O  16 SI(0.8) 42 O (0.2)  0.0
            (S)  31 O  17 SI(0.9)         0.0
            (S)  39 O  17 SI(0.8) 43 O (0.2)  0.0
            (S)  32 O  18 SI(0.9)         0.0
            (S)  40 O  18 SI(0.8) 44 O (0.2)  0.0
120  830.5843 (B2 )
            (B)  21 O   3 CA(0.0) 32 O (1.0)  0.0
            (B)  24 O   3 CA(0.0) 29 O (1.0)  0.0
            (B)  27 O   3 CA(0.2) 26 O (0.8)  0.0
            (B)  22 O   4 CA(0.0) 31 O (1.0)  0.0
            (B)  23 O   4 CA(0.0) 30 O (1.0)  0.0
            (B)   4 CA 28 O (0.2) 14 SI(0.8)  0.0
            (B)  21 O   5 CA(0.0) 13 SI(1.0)  0.0
            (B)  27 O   5 CA(0.4) 13 SI(0.6)  0.0
            (B)  22 O   6 CA(0.0) 14 SI(1.0)  0.1
            (B)  28 O   6 CA(0.4) 14 SI(0.6)  0.0
            (B)  23 O   7 CA(0.0) 14 SI(1.0)  0.0
            (B)  28 O   7 CA(0.4) 14 SI(0.6)  0.1
            (B)  24 O   8 CA(0.0) 13 SI(1.0)  0.0
            (B)  27 O   8 CA(0.4) 13 SI(0.6)  0.0
            (S)   9 CA 21 O (0.5) 13 SI(0.5)  0.0
            (S)  10 CA 22 O (0.5) 14 SI(0.5)  0.1
            (S)  11 CA 23 O (0.5) 14 SI(0.5)  0.0
            (S)  12 CA 24 O (0.5) 13 SI(0.5)  0.0
            (S)  27 O  13 SI(1.0)         0.0
            (S)  28 O  14 SI(1.0)         0.0
121  848.2964 (A2 )
            (S)  29 O  15 SI(0.9)         0.0
            (S)  30 O  16 SI(0.9)         0.0
            (S)  31 O  17 SI(0.9)         0.0
            (S)  32 O  18 SI(0.9)         0.0
122  850.9464 (A1 )
            (S)  29 O  15 SI(0.8)  9 CA(0.2)  0.0
            (S)  41 O  15 SI(0.8) 37 O (0.2)  0.0
            (S)  16 SI 30 O (0.8) 10 CA(0.2)  0.0
            (S)  42 O  16 SI(0.8) 38 O (0.2)  0.0
            (S)  17 SI 31 O (0.8) 11 CA(0.2)  0.0
            (S)  43 O  17 SI(0.8) 39 O (0.2)  0.0
            (S)  18 SI 32 O (0.8) 12 CA(0.2)  0.0
            (S)  44 O  18 SI(0.8) 40 O (0.2)  0.0
123  864.0546 (A1 )
            (S)  25 O  13 SI(1.0)         0.1
            (S)  26 O  14 SI(1.0)         0.1
124  882.4412 (B2 )
            (S)  25 O  13 SI(1.0)         0.1
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              (S)  26 O   14 SI(1.0)              0.1
125  884.5126  (A2 )
              (S)  21 O   13 SI(0.9)              0.0
              (S)  24 O   13 SI(0.9)              0.1
              (S)  22 O   14 SI(0.9)              0.1
              (S)  23 O   14 SI(0.9)              0.0
126  888.4763  (B1 )
              (S)  21 O   13 SI(0.9)              0.0
              (S)  24 O   13 SI(0.9)              0.0
              (S)  22 O   14 SI(0.9)              0.1
              (S)  23 O   14 SI(0.9)              0.0
127  896.0043  (B2 )
              (S)  37 O   19 SI(0.9)              0.0
              (S)  38 O   19 SI(0.9)              0.0
              (S)  39 O   20 SI(0.9)              0.0
              (S)  40 O   20 SI(0.9)              0.0
128  897.6453  (A1 )
              (S)  15 SI  37 O (0.7)  19 SI(0.3)  0.1
              (S)  16 SI  38 O (0.7)  19 SI(0.3)  0.0
              (S)  17 SI  39 O (0.7)  20 SI(0.3)  0.0
              (S)  18 SI  40 O (0.7)  20 SI(0.3)  0.0
              (S)  37 O   19 SI(0.8)  46 O (0.2)  0.0
              (S)  38 O   19 SI(0.8)  45 O (0.2)  0.0
              (S)  39 O   20 SI(0.8)  48 O (0.2)  0.0
              (S)  40 O   20 SI(0.8)  47 O (0.2)  0.0
129  903.8423  (A2 )
              (S)  37 O   15 SI(0.7)  41 O (0.3)  0.0
              (S)  38 O   16 SI(0.7)  42 O (0.3)  0.0
              (S)  39 O   17 SI(0.7)  43 O (0.3)  0.0
              (S)  40 O   18 SI(0.7)  44 O (0.3)  0.0
              (S)  37 O   19 SI(0.8)  46 O (0.2)  0.0
              (S)  38 O   19 SI(0.8)  45 O (0.2)  0.0
              (S)  39 O   20 SI(0.8)  48 O (0.2)  0.0
              (S)  40 O   20 SI(0.8)  47 O (0.2)  0.0
130  915.9512  (B1 )
              (S)  13 SI  21 O (0.8)   3 CA(0.2)  0.0
              (S)  13 SI  24 O (0.8)   3 CA(0.2)  0.0
              (S)  22 O   14 SI(0.8)   4 CA(0.2)  0.1
              (S)  23 O   14 SI(0.8)   4 CA(0.2)  0.0
131  922.8638  (B1 )
              (S)  15 SI  35 O (0.8)   7 CA(0.2)  0.0
              (S)  36 O   16 SI(0.8)   8 CA(0.2)  0.0
              (S)  33 O   17 SI(0.8)   5 CA(0.2)  0.0
              (S)  34 O   18 SI(0.8)   6 CA(0.2)  0.0
132  932.3091  (A1 )
              (S)  27 O   13 SI(1.0)              0.1
              (S)  28 O   14 SI(1.0)              0.0
133  934.8533  (B2 )
              (S)  27 O   13 SI(1.0)              0.1
              (S)  28 O   14 SI(1.0)              0.0
134  947.5727  (A1 )
              (S)  29 O   15 SI(0.9)              0.0
              (S)  35 O   15 SI(0.8)  29 O (0.2)  0.0
              (S)  30 O   16 SI(0.9)              0.0
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              (S)   36 O   16 SI(0.8)  30 O (0.2)   0.0
              (S)   31 O   17 SI(0.9)             0.0
              (S)   33 O   17 SI(0.8)  31 O (0.2)   0.0
              (S)   32 O   18 SI(0.9)             0.0
              (S)   34 O   18 SI(0.8)  32 O (0.2)   0.0
135  948.7198  (A2 )
              (S)   41 O   15 SI(0.8)  35 O (0.2)   0.0
              (S)   42 O   16 SI(0.8)  36 O (0.2)   0.0
              (S)   43 O   17 SI(0.8)  33 O (0.2)   0.0
              (S)   44 O   18 SI(0.8)  34 O (0.2)   0.0
136  959.9044  (B2 )
              (S)   29 O   15 SI(1.0)             0.0
              (S)   30 O   16 SI(1.0)             0.0
              (S)   31 O   17 SI(1.0)             0.0
              (S)   32 O   18 SI(1.0)             0.0
137  975.3016  (A1 )
              (S)   41 O   15 SI(1.0)             0.0
              (S)   42 O   16 SI(1.0)             0.0
              (S)   43 O   17 SI(1.0)             0.0
              (S)   44 O   18 SI(1.0)             0.0
138  977.6905  (B1 )
              (S)   41 O   15 SI(1.0)             0.0
              (S)   42 O   16 SI(1.0)             0.0
              (S)   43 O   17 SI(1.0)             0.0
              (S)   44 O   18 SI(1.0)             0.0
139  982.2283  (B2 )
              (S)   41 O   15 SI(1.0)             0.0
              (S)   42 O   16 SI(1.0)             0.0
              (S)   43 O   17 SI(1.0)             0.0
              (S)   44 O   18 SI(1.0)             0.0
140  994.8184  (A1 )
              (S)   45 O   19 SI(0.8)   1 CA(0.2)   0.0
              (S)   19 SI  46 O (0.8)   1 CA(0.2)   0.0
              (S)   20 SI  47 O (0.8)   2 CA(0.2)  -0.1
              (S)   48 O   20 SI(0.8)   2 CA(0.2)   0.0
141  999.4520  (A2 )
              (S)   35 O   15 SI(1.0)             0.0
              (S)   36 O   16 SI(1.0)             0.0
              (S)   33 O   17 SI(1.0)             0.0
              (S)   34 O   18 SI(1.0)             0.0
142  1016.1355  (A2 )
              (S)   45 O   19 SI(0.8)   1 CA(0.2)   0.0
              (S)   46 O   19 SI(0.8)  45 O (0.2)   0.0
              (S)   47 O   20 SI(0.8)   2 CA(0.2)  -0.1
              (S)   48 O   20 SI(0.8)   2 CA(0.2)   0.0
143  1039.6749  (B2 )
              (S)   45 O   19 SI(0.9)             0.0
              (S)   46 O   19 SI(0.9)             0.0
              (S)   47 O   20 SI(0.9)             0.0
              (S)   48 O   20 SI(0.9)             0.0
144  1043.9050  (B1 )
              (S)   45 O   19 SI(0.9)             0.0
              (S)   46 O   19 SI(0.9)             0.0
              (S)   47 O   20 SI(0.9)             0.0
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(S)　48 O　20 SI(0.9)　　　　0.0

NORMAL MODES NORMALIZED TO CLASSICAL AMPLITUDES

FREQ(CM**-1)　-2.12　　-1.95　　-1.51　　91.07　　94.32　　99.74

AT.　1 CA X　0.0000　0.2298　0.0000　0.0000　0.0000　0.0013
　　　　Y　0.2194　0.0000　0.0002　-0.0011　-0.0467　0.0000
　　　　Z　-0.0004　0.0000　0.2608　0.0060　0.0039　0.0000
AT.　2 CA X　0.0000　0.2298　0.0000　0.0000　0.0000　-0.0013
　　　　Y　0.2194　0.0000　-0.0002　0.0011　-0.0467　0.0000
　　　　Z　0.0004　0.0000　0.2608　0.0060　-0.0039　0.0000
AT.　3 CA X　0.0003　0.2322　0.0000　0.0000　-0.0007　0.0000
　　　　Y　0.2223　0.0002　0.0000　0.0000　0.0044　0.0000
　　　　Z　0.0000　0.0000　0.2635　0.0027　0.0000　-0.0287
AT.　4 CA X　-0.0003　0.2322　0.0000　0.0000　0.0007　0.0000
　　　　Y　0.2223　-0.0002　0.0000　0.0000　0.0044　0.0000
　　　　Z　0.0000　0.0000　0.2635　0.0027　0.0000　0.0287
AT.　5 CA X　0.0000　0.2317　0.0009　-0.0455　0.0327　-0.0448
　　　　Y　0.2220　0.0000　0.0001　-0.0007　0.0130　-0.0076
　　　　Z　-0.0003　-0.0002　0.2630　0.0271　-0.0016　0.0511
AT.　6 CA X　0.0000　0.2317　-0.0009　0.0455　-0.0327　-0.0448
　　　　Y　0.2220　0.0000　0.0001　-0.0007　0.0130　0.0076
　　　　Z　-0.0003　0.0002　0.2630　0.0271　-0.0016　-0.0511
AT.　7 CA X　0.0000　0.2317　0.0009　-0.0455　-0.0327　0.0448
　　　　Y　0.2220　0.0000　-0.0001　0.0007　0.0130　-0.0076
　　　　Z　0.0003　-0.0002　0.2630　0.0271　0.0016　-0.0511
AT.　8 CA X　0.0000　0.2317　-0.0009　0.0455　0.0327　0.0448
　　　　Y　0.2220　0.0000　-0.0001　0.0007　0.0130　0.0076
　　　　Z　0.0003　0.0002　0.2630　0.0271　0.0016　0.0511
AT.　9 CA X　-0.0003　0.2314　0.0011　-0.0372　-0.0013　-0.0101
　　　　Y　0.2222　0.0006　-0.0003　0.0058　-0.0006　-0.0064
　　　　Z　-0.0008　-0.0004　0.2629　-0.0068　-0.0343　0.0118
AT.　10 CA X　0.0003　0.2314　-0.0011　0.0372　0.0013　-0.0101
　　　　Y　0.2222　-0.0006　-0.0003　0.0058　-0.0006　0.0064
　　　　Z　-0.0008　0.0004　0.2629　-0.0068　-0.0343　-0.0118
AT.　11 CA X　0.0003　0.2314　0.0011　-0.0372　0.0013　0.0101
　　　　Y　0.2222　-0.0006　0.0003　-0.0058　-0.0006　-0.0064
　　　　Z　0.0008　-0.0004　0.2629　-0.0068　0.0343　-0.0118
AT.　12 CA X　-0.0003　0.2314　-0.0011　0.0372　-0.0013　0.0101
　　　　Y　0.2222　0.0006　0.0003　-0.0058　-0.0006　0.0064
　　　　Z　0.0008　0.0004　0.2629　-0.0068　0.0343　0.0118
AT.　13 SI X　0.0002　0.2325　0.0000　0.0000　0.0242　0.0000
　　　　Y　0.2221　0.0004　0.0000　0.0000　0.0224　0.0000
　　　　Z　0.0000　0.0000　0.2643　0.0010　0.0000　0.0213
AT.　14 SI X　-0.0002　0.2325　0.0000　0.0000　-0.0242　0.0000
　　　　Y　0.2221　-0.0004　0.0000　0.0000　0.0224　0.0000
　　　　Z　0.0000　0.0000　0.2643　0.0010　0.0000　-0.0213
AT.　15 SI X　0.0010　0.2310　0.0012　-0.0277　0.0073　0.0010
　　　　Y　0.2215　0.0004　0.0003　-0.0074　0.0013　-0.0045
　　　　Z　-0.0007　-0.0001　0.2629　-0.0023　-0.0245　-0.0147
AT.　16 SI X　-0.0010　0.2310　-0.0012　0.0277　-0.0073　0.0010
　　　　Y　0.2215　-0.0004　0.0003　-0.0074　0.0013　0.0045
　　　　Z　-0.0007　0.0001　0.2629　-0.0023　-0.0245　0.0147

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AT. 17 SI X  -0.0010   0.2310   0.0012  -0.0277  -0.0073  -0.0010
        Y   0.2215  -0.0004  -0.0003   0.0074   0.0013  -0.0045
        Z   0.0007  -0.0001   0.2629  -0.0023   0.0245   0.0147
AT. 18 SI X   0.0010   0.2310  -0.0012   0.0277   0.0073  -0.0010
        Y   0.2215   0.0004  -0.0003   0.0074   0.0013   0.0045
        Z   0.0007   0.0001   0.2629  -0.0023   0.0245  -0.0147
AT. 19 SI X   0.0000   0.2299   0.0000   0.0000   0.0000  -0.0103
        Y   0.2215   0.0000  -0.0007   0.0176  -0.0208   0.0000
        Z  -0.0005   0.0000   0.2628  -0.0241  -0.0150   0.0000
AT. 20 SI X   0.0000   0.2299   0.0000   0.0000   0.0000   0.0103
        Y   0.2215   0.0000   0.0007  -0.0176  -0.0208   0.0000
        Z   0.0005   0.0000   0.2628  -0.0241   0.0150   0.0000
AT. 21 O  X   0.0005   0.2322   0.0008  -0.0243   0.0251  -0.0229
        Y   0.2231   0.0004  -0.0009  -0.0037   0.0264  -0.0069
        Z  -0.0003  -0.0004   0.2643  -0.0106  -0.0027   0.0105
AT. 22 O  X  -0.0005   0.2322  -0.0008   0.0243  -0.0251  -0.0229
        Y   0.2231  -0.0004  -0.0009  -0.0037   0.0264   0.0069
        Z  -0.0003   0.0004   0.2643  -0.0106  -0.0027  -0.0105
AT. 23 O  X  -0.0005   0.2322   0.0008  -0.0243  -0.0251   0.0229
        Y   0.2231  -0.0004   0.0009   0.0037   0.0264  -0.0069
        Z   0.0003  -0.0004   0.2643  -0.0106   0.0027  -0.0105
AT. 24 O  X   0.0005   0.2322  -0.0008   0.0243   0.0251   0.0229
        Y   0.2231   0.0004   0.0009   0.0037   0.0264   0.0069
        Z   0.0003   0.0004   0.2643  -0.0106   0.0027   0.0105
AT. 25 O  X  -0.0001   0.2314   0.0000   0.0000   0.0250   0.0000
        Y   0.2228  -0.0018   0.0000   0.0000   0.0208   0.0000
        Z   0.0000   0.0000   0.2636   0.0263   0.0000   0.0480
AT. 26 O  X   0.0001   0.2314   0.0000   0.0000  -0.0250   0.0000
        Y   0.2228   0.0018   0.0000   0.0000   0.0208   0.0000
        Z   0.0000   0.0000   0.2636   0.0263   0.0000  -0.0480
AT. 27 O  X   0.0003   0.2314   0.0000   0.0000   0.0272   0.0000
        Y   0.2242  -0.0001   0.0000   0.0000   0.0232   0.0000
        Z   0.0000   0.0000   0.2640   0.0022   0.0000   0.0198
AT. 28 O  X  -0.0003   0.2314   0.0000   0.0000  -0.0272   0.0000
        Y   0.2242   0.0001   0.0000   0.0000   0.0232   0.0000
        Z   0.0000   0.0000   0.2640   0.0022   0.0000  -0.0198
AT. 29 O  X   0.0000   0.2319   0.0004  -0.0231  -0.0122   0.0192
        Y   0.2230   0.0007  -0.0013  -0.0056   0.0169  -0.0118
        Z  -0.0002   0.0009   0.2636   0.0017  -0.0258  -0.0098
AT. 30 O  X   0.0000   0.2319  -0.0004   0.0231   0.0122   0.0192
        Y   0.2230  -0.0007  -0.0013  -0.0056   0.0169   0.0118
        Z  -0.0002  -0.0009   0.2636   0.0017  -0.0258   0.0098
AT. 31 O  X   0.0000   0.2319   0.0004  -0.0231   0.0122  -0.0192
        Y   0.2230  -0.0007   0.0013   0.0056   0.0169  -0.0118
        Z   0.0002   0.0009   0.2636   0.0017   0.0258   0.0098
AT. 32 O  X   0.0000   0.2319  -0.0004   0.0231  -0.0122  -0.0192
        Y   0.2230   0.0007   0.0013   0.0056   0.0169   0.0118
        Z   0.0002  -0.0009   0.2636   0.0017   0.0258  -0.0098
AT. 33 O  X  -0.0010   0.2317   0.0012  -0.0320  -0.0077  -0.0038
        Y   0.2215   0.0020  -0.0011   0.0197  -0.0040   0.0037
        Z  -0.0007  -0.0015   0.2632  -0.0095  -0.0036   0.0361
AT. 34 O  X   0.0010   0.2317  -0.0012   0.0320   0.0077  -0.0038
        Y   0.2215  -0.0020  -0.0011   0.0197  -0.0040  -0.0037
        Z  -0.0007   0.0015   0.2632  -0.0095  -0.0036  -0.0361
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AT. 35 O  X    0.0010   0.2317   0.0012  -0.0320   0.0077   0.0038
         Y    0.2215  -0.0020   0.0011  -0.0197  -0.0040   0.0037
         Z    0.0007  -0.0015   0.2632  -0.0095   0.0036  -0.0361
AT. 36 O  X   -0.0010   0.2317  -0.0012   0.0320  -0.0077   0.0038
         Y    0.2215   0.0020   0.0011  -0.0197  -0.0040  -0.0037
         Z    0.0007   0.0015   0.2632  -0.0095   0.0036   0.0361
AT. 37 O  X    0.0016   0.2305   0.0006  -0.0346   0.0250  -0.0123
         Y    0.2222  -0.0004  -0.0008   0.0025  -0.0094  -0.0023
         Z   -0.0010   0.0003   0.2622  -0.0003  -0.0300  -0.0018
AT. 38 O  X   -0.0016   0.2305  -0.0006   0.0346  -0.0250  -0.0123
         Y    0.2222   0.0004  -0.0008   0.0025  -0.0094   0.0023
         Z   -0.0010  -0.0003   0.2622  -0.0003  -0.0300   0.0018
AT. 39 O  X   -0.0016   0.2305   0.0006  -0.0346  -0.0250   0.0123
         Y    0.2222   0.0004   0.0008  -0.0025  -0.0094  -0.0023
         Z    0.0010   0.0003   0.2622  -0.0003   0.0300   0.0018
AT. 40 O  X    0.0016   0.2305  -0.0006   0.0346   0.0250   0.0123
         Y    0.2222  -0.0004   0.0008  -0.0025  -0.0094   0.0023
         Z    0.0010  -0.0003   0.2622  -0.0003   0.0300  -0.0018
AT. 41 O  X    0.0012   0.2320  -0.0001  -0.0197   0.0090   0.0009
         Y    0.2235   0.0000  -0.0003  -0.0070   0.0022  -0.0041
         Z   -0.0018  -0.0008   0.2628   0.0113  -0.0389  -0.0130
AT. 42 O  X   -0.0012   0.2320   0.0001   0.0197  -0.0090   0.0009
         Y    0.2235   0.0000  -0.0003  -0.0070   0.0022   0.0041
         Z   -0.0018   0.0008   0.2628   0.0113  -0.0389   0.0130
AT. 43 O  X   -0.0012   0.2320  -0.0001  -0.0197  -0.0090  -0.0009
         Y    0.2235   0.0000   0.0003   0.0070   0.0022  -0.0041
         Z    0.0018  -0.0008   0.2628   0.0113   0.0389   0.0130
AT. 44 O  X    0.0012   0.2320   0.0001   0.0197   0.0090  -0.0009
         Y    0.2235   0.0000   0.0003   0.0070   0.0022   0.0041
         Z    0.0018   0.0008   0.2628   0.0113   0.0389  -0.0130
AT. 45 O  X   -0.0007   0.2309  -0.0001  -0.0059   0.0023  -0.0098
         Y    0.2200   0.0007  -0.0003   0.0303  -0.0388   0.0087
         Z    0.0007   0.0006   0.2624  -0.0431   0.0075  -0.0086
AT. 46 O  X    0.0007   0.2309   0.0001   0.0059  -0.0023  -0.0098
         Y    0.2200  -0.0007  -0.0003   0.0303  -0.0388  -0.0087
         Z    0.0007  -0.0006   0.2624  -0.0431   0.0075   0.0086
AT. 47 O  X    0.0007   0.2309  -0.0001  -0.0059  -0.0023   0.0098
         Y    0.2200  -0.0007   0.0003  -0.0303  -0.0388   0.0087
         Z   -0.0007   0.0006   0.2624  -0.0431  -0.0075   0.0086
AT. 48 O  X   -0.0007   0.2309   0.0001   0.0059   0.0023   0.0098
         Y    0.2200   0.0007   0.0003  -0.0303  -0.0388  -0.0087
         Z   -0.0007  -0.0006   0.2624  -0.0431  -0.0075  -0.0086


FREQ(CM**-1)   110.69   113.40   115.39   116.76   125.84   127.40


AT.  1 CA X   -0.0240   0.0000   0.0000  -0.0380   0.0000  -0.0131
         Y    0.0000  -0.0312   0.0928   0.0000  -0.0010   0.0000
         Z    0.0000  -0.0072   0.0154   0.0000   0.0308   0.0000
AT.  2 CA X    0.0240   0.0000   0.0000  -0.0380   0.0000  -0.0131
         Y    0.0000  -0.0312  -0.0928   0.0000   0.0010   0.0000
         Z    0.0000   0.0072   0.0154   0.0000   0.0308   0.0000
AT.  3 CA X    0.0000  -0.0059   0.0000   0.0419   0.0000   0.0081
         Y    0.0000   0.0315   0.0000   0.0006   0.0000   0.0009
         Z    0.0112   0.0000  -0.0019   0.0000   0.0064   0.0000
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AT.  4 CA X   0.0000   0.0059   0.0000   0.0419   0.0000   0.0081
        Y   0.0000   0.0315   0.0000  -0.0006   0.0000  -0.0009
        Z  -0.0112   0.0000  -0.0019   0.0000   0.0064   0.0000
AT.  5 CA X   0.0253  -0.0105  -0.0015   0.0284   0.0051   0.0094
        Y  -0.0163   0.0103   0.0096  -0.0171  -0.0185   0.0423
        Z  -0.0002  -0.0195   0.0066  -0.0168   0.0087  -0.0071
AT.  6 CA X   0.0253   0.0105   0.0015   0.0284  -0.0051   0.0094
        Y   0.0163   0.0103   0.0096   0.0171  -0.0185  -0.0423
        Z   0.0002  -0.0195   0.0066   0.0168   0.0087   0.0071
AT.  7 CA X  -0.0253   0.0105  -0.0015   0.0284   0.0051   0.0094
        Y  -0.0163   0.0103  -0.0096   0.0171   0.0185  -0.0423
        Z   0.0002   0.0195   0.0066  -0.0168   0.0087  -0.0071
AT.  8 CA X  -0.0253  -0.0105   0.0015   0.0284  -0.0051   0.0094
        Y   0.0163   0.0103  -0.0096  -0.0171   0.0185   0.0423
        Z  -0.0002   0.0195   0.0066   0.0168   0.0087   0.0071
AT.  9 CA X   0.0077  -0.0022   0.0027  -0.0034   0.0105  -0.0086
        Y  -0.0315   0.0052   0.0062  -0.0054   0.0329   0.0102
        Z   0.0103   0.0056   0.0082   0.0000   0.0056  -0.0137
AT. 10 CA X   0.0077   0.0022  -0.0027  -0.0034  -0.0105  -0.0086
        Y   0.0315   0.0052   0.0062   0.0054   0.0329  -0.0102
        Z  -0.0103   0.0056   0.0082   0.0000   0.0056   0.0137
AT. 11 CA X  -0.0077   0.0022   0.0027  -0.0034   0.0105  -0.0086
        Y  -0.0315   0.0052  -0.0062   0.0054  -0.0329  -0.0102
        Z  -0.0103  -0.0056   0.0082   0.0000   0.0056  -0.0137
AT. 12 CA X  -0.0077  -0.0022  -0.0027  -0.0034  -0.0105  -0.0086
        Y   0.0315   0.0052  -0.0062  -0.0054  -0.0329   0.0102
        Z   0.0103  -0.0056   0.0082   0.0000   0.0056   0.0137
AT. 13 SI X   0.0000  -0.0226   0.0000   0.0251   0.0000   0.0250
        Y   0.0000   0.0141   0.0000  -0.0219   0.0000   0.0396
        Z   0.0146   0.0000   0.0055   0.0000  -0.0076   0.0000
AT. 14 SI X   0.0000   0.0226   0.0000   0.0251   0.0000   0.0250
        Y   0.0000   0.0141   0.0000   0.0219   0.0000  -0.0396
        Z  -0.0146   0.0000   0.0055   0.0000  -0.0076   0.0000
AT. 15 SI X  -0.0141   0.0173   0.0112  -0.0140   0.0091  -0.0060
        Y  -0.0258  -0.0038  -0.0204   0.0092   0.0270  -0.0208
        Z  -0.0174   0.0224  -0.0133  -0.0119  -0.0092  -0.0004
AT. 16 SI X  -0.0141  -0.0173  -0.0112  -0.0140  -0.0091  -0.0060
        Y   0.0258  -0.0038  -0.0204  -0.0092   0.0270   0.0208
        Z   0.0174   0.0224  -0.0133   0.0119  -0.0092   0.0004
AT. 17 SI X   0.0141  -0.0173   0.0112  -0.0140   0.0091  -0.0060
        Y  -0.0258  -0.0038   0.0204  -0.0092  -0.0270   0.0208
        Z   0.0174  -0.0224  -0.0133  -0.0119  -0.0092  -0.0004
AT. 18 SI X   0.0141   0.0173  -0.0112  -0.0140  -0.0091  -0.0060
        Y   0.0258  -0.0038   0.0204   0.0092  -0.0270  -0.0208
        Z  -0.0174  -0.0224  -0.0133   0.0119  -0.0092   0.0004
AT. 19 SI X  -0.0265   0.0000   0.0000  -0.0360   0.0000  -0.0121
        Y   0.0000  -0.0203  -0.0077   0.0000   0.0434   0.0000
        Z   0.0000   0.0403  -0.0015   0.0000  -0.0059   0.0000
AT. 20 SI X   0.0265   0.0000   0.0000  -0.0360   0.0000  -0.0121
        Y   0.0000  -0.0203   0.0077   0.0000  -0.0434   0.0000
        Z   0.0000  -0.0403  -0.0015   0.0000  -0.0059   0.0000
AT. 21 O  X   0.0174  -0.0170   0.0022   0.0246   0.0014   0.0196
        Y  -0.0053   0.0173   0.0019  -0.0187   0.0042   0.0343
        Z   0.0264   0.0009   0.0040  -0.0017  -0.0085  -0.0003
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AT. 22 O  X    0.0174   0.0170  -0.0022   0.0246  -0.0014   0.0196
          Y    0.0053   0.0173   0.0019   0.0187   0.0042  -0.0343
          Z   -0.0264   0.0009   0.0040   0.0017  -0.0085   0.0003
AT. 23 O  X   -0.0174   0.0170   0.0022   0.0246   0.0014   0.0196
          Y   -0.0053   0.0173  -0.0019   0.0187  -0.0042  -0.0343
          Z   -0.0264  -0.0009   0.0040  -0.0017  -0.0085  -0.0003
AT. 24 O  X   -0.0174  -0.0170  -0.0022   0.0246  -0.0014   0.0196
          Y    0.0053   0.0173  -0.0019  -0.0187  -0.0042   0.0343
          Z    0.0264  -0.0009   0.0040   0.0017  -0.0085   0.0003
AT. 25 O  X    0.0000  -0.0168   0.0000   0.0270   0.0000   0.0234
          Y    0.0000   0.0052   0.0000  -0.0269   0.0000   0.0418
          Z   -0.0068   0.0000   0.0021   0.0000  -0.0065   0.0000
AT. 26 O  X    0.0000   0.0168   0.0000   0.0270   0.0000   0.0234
          Y    0.0000   0.0052   0.0000   0.0269   0.0000  -0.0418
          Z    0.0068   0.0000   0.0021   0.0000  -0.0065   0.0000
AT. 27 O  X    0.0000  -0.0289   0.0000   0.0199   0.0000   0.0221
          Y    0.0000   0.0147   0.0000  -0.0220   0.0000   0.0404
          Z    0.0159   0.0000  -0.0001   0.0000  -0.0061   0.0000
AT. 28 O  X    0.0000   0.0289   0.0000   0.0199   0.0000   0.0221
          Y    0.0000   0.0147   0.0000   0.0220   0.0000  -0.0404
          Z   -0.0159   0.0000  -0.0001   0.0000  -0.0061   0.0000
AT. 29 O  X   -0.0069   0.0139   0.0090   0.0054   0.0063  -0.0012
          Y   -0.0145   0.0021  -0.0074   0.0054   0.0320  -0.0212
          Z   -0.0064   0.0243  -0.0062  -0.0044  -0.0077  -0.0003
AT. 30 O  X   -0.0069  -0.0139  -0.0090   0.0054  -0.0063  -0.0012
          Y    0.0145   0.0021  -0.0074  -0.0054   0.0320   0.0212
          Z    0.0064   0.0243  -0.0062   0.0044  -0.0077   0.0003
AT. 31 O  X    0.0069  -0.0139   0.0090   0.0054   0.0063  -0.0012
          Y   -0.0145   0.0021   0.0074  -0.0054  -0.0320   0.0212
          Z    0.0064  -0.0243  -0.0062  -0.0044  -0.0077  -0.0003
AT. 32 O  X    0.0069   0.0139  -0.0090   0.0054  -0.0063  -0.0012
          Y    0.0145   0.0021   0.0074   0.0054  -0.0320  -0.0212
          Z   -0.0064  -0.0243  -0.0062   0.0044  -0.0077   0.0003
AT. 33 O  X    0.0189  -0.0160   0.0087  -0.0122   0.0002  -0.0086
          Y   -0.0372  -0.0068   0.0258  -0.0161  -0.0048   0.0247
          Z    0.0276  -0.0182  -0.0064  -0.0231  -0.0101  -0.0084
AT. 34 O  X    0.0189   0.0160  -0.0087  -0.0122  -0.0002  -0.0086
          Y    0.0372  -0.0068   0.0258   0.0161  -0.0048  -0.0247
          Z   -0.0276  -0.0182  -0.0064   0.0231  -0.0101   0.0084
AT. 35 O  X   -0.0189   0.0160   0.0087  -0.0122   0.0002  -0.0086
          Y   -0.0372  -0.0068  -0.0258   0.0161   0.0048  -0.0247
          Z   -0.0276   0.0182  -0.0064  -0.0231  -0.0101  -0.0084
AT. 36 O  X   -0.0189  -0.0160  -0.0087  -0.0122  -0.0002  -0.0086
          Y    0.0372  -0.0068  -0.0258  -0.0161   0.0048   0.0247
          Z    0.0276   0.0182  -0.0064   0.0231  -0.0101   0.0084
AT. 37 O  X   -0.0271   0.0179  -0.0030  -0.0299   0.0014  -0.0138
          Y   -0.0158  -0.0113  -0.0172   0.0027   0.0406  -0.0078
          Z   -0.0128   0.0271  -0.0060  -0.0011  -0.0081  -0.0042
AT. 38 O  X   -0.0271  -0.0179   0.0030  -0.0299  -0.0014  -0.0138
          Y    0.0158  -0.0113  -0.0172  -0.0027   0.0406   0.0078
          Z    0.0128   0.0271  -0.0060   0.0011  -0.0081   0.0042
AT. 39 O  X    0.0271  -0.0179  -0.0030  -0.0299   0.0014  -0.0138
          Y   -0.0158  -0.0113   0.0172  -0.0027  -0.0406   0.0078
          Z    0.0128  -0.0271  -0.0060  -0.0011  -0.0081  -0.0042
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AT. 40 O  X   0.0271   0.0179   0.0030  -0.0299  -0.0014  -0.0138
          Y   0.0158  -0.0113   0.0172   0.0027  -0.0406  -0.0078
          Z  -0.0128  -0.0271  -0.0060   0.0011  -0.0081   0.0042
AT. 41 O  X  -0.0006   0.0168   0.0225  -0.0140   0.0204  -0.0044
          Y  -0.0253  -0.0038  -0.0188   0.0101   0.0285  -0.0210
          Z  -0.0099   0.0180  -0.0187  -0.0095  -0.0116  -0.0001
AT. 42 O  X  -0.0006  -0.0168  -0.0225  -0.0140  -0.0204  -0.0044
          Y   0.0253  -0.0038  -0.0188  -0.0101   0.0285   0.0210
          Z   0.0099   0.0180  -0.0187   0.0095  -0.0116   0.0001
AT. 43 O  X   0.0006  -0.0168   0.0225  -0.0140   0.0204  -0.0044
          Y  -0.0253  -0.0038   0.0188  -0.0101  -0.0285   0.0210
          Z   0.0099  -0.0180  -0.0187  -0.0095  -0.0116  -0.0001
AT. 44 O  X   0.0006   0.0168  -0.0225  -0.0140  -0.0204  -0.0044
          Y   0.0253  -0.0038   0.0188   0.0101  -0.0285  -0.0210
          Z  -0.0099  -0.0180  -0.0187   0.0095  -0.0116   0.0001
AT. 45 O  X  -0.0282  -0.0034   0.0220  -0.0318   0.0040  -0.0118
          Y  -0.0277  -0.0358   0.0166  -0.0099   0.0422  -0.0034
          Z   0.0265   0.0526  -0.0016   0.0135  -0.0017   0.0042
AT. 46 O  X  -0.0282   0.0034  -0.0220  -0.0318  -0.0040  -0.0118
          Y   0.0277  -0.0358   0.0166   0.0099   0.0422   0.0034
          Z  -0.0265   0.0526  -0.0016  -0.0135  -0.0017  -0.0042
AT. 47 O  X   0.0282   0.0034   0.0220  -0.0318   0.0040  -0.0118
          Y  -0.0277  -0.0358  -0.0166   0.0099  -0.0422   0.0034
          Z  -0.0265  -0.0526  -0.0016   0.0135  -0.0017   0.0042
AT. 48 O  X   0.0282  -0.0034  -0.0220  -0.0318  -0.0040  -0.0118
          Y   0.0277  -0.0358  -0.0166  -0.0099  -0.0422  -0.0034
          Z   0.0265  -0.0526  -0.0016  -0.0135  -0.0017  -0.0042


FREQ(CM**-1)   128.84   129.97   142.94   145.39   147.04   150.25

AT.  1 CA X  -0.0079   0.0000   0.0000   0.0000  -0.0421  -0.0064
          Y   0.0000   0.0094   0.0034  -0.0503   0.0000   0.0000
          Z   0.0000   0.0608   0.0429  -0.0156   0.0000   0.0000
AT.  2 CA X   0.0079   0.0000   0.0000   0.0000   0.0421  -0.0064
          Y   0.0000   0.0094  -0.0034  -0.0503   0.0000   0.0000
          Z   0.0000  -0.0608   0.0429   0.0156   0.0000   0.0000
AT.  3 CA X   0.0000   0.0221   0.0000   0.0129   0.0000   0.0044
          Y   0.0000  -0.0074   0.0000   0.0296   0.0000   0.0650
          Z   0.0238   0.0000  -0.0086   0.0000  -0.0332   0.0000
AT.  4 CA X   0.0000  -0.0221   0.0000  -0.0129   0.0000   0.0044
          Y   0.0000  -0.0074   0.0000   0.0296   0.0000  -0.0650
          Z  -0.0238   0.0000  -0.0086   0.0000   0.0332   0.0000
AT.  5 CA X   0.0214  -0.0174  -0.0133  -0.0304  -0.0030   0.0069
          Y   0.0236  -0.0019  -0.0192   0.0046   0.0073  -0.0083
          Z   0.0134   0.0210   0.0236   0.0217  -0.0122   0.0044
AT.  6 CA X   0.0214   0.0174   0.0133   0.0304  -0.0030   0.0069
          Y  -0.0236  -0.0019  -0.0192   0.0046  -0.0073   0.0083
          Z  -0.0134   0.0210   0.0236   0.0217   0.0122  -0.0044
AT.  7 CA X  -0.0214   0.0174  -0.0133   0.0304   0.0030   0.0069
          Y   0.0236  -0.0019   0.0192   0.0046   0.0073   0.0083
          Z  -0.0134  -0.0210   0.0236  -0.0217   0.0122   0.0044
AT.  8 CA X  -0.0214  -0.0174   0.0133  -0.0304   0.0030   0.0069
          Y  -0.0236  -0.0019   0.0192   0.0046  -0.0073  -0.0083
          Z   0.0134  -0.0210   0.0236  -0.0217  -0.0122  -0.0044
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AT.  9 CA X   -0.0058   0.0125  -0.0042  -0.0059   0.0010   0.0003
        Y    0.0138   0.0093  -0.0123  -0.0094   0.0091   0.0241
        Z   -0.0008   0.0149  -0.0205   0.0047  -0.0318  -0.0121
AT. 10 CA X   -0.0058  -0.0125   0.0042   0.0059   0.0010   0.0003
        Y   -0.0138   0.0093  -0.0123  -0.0094  -0.0091  -0.0241
        Z    0.0008   0.0149  -0.0205   0.0047   0.0318   0.0121
AT. 11 CA X    0.0058  -0.0125  -0.0042   0.0059  -0.0010   0.0003
        Y    0.0138   0.0093   0.0123  -0.0094   0.0091  -0.0241
        Z    0.0008  -0.0149  -0.0205  -0.0047   0.0318  -0.0121
AT. 12 CA X    0.0058   0.0125   0.0042  -0.0059  -0.0010   0.0003
        Y   -0.0138   0.0093   0.0123  -0.0094  -0.0091   0.0241
        Z   -0.0008  -0.0149  -0.0205  -0.0047  -0.0318   0.0121
AT. 13 SI X    0.0000   0.0073   0.0000  -0.0143   0.0000  -0.0047
        Y    0.0000  -0.0041   0.0000   0.0129   0.0000   0.0205
        Z    0.0276   0.0000  -0.0064   0.0000  -0.0276   0.0000
AT. 14 SI X    0.0000  -0.0073   0.0000   0.0143   0.0000  -0.0047
        Y    0.0000  -0.0041   0.0000   0.0129   0.0000  -0.0205
        Z   -0.0276   0.0000  -0.0064   0.0000   0.0276   0.0000
AT. 15 SI X   -0.0141   0.0218   0.0011  -0.0042   0.0080   0.0009
        Y    0.0262   0.0000   0.0094  -0.0050   0.0006   0.0197
        Z   -0.0106  -0.0178  -0.0076  -0.0134  -0.0181   0.0057
AT. 16 SI X   -0.0141  -0.0218  -0.0011   0.0042   0.0080   0.0009
        Y   -0.0262   0.0000   0.0094  -0.0050  -0.0006  -0.0197
        Z    0.0106  -0.0178  -0.0076  -0.0134   0.0181  -0.0057
AT. 17 SI X    0.0141  -0.0218   0.0011   0.0042  -0.0080   0.0009
        Y    0.0262   0.0000  -0.0094  -0.0050   0.0006  -0.0197
        Z    0.0106   0.0178  -0.0076   0.0134   0.0181   0.0057
AT. 18 SI X    0.0141   0.0218  -0.0011  -0.0042  -0.0080   0.0009
        Y   -0.0262   0.0000  -0.0094  -0.0050  -0.0006   0.0197
        Z   -0.0106   0.0178  -0.0076   0.0134  -0.0181  -0.0057
AT. 19 SI X   -0.0243   0.0000   0.0000   0.0000  -0.0258  -0.0032
        Y    0.0000  -0.0003  -0.0300   0.0041   0.0000   0.0000
        Z    0.0000   0.0107  -0.0106  -0.0153   0.0000   0.0000
AT. 20 SI X    0.0243   0.0000   0.0000   0.0000   0.0258  -0.0032
        Y    0.0000  -0.0003   0.0300   0.0041   0.0000   0.0000
        Z    0.0000  -0.0107  -0.0106   0.0153   0.0000   0.0000
AT. 21 O  X    0.0112   0.0028  -0.0051  -0.0164   0.0005  -0.0017
        Y    0.0214  -0.0089   0.0009   0.0053   0.0038   0.0309
        Z    0.0221   0.0012  -0.0087   0.0024  -0.0289  -0.0034
AT. 22 O  X    0.0112  -0.0028   0.0051   0.0164   0.0005  -0.0017
        Y   -0.0214  -0.0089   0.0009   0.0053  -0.0038  -0.0309
        Z   -0.0221   0.0012  -0.0087   0.0024   0.0289   0.0034
AT. 23 O  X   -0.0112  -0.0028  -0.0051   0.0164  -0.0005  -0.0017
        Y    0.0214  -0.0089  -0.0009   0.0053   0.0038  -0.0309
        Z   -0.0221  -0.0012  -0.0087  -0.0024   0.0289  -0.0034
AT. 24 O  X   -0.0112   0.0028   0.0051  -0.0164  -0.0005  -0.0017
        Y   -0.0214  -0.0089  -0.0009   0.0053  -0.0038   0.0309
        Z    0.0221  -0.0012  -0.0087  -0.0024  -0.0289   0.0034
AT. 25 O  X    0.0000  -0.0006   0.0000  -0.0183   0.0000   0.0070
        Y    0.0000   0.0091   0.0000   0.0218   0.0000  -0.0062
        Z    0.0122   0.0000   0.0002   0.0000  -0.0170   0.0000
AT. 26 O  X    0.0000   0.0006   0.0000   0.0183   0.0000   0.0070
        Y    0.0000   0.0091   0.0000   0.0218   0.0000   0.0062
        Z   -0.0122   0.0000   0.0002   0.0000   0.0170   0.0000
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AT. 27 O  X   0.0000   0.0113   0.0000  -0.0134   0.0000  -0.0159
        Y   0.0000  -0.0036   0.0000   0.0124   0.0000   0.0202
        Z   0.0391   0.0000   0.0077   0.0000  -0.0196   0.0000
AT. 28 O  X   0.0000  -0.0113   0.0000   0.0134   0.0000  -0.0159
        Y   0.0000  -0.0036   0.0000   0.0124   0.0000  -0.0202
        Z  -0.0391   0.0000   0.0077   0.0000   0.0196   0.0000
AT. 29 O  X  -0.0109   0.0280  -0.0156   0.0097   0.0174  -0.0032
        Y   0.0353   0.0010   0.0139   0.0042   0.0009   0.0328
        Z  -0.0030  -0.0118  -0.0153  -0.0018  -0.0119   0.0090
AT. 30 O  X  -0.0109  -0.0280   0.0156  -0.0097   0.0174  -0.0032
        Y  -0.0353   0.0010   0.0139   0.0042  -0.0009  -0.0328
        Z   0.0030  -0.0118  -0.0153  -0.0018   0.0119  -0.0090
AT. 31 O  X   0.0109  -0.0280  -0.0156  -0.0097  -0.0174  -0.0032
        Y   0.0353   0.0010  -0.0139   0.0042   0.0009  -0.0328
        Z   0.0030   0.0118  -0.0153   0.0018   0.0119   0.0090
AT. 32 O  X   0.0109   0.0280   0.0156   0.0097  -0.0174  -0.0032
        Y  -0.0353   0.0010  -0.0139   0.0042  -0.0009   0.0328
        Z  -0.0030   0.0118  -0.0153   0.0018  -0.0119  -0.0090
AT. 33 O  X   0.0127  -0.0187   0.0038   0.0032  -0.0047  -0.0042
        Y   0.0283  -0.0034  -0.0111  -0.0008  -0.0062  -0.0079
        Z   0.0137   0.0248   0.0168   0.0218   0.0242   0.0048
AT. 34 O  X   0.0127   0.0187  -0.0038  -0.0032  -0.0047  -0.0042
        Y  -0.0283  -0.0034  -0.0111  -0.0008   0.0062   0.0079
        Z  -0.0137   0.0248   0.0168   0.0218  -0.0242  -0.0048
AT. 35 O  X  -0.0127   0.0187   0.0038  -0.0032   0.0047  -0.0042
        Y   0.0283  -0.0034   0.0111  -0.0008  -0.0062   0.0079
        Z  -0.0137  -0.0248   0.0168  -0.0218  -0.0242   0.0048
AT. 36 O  X  -0.0127  -0.0187  -0.0038   0.0032   0.0047  -0.0042
        Y  -0.0283  -0.0034   0.0111  -0.0008   0.0062  -0.0079
        Z   0.0137  -0.0248   0.0168  -0.0218   0.0242  -0.0048
AT. 37 O  X  -0.0216   0.0180   0.0293  -0.0181  -0.0161  -0.0014
        Y   0.0114  -0.0016  -0.0079  -0.0051   0.0062   0.0135
        Z   0.0052  -0.0131  -0.0194  -0.0039  -0.0035   0.0098
AT. 38 O  X  -0.0216  -0.0180  -0.0293   0.0181  -0.0161  -0.0014
        Y  -0.0114  -0.0016  -0.0079  -0.0051  -0.0062  -0.0135
        Z  -0.0052  -0.0131  -0.0194  -0.0039   0.0035  -0.0098
AT. 39 O  X   0.0216  -0.0180   0.0293   0.0181   0.0161  -0.0014
        Y   0.0114  -0.0016   0.0079  -0.0051   0.0062  -0.0135
        Z  -0.0052   0.0131  -0.0194   0.0039   0.0035   0.0098
AT. 40 O  X   0.0216   0.0180  -0.0293  -0.0181   0.0161  -0.0014
        Y  -0.0114  -0.0016   0.0079  -0.0051  -0.0062   0.0135
        Z   0.0052   0.0131  -0.0194   0.0039  -0.0035  -0.0098
AT. 41 O  X  -0.0114   0.0168   0.0088   0.0031   0.0158   0.0052
        Y   0.0270  -0.0007   0.0104  -0.0029   0.0014   0.0203
        Z  -0.0257  -0.0151  -0.0157  -0.0167  -0.0104  -0.0063
AT. 42 O  X  -0.0114  -0.0168  -0.0088  -0.0031   0.0158   0.0052
        Y  -0.0270  -0.0007   0.0104  -0.0029  -0.0014  -0.0203
        Z   0.0257  -0.0151  -0.0157  -0.0167   0.0104   0.0063
AT. 43 O  X   0.0114  -0.0168   0.0088  -0.0031  -0.0158   0.0052
        Y   0.0270  -0.0007  -0.0104  -0.0029   0.0014  -0.0203
        Z   0.0257   0.0151  -0.0157   0.0167   0.0104  -0.0063
AT. 44 O  X   0.0114   0.0168  -0.0088   0.0031  -0.0158   0.0052
        Y  -0.0270  -0.0007  -0.0104  -0.0029  -0.0014   0.0203
        Z  -0.0257   0.0151  -0.0157   0.0167  -0.0104   0.0063
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AT. 45 O  X  -0.0202   0.0149   0.0107  -0.0051  -0.0293  -0.0010
        Y   0.0158  -0.0068  -0.0450   0.0134   0.0080   0.0171
        Z  -0.0103   0.0335   0.0165  -0.0317  -0.0117  -0.0148
AT. 46 O  X  -0.0202  -0.0149  -0.0107   0.0051  -0.0293  -0.0010
        Y  -0.0158  -0.0068  -0.0450   0.0134  -0.0080  -0.0171
        Z   0.0103   0.0335   0.0165  -0.0317   0.0117   0.0148
AT. 47 O  X   0.0202  -0.0149   0.0107   0.0051   0.0293  -0.0010
        Y   0.0158  -0.0068   0.0450   0.0134   0.0080  -0.0171
        Z   0.0103  -0.0335   0.0165   0.0317   0.0117  -0.0148
AT. 48 O  X   0.0202   0.0149  -0.0107  -0.0051   0.0293  -0.0010
        Y  -0.0158  -0.0068   0.0450   0.0134  -0.0080   0.0171
        Z  -0.0103  -0.0335   0.0165   0.0317  -0.0117   0.0148


FREQ(CM**-1)   152.83   157.29   162.67   164.83   170.20   174.88


AT.  1 CA X   0.0000   0.0036   0.0000   0.0032   0.0000   0.0000
        Y  -0.0220   0.0000   0.0071   0.0000  -0.0468  -0.0362
        Z  -0.0519   0.0000   0.0352   0.0000   0.0329   0.0463
AT.  2 CA X   0.0000   0.0036   0.0000  -0.0032   0.0000   0.0000
        Y  -0.0220   0.0000  -0.0071   0.0000  -0.0468   0.0362
        Z   0.0519   0.0000   0.0352   0.0000  -0.0329   0.0463
AT.  3 CA X   0.0002  -0.0169   0.0000   0.0000  -0.0138   0.0000
        Y  -0.0386   0.0088   0.0000   0.0000  -0.0201   0.0000
        Z   0.0000   0.0000   0.0010  -0.0161   0.0000  -0.0043
AT.  4 CA X  -0.0002  -0.0169   0.0000   0.0000   0.0138   0.0000
        Y  -0.0386  -0.0088   0.0000   0.0000  -0.0201   0.0000
        Z   0.0000   0.0000   0.0010   0.0161   0.0000  -0.0043
AT.  5 CA X  -0.0056   0.0098   0.0052   0.0210  -0.0059   0.0092
        Y   0.0047   0.0054   0.0181  -0.0218  -0.0076   0.0093
        Z  -0.0080  -0.0281  -0.0261   0.0181   0.0009   0.0065
AT.  6 CA X   0.0056   0.0098  -0.0052   0.0210   0.0059  -0.0092
        Y   0.0047  -0.0054   0.0181   0.0218  -0.0076   0.0093
        Z  -0.0080   0.0281  -0.0261  -0.0181   0.0009   0.0065
AT.  7 CA X   0.0056   0.0098   0.0052  -0.0210   0.0059   0.0092
        Y   0.0047  -0.0054  -0.0181  -0.0218  -0.0076  -0.0093
        Z   0.0080  -0.0281  -0.0261  -0.0181  -0.0009   0.0065
AT.  8 CA X  -0.0056   0.0098  -0.0052  -0.0210  -0.0059  -0.0092
        Y   0.0047   0.0054  -0.0181   0.0218  -0.0076  -0.0093
        Z   0.0080   0.0281  -0.0261   0.0181  -0.0009   0.0065
AT.  9 CA X  -0.0070   0.0121  -0.0221  -0.0221  -0.0031   0.0081
        Y   0.0180  -0.0036   0.0280   0.0058   0.0171  -0.0053
        Z   0.0105  -0.0020  -0.0075  -0.0298  -0.0030  -0.0097
AT. 10 CA X   0.0070   0.0121   0.0221  -0.0221   0.0031  -0.0081
        Y   0.0180   0.0036   0.0280  -0.0058   0.0171  -0.0053
        Z   0.0105   0.0020  -0.0075   0.0298  -0.0030  -0.0097
AT. 11 CA X   0.0070   0.0121  -0.0221   0.0221   0.0031   0.0081
        Y   0.0180   0.0036  -0.0280   0.0058   0.0171   0.0053
        Z  -0.0105  -0.0020  -0.0075   0.0298   0.0030  -0.0097
AT. 12 CA X  -0.0070   0.0121   0.0221   0.0221  -0.0031  -0.0081
        Y   0.0180  -0.0036  -0.0280  -0.0058   0.0171   0.0053
        Z  -0.0105   0.0020  -0.0075  -0.0298   0.0030  -0.0097
AT. 13 SI X   0.0203  -0.0319   0.0000   0.0000  -0.0108   0.0000
        Y  -0.0153   0.0090   0.0000   0.0000  -0.0152   0.0000
        Z   0.0000   0.0000  -0.0171   0.0029   0.0000  -0.0016
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AT. 14 SI X  -0.0203  -0.0319   0.0000   0.0000   0.0108   0.0000
        Y  -0.0153  -0.0090   0.0000   0.0000  -0.0152   0.0000
        Z   0.0000   0.0000  -0.0171  -0.0029   0.0000  -0.0016
AT. 15 SI X   0.0170   0.0050  -0.0170  -0.0045  -0.0043   0.0108
        Y   0.0061   0.0006   0.0011  -0.0060   0.0081  -0.0171
        Z  -0.0054  -0.0242   0.0119  -0.0043   0.0067  -0.0034
AT. 16 SI X  -0.0170   0.0050   0.0170  -0.0045   0.0043  -0.0108
        Y   0.0061  -0.0006   0.0011   0.0060   0.0081  -0.0171
        Z  -0.0054   0.0242   0.0119   0.0043   0.0067  -0.0034
AT. 17 SI X  -0.0170   0.0050  -0.0170   0.0045   0.0043   0.0108
        Y   0.0061  -0.0006  -0.0011  -0.0060   0.0081   0.0171
        Z   0.0054  -0.0242   0.0119   0.0043  -0.0067  -0.0034
AT. 18 SI X   0.0170   0.0050   0.0170   0.0045  -0.0043  -0.0108
        Y   0.0061   0.0006  -0.0011   0.0060   0.0081   0.0171
        Z   0.0054   0.0242   0.0119  -0.0043  -0.0067  -0.0034
AT. 19 SI X   0.0000   0.0023   0.0000   0.0134   0.0000   0.0000
        Y   0.0187   0.0000  -0.0019   0.0000   0.0187  -0.0023
        Z   0.0127   0.0000   0.0144   0.0000   0.0004  -0.0045
AT. 20 SI X   0.0000   0.0023   0.0000  -0.0134   0.0000   0.0000
        Y   0.0187   0.0000   0.0019   0.0000   0.0187   0.0023
        Z  -0.0127   0.0000   0.0144   0.0000  -0.0004  -0.0045
AT. 21 O  X   0.0156  -0.0208   0.0018  -0.0127  -0.0111  -0.0039
        Y  -0.0177   0.0174   0.0021   0.0154  -0.0046   0.0078
        Z  -0.0011   0.0003  -0.0154  -0.0123  -0.0044  -0.0101
AT. 22 O  X  -0.0156  -0.0208  -0.0018  -0.0127   0.0111   0.0039
        Y  -0.0177  -0.0174   0.0021  -0.0154  -0.0046   0.0078
        Z  -0.0011  -0.0003  -0.0154   0.0123  -0.0044  -0.0101
AT. 23 O  X  -0.0156  -0.0208   0.0018   0.0127   0.0111  -0.0039
        Y  -0.0177  -0.0174  -0.0021   0.0154  -0.0046  -0.0078
        Z   0.0011   0.0003  -0.0154   0.0123   0.0044  -0.0101
AT. 24 O  X   0.0156  -0.0208  -0.0018   0.0127  -0.0111   0.0039
        Y  -0.0177   0.0174  -0.0021  -0.0154  -0.0046  -0.0078
        Z   0.0011  -0.0003  -0.0154  -0.0123   0.0044  -0.0101
AT. 25 O  X   0.0144  -0.0225   0.0000   0.0000  -0.0051   0.0000
        Y  -0.0064  -0.0079   0.0000   0.0000  -0.0278   0.0000
        Z   0.0000   0.0000  -0.0193   0.0167   0.0000   0.0018
AT. 26 O  X  -0.0144  -0.0225   0.0000   0.0000   0.0051   0.0000
        Y  -0.0064   0.0079   0.0000   0.0000  -0.0278   0.0000
        Z   0.0000   0.0000  -0.0193  -0.0167   0.0000   0.0018
AT. 27 O  X   0.0238  -0.0311   0.0000   0.0000  -0.0196   0.0000
        Y  -0.0152   0.0099   0.0000   0.0000  -0.0154   0.0000
        Z   0.0000   0.0000  -0.0194   0.0205   0.0000  -0.0053
AT. 28 O  X  -0.0238  -0.0311   0.0000   0.0000   0.0196   0.0000
        Y  -0.0152  -0.0099   0.0000   0.0000  -0.0154   0.0000
        Z   0.0000   0.0000  -0.0194  -0.0205   0.0000  -0.0053
AT. 29 O  X   0.0222   0.0044  -0.0143  -0.0285  -0.0237   0.0283
        Y   0.0054   0.0123   0.0003  -0.0063   0.0013  -0.0184
        Z  -0.0031  -0.0179   0.0095  -0.0184  -0.0059   0.0046
AT. 30 O  X  -0.0222   0.0044   0.0143  -0.0285   0.0237  -0.0283
        Y   0.0054  -0.0123   0.0003   0.0063   0.0013  -0.0184
        Z  -0.0031   0.0179   0.0095   0.0184  -0.0059   0.0046
AT. 31 O  X  -0.0222   0.0044  -0.0143   0.0285   0.0237   0.0283
        Y   0.0054  -0.0123  -0.0003  -0.0063   0.0013   0.0184
        Z   0.0031  -0.0179   0.0095   0.0184   0.0059   0.0046
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AT. 32 O   X    0.0222   0.0044   0.0143   0.0285  -0.0237  -0.0283
          Y    0.0054   0.0123  -0.0003   0.0063   0.0013   0.0184
          Z    0.0031   0.0179   0.0095  -0.0184   0.0059   0.0046
AT. 33 O   X   -0.0108   0.0065  -0.0174  -0.0039  -0.0037   0.0035
          Y   -0.0044  -0.0049  -0.0010   0.0064   0.0220   0.0295
          Z    0.0149  -0.0259   0.0071  -0.0249  -0.0371  -0.0360
AT. 34 O   X    0.0108   0.0065   0.0174  -0.0039   0.0037  -0.0035
          Y   -0.0044   0.0049  -0.0010  -0.0064   0.0220   0.0295
          Z    0.0149   0.0259   0.0071   0.0249  -0.0371  -0.0360
AT. 35 O   X    0.0108   0.0065  -0.0174   0.0039   0.0037   0.0035
          Y   -0.0044   0.0049   0.0010   0.0064   0.0220  -0.0295
          Z   -0.0149  -0.0259   0.0071   0.0249   0.0371  -0.0360
AT. 36 O   X   -0.0108   0.0065   0.0174   0.0039  -0.0037  -0.0035
          Y   -0.0044  -0.0049   0.0010  -0.0064   0.0220  -0.0295
          Z   -0.0149   0.0259   0.0071  -0.0249   0.0371  -0.0360
AT. 37 O   X    0.0005   0.0050  -0.0038   0.0154   0.0102  -0.0145
          Y    0.0128  -0.0144  -0.0068  -0.0122   0.0198  -0.0105
          Z    0.0056  -0.0185   0.0116  -0.0160  -0.0089   0.0092
AT. 38 O   X   -0.0005   0.0050   0.0038   0.0154  -0.0102   0.0145
          Y    0.0128   0.0144  -0.0068   0.0122   0.0198  -0.0105
          Z    0.0056   0.0185   0.0116   0.0160  -0.0089   0.0092
AT. 39 O   X   -0.0005   0.0050  -0.0038  -0.0154  -0.0102  -0.0145
          Y    0.0128   0.0144   0.0068  -0.0122   0.0198   0.0105
          Z   -0.0056  -0.0185   0.0116   0.0160   0.0089   0.0092
AT. 40 O   X    0.0005   0.0050   0.0038  -0.0154   0.0102   0.0145
          Y    0.0128  -0.0144   0.0068   0.0122   0.0198   0.0105
          Z   -0.0056   0.0185   0.0116  -0.0160   0.0089   0.0092
AT. 41 O   X    0.0241   0.0054  -0.0120  -0.0156  -0.0093   0.0173
          Y    0.0072   0.0009   0.0002  -0.0070   0.0096  -0.0176
          Z   -0.0147  -0.0308  -0.0040  -0.0148   0.0026   0.0064
AT. 42 O   X   -0.0241   0.0054   0.0120  -0.0156   0.0093  -0.0173
          Y    0.0072  -0.0009   0.0002   0.0070   0.0096  -0.0176
          Z   -0.0147   0.0308  -0.0040   0.0148   0.0026   0.0064
AT. 43 O   X   -0.0241   0.0054  -0.0120   0.0156   0.0093   0.0173
          Y    0.0072  -0.0009  -0.0002  -0.0070   0.0096   0.0176
          Z    0.0147  -0.0308  -0.0040   0.0148  -0.0026   0.0064
AT. 44 O   X    0.0241   0.0054   0.0120   0.0156  -0.0093  -0.0173
          Y    0.0072   0.0009  -0.0002   0.0070   0.0096   0.0176
          Z    0.0147   0.0308  -0.0040  -0.0148  -0.0026   0.0064
AT. 45 O   X   -0.0063   0.0054   0.0021   0.0057  -0.0042   0.0052
          Y    0.0121  -0.0331  -0.0147  -0.0136   0.0156   0.0044
          Z    0.0116   0.0362   0.0318   0.0041  -0.0023  -0.0054
AT. 46 O   X    0.0063   0.0054  -0.0021   0.0057   0.0042  -0.0052
          Y    0.0121   0.0331  -0.0147   0.0136   0.0156   0.0044
          Z    0.0116  -0.0362   0.0318  -0.0041  -0.0023  -0.0054
AT. 47 O   X    0.0063   0.0054   0.0021  -0.0057   0.0042   0.0052
          Y    0.0121   0.0331   0.0147  -0.0136   0.0156  -0.0044
          Z   -0.0116   0.0362   0.0318  -0.0041   0.0023  -0.0054
AT. 48 O   X   -0.0063   0.0054  -0.0021  -0.0057  -0.0042  -0.0052
          Y    0.0121  -0.0331   0.0147   0.0136   0.0156  -0.0044
          Z   -0.0116  -0.0362   0.0318   0.0041   0.0023  -0.0054

FREQ(CM**-1)   179.96   181.93   182.21   185.06   191.99   194.22
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AT.  1 CA X    0.0000   0.0000   0.0091  -0.0050   0.0000   0.0000
        Y    0.0322  -0.0187   0.0000   0.0000  -0.0067   0.0212
        Z   -0.0225  -0.0223   0.0000   0.0000   0.0003  -0.0178
AT.  2 CA X    0.0000   0.0000  -0.0091  -0.0050   0.0000   0.0000
        Y    0.0322   0.0187   0.0000   0.0000  -0.0067  -0.0212
        Z    0.0225  -0.0223   0.0000   0.0000  -0.0003  -0.0178
AT.  3 CA X   -0.0034   0.0000   0.0000  -0.0034   0.0408   0.0000
        Y   -0.0019   0.0000   0.0000  -0.0300   0.0202   0.0000
        Z    0.0000  -0.0229  -0.0250   0.0000   0.0000   0.0072
AT.  4 CA X    0.0034   0.0000   0.0000  -0.0034  -0.0408   0.0000
        Y   -0.0019   0.0000   0.0000   0.0300   0.0202   0.0000
        Z    0.0000  -0.0229   0.0250   0.0000   0.0000   0.0072
AT.  5 CA X   -0.0191  -0.0198  -0.0013  -0.0184   0.0233   0.0106
        Y   -0.0110   0.0255   0.0204  -0.0016  -0.0168  -0.0070
        Z    0.0127   0.0089  -0.0078  -0.0009   0.0162   0.0092
AT.  6 CA X    0.0191   0.0198  -0.0013  -0.0184  -0.0233  -0.0106
        Y   -0.0110   0.0255  -0.0204   0.0016  -0.0168  -0.0070
        Z    0.0127   0.0089   0.0078   0.0009   0.0162   0.0092
AT.  7 CA X    0.0191  -0.0198   0.0013  -0.0184  -0.0233   0.0106
        Y   -0.0110  -0.0255   0.0204   0.0016  -0.0168   0.0070
        Z   -0.0127   0.0089   0.0078  -0.0009  -0.0162   0.0092
AT.  8 CA X   -0.0191   0.0198   0.0013  -0.0184   0.0233  -0.0106
        Y   -0.0110  -0.0255  -0.0204  -0.0016  -0.0168   0.0070
        Z   -0.0127   0.0089  -0.0078   0.0009  -0.0162   0.0092
AT.  9 CA X   -0.0267  -0.0024   0.0075  -0.0064  -0.0283   0.0051
        Y    0.0057   0.0244   0.0077   0.0177   0.0170   0.0091
        Z   -0.0214  -0.0044   0.0098  -0.0249   0.0012  -0.0388
AT. 10 CA X    0.0267   0.0024   0.0075  -0.0064   0.0283  -0.0051
        Y    0.0057   0.0244  -0.0077  -0.0177   0.0170   0.0091
        Z   -0.0214  -0.0044  -0.0098   0.0249   0.0012  -0.0388
AT. 11 CA X    0.0267  -0.0024  -0.0075  -0.0064   0.0283   0.0051
        Y    0.0057  -0.0244   0.0077  -0.0177   0.0170  -0.0091
        Z    0.0214  -0.0044  -0.0098  -0.0249  -0.0012  -0.0388
AT. 12 CA X   -0.0267   0.0024  -0.0075  -0.0064  -0.0283  -0.0051
        Y    0.0057  -0.0244  -0.0077   0.0177   0.0170  -0.0091
        Z    0.0214  -0.0044   0.0098   0.0249  -0.0012  -0.0388
AT. 13 SI X   -0.0173   0.0000   0.0000   0.0059   0.0043   0.0000
        Y   -0.0087   0.0000   0.0000  -0.0107  -0.0055   0.0000
        Z    0.0000   0.0137   0.0140   0.0000   0.0000  -0.0069
AT. 14 SI X    0.0173   0.0000   0.0000   0.0059  -0.0043   0.0000
        Y   -0.0087   0.0000   0.0000   0.0107  -0.0055   0.0000
        Z    0.0000   0.0137  -0.0140   0.0000   0.0000  -0.0069
AT. 15 SI X    0.0079   0.0180   0.0164   0.0155  -0.0006   0.0060
        Y    0.0056  -0.0046   0.0054   0.0056  -0.0039   0.0028
        Z   -0.0049  -0.0051  -0.0222  -0.0190   0.0063   0.0183
AT. 16 SI X   -0.0079  -0.0180   0.0164   0.0155   0.0006  -0.0060
        Y    0.0056  -0.0046  -0.0054  -0.0056  -0.0039   0.0028
        Z   -0.0049  -0.0051   0.0222   0.0190   0.0063   0.0183
AT. 17 SI X   -0.0079   0.0180  -0.0164   0.0155   0.0006   0.0060
        Y    0.0056   0.0046   0.0054  -0.0056  -0.0039  -0.0028
        Z    0.0049  -0.0051   0.0222  -0.0190  -0.0063   0.0183
AT. 18 SI X    0.0079  -0.0180  -0.0164   0.0155  -0.0006  -0.0060
        Y    0.0056   0.0046  -0.0054   0.0056  -0.0039  -0.0028
        Z    0.0049  -0.0051  -0.0222   0.0190  -0.0063   0.0183
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AT. 19 SI  X   0.0000   0.0000   0.0155  -0.0067   0.0000   0.0000
          Y  -0.0123   0.0086   0.0000   0.0000   0.0047  -0.0018
          Z  -0.0093   0.0111   0.0000   0.0000   0.0146   0.0071
AT. 20 SI  X   0.0000   0.0000  -0.0155  -0.0067   0.0000   0.0000
          Y  -0.0123  -0.0086   0.0000   0.0000   0.0047   0.0018
          Z   0.0093   0.0111   0.0000   0.0000  -0.0146   0.0071
AT. 21 O   X  -0.0173  -0.0040   0.0060   0.0027   0.0055  -0.0127
          Y  -0.0002   0.0167   0.0110  -0.0029  -0.0058   0.0206
          Z  -0.0043   0.0026   0.0099  -0.0073   0.0007  -0.0219
AT. 22 O   X   0.0173   0.0040   0.0060   0.0027  -0.0055   0.0127
          Y  -0.0002   0.0167  -0.0110   0.0029  -0.0058   0.0206
          Z  -0.0043   0.0026  -0.0099   0.0073   0.0007  -0.0219
AT. 23 O   X   0.0173  -0.0040  -0.0060   0.0027  -0.0055  -0.0127
          Y  -0.0002  -0.0167   0.0110   0.0029  -0.0058  -0.0206
          Z   0.0043   0.0026  -0.0099  -0.0073  -0.0007  -0.0219
AT. 24 O   X  -0.0173   0.0040  -0.0060   0.0027   0.0055   0.0127
          Y  -0.0002  -0.0167  -0.0110  -0.0029  -0.0058  -0.0206
          Z   0.0043   0.0026   0.0099   0.0073  -0.0007  -0.0219
AT. 25 O   X  -0.0146   0.0000   0.0000   0.0006  -0.0014   0.0000
          Y  -0.0158   0.0000   0.0000  -0.0052   0.0072   0.0000
          Z   0.0000   0.0172   0.0069   0.0000   0.0000   0.0141
AT. 26 O   X   0.0146   0.0000   0.0000   0.0006   0.0014   0.0000
          Y  -0.0158   0.0000   0.0000   0.0052   0.0072   0.0000
          Z   0.0000   0.0172  -0.0069   0.0000   0.0000   0.0141
AT. 27 O   X  -0.0260   0.0000   0.0000   0.0047   0.0192   0.0000
          Y  -0.0085   0.0000   0.0000  -0.0087  -0.0050   0.0000
          Z   0.0000   0.0225   0.0071   0.0000   0.0000   0.0293
AT. 28 O   X   0.0260   0.0000   0.0000   0.0047  -0.0192   0.0000
          Y  -0.0085   0.0000   0.0000   0.0087  -0.0050   0.0000
          Z   0.0000   0.0225  -0.0071   0.0000   0.0000   0.0293
AT. 29 O   X  -0.0037   0.0045   0.0013   0.0222   0.0050   0.0135
          Y   0.0037  -0.0041   0.0143   0.0133  -0.0066   0.0002
          Z  -0.0131  -0.0109  -0.0240  -0.0095   0.0085   0.0206
AT. 30 O   X   0.0037  -0.0045   0.0013   0.0222  -0.0050  -0.0135
          Y   0.0037  -0.0041  -0.0143  -0.0133  -0.0066   0.0002
          Z  -0.0131  -0.0109   0.0240   0.0095   0.0085   0.0206
AT. 31 O   X   0.0037   0.0045  -0.0013   0.0222  -0.0050   0.0135
          Y   0.0037   0.0041   0.0143  -0.0133  -0.0066  -0.0002
          Z   0.0131  -0.0109   0.0240  -0.0095  -0.0085   0.0206
AT. 32 O   X  -0.0037  -0.0045  -0.0013   0.0222   0.0050  -0.0135
          Y   0.0037   0.0041  -0.0143   0.0133  -0.0066  -0.0002
          Z   0.0131  -0.0109  -0.0240   0.0095  -0.0085   0.0206
AT. 33 O   X  -0.0127   0.0124  -0.0116   0.0055  -0.0042   0.0025
          Y   0.0075   0.0166  -0.0052   0.0143   0.0083   0.0002
          Z  -0.0084   0.0115   0.0035  -0.0270  -0.0030   0.0035
AT. 34 O   X   0.0127  -0.0124  -0.0116   0.0055   0.0042  -0.0025
          Y   0.0075   0.0166   0.0052  -0.0143   0.0083   0.0002
          Z  -0.0084   0.0115  -0.0035   0.0270  -0.0030   0.0035
AT. 35 O   X   0.0127   0.0124   0.0116   0.0055   0.0042   0.0025
          Y   0.0075  -0.0166  -0.0052  -0.0143   0.0083  -0.0002
          Z   0.0084   0.0115  -0.0035  -0.0270   0.0030   0.0035
AT. 36 O   X  -0.0127  -0.0124   0.0116   0.0055  -0.0042  -0.0025
          Y   0.0075  -0.0166   0.0052   0.0143   0.0083  -0.0002
          Z   0.0084   0.0115   0.0035   0.0270   0.0030   0.0035
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AT. 37 O  X   0.0246   0.0268   0.0206  -0.0061  -0.0099  -0.0065
         Y   0.0025   0.0088  -0.0118   0.0049  -0.0058   0.0060
         Z  -0.0185  -0.0159  -0.0203   0.0011   0.0143   0.0210
AT. 38 O  X  -0.0246  -0.0268   0.0206  -0.0061   0.0099   0.0065
         Y   0.0025   0.0088   0.0118  -0.0049  -0.0058   0.0060
         Z  -0.0185  -0.0159   0.0203  -0.0011   0.0143   0.0210
AT. 39 O  X  -0.0246   0.0268  -0.0206  -0.0061   0.0099  -0.0065
         Y   0.0025  -0.0088  -0.0118  -0.0049  -0.0058  -0.0060
         Z   0.0185  -0.0159   0.0203   0.0011  -0.0143   0.0210
AT. 40 O  X   0.0246  -0.0268  -0.0206  -0.0061  -0.0099   0.0065
         Y   0.0025  -0.0088   0.0118   0.0049  -0.0058  -0.0060
         Z   0.0185  -0.0159  -0.0203  -0.0011  -0.0143   0.0210
AT. 41 O  X   0.0057   0.0114   0.0185   0.0208  -0.0192   0.0003
         Y   0.0060  -0.0056   0.0051   0.0052  -0.0048   0.0022
         Z  -0.0116   0.0002  -0.0213  -0.0314   0.0021   0.0166
AT. 42 O  X  -0.0057  -0.0114   0.0185   0.0208   0.0192  -0.0003
         Y   0.0060  -0.0056  -0.0051  -0.0052  -0.0048   0.0022
         Z  -0.0116   0.0002   0.0213   0.0314   0.0021   0.0166
AT. 43 O  X  -0.0057   0.0114  -0.0185   0.0208   0.0192   0.0003
         Y   0.0060   0.0056   0.0051  -0.0052  -0.0048  -0.0022
         Z   0.0116   0.0002   0.0213  -0.0314  -0.0021   0.0166
AT. 44 O  X   0.0057  -0.0114  -0.0185   0.0208  -0.0192  -0.0003
         Y   0.0060   0.0056  -0.0051   0.0052  -0.0048  -0.0022
         Z   0.0116   0.0002  -0.0213   0.0314  -0.0021   0.0166
AT. 45 O  X   0.0015   0.0032   0.0144  -0.0023  -0.0059  -0.0144
         Y  -0.0237  -0.0052  -0.0356   0.0239   0.0040  -0.0032
         Z   0.0039   0.0249   0.0378  -0.0223   0.0080  -0.0068
AT. 46 O  X  -0.0015  -0.0032   0.0144  -0.0023   0.0059   0.0144
         Y  -0.0237  -0.0052   0.0356  -0.0239   0.0040  -0.0032
         Z   0.0039   0.0249  -0.0378   0.0223   0.0080  -0.0068
AT. 47 O  X  -0.0015   0.0032  -0.0144  -0.0023   0.0059  -0.0144
         Y  -0.0237   0.0052  -0.0356  -0.0239   0.0040   0.0032
         Z  -0.0039   0.0249  -0.0378  -0.0223  -0.0080  -0.0068
AT. 48 O  X   0.0015  -0.0032  -0.0144  -0.0023  -0.0059   0.0144
         Y  -0.0237   0.0052   0.0356   0.0239   0.0040   0.0032
         Z  -0.0039   0.0249   0.0378   0.0223  -0.0080  -0.0068


FREQ(CM**-1)   199.83   200.42   203.16   207.64   207.88   208.58


AT.  1 CA X   0.0085   0.0247   0.0000   0.0000   0.0104   0.0000
         Y   0.0000   0.0000   0.0052   0.0017   0.0000  -0.0082
         Z   0.0000   0.0000  -0.0048  -0.0093   0.0000  -0.0075
AT.  2 CA X  -0.0085   0.0247   0.0000   0.0000   0.0104   0.0000
         Y   0.0000   0.0000  -0.0052   0.0017   0.0000   0.0082
         Z   0.0000   0.0000  -0.0048   0.0093   0.0000  -0.0075
AT.  3 CA X   0.0000   0.0300   0.0000  -0.0095  -0.0037   0.0000
         Y   0.0000   0.0341   0.0000   0.0407  -0.0248   0.0000
         Z   0.0336   0.0000  -0.0179   0.0000   0.0000   0.0610
AT.  4 CA X   0.0000   0.0300   0.0000   0.0095  -0.0037   0.0000
         Y   0.0000  -0.0341   0.0000   0.0407   0.0248   0.0000
         Z  -0.0336   0.0000  -0.0179   0.0000   0.0000   0.0610
AT.  5 CA X   0.0086  -0.0204  -0.0294   0.0133   0.0012  -0.0162
         Y  -0.0200  -0.0065  -0.0130  -0.0213   0.0053   0.0080
         Z   0.0172   0.0065  -0.0005  -0.0109  -0.0052  -0.0101
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AT.  6 CA X    0.0086  -0.0204   0.0294  -0.0133   0.0012   0.0162
        Y    0.0200   0.0065  -0.0130  -0.0213  -0.0053   0.0080
        Z   -0.0172  -0.0065  -0.0005  -0.0109   0.0052  -0.0101
AT.  7 CA X   -0.0086  -0.0204  -0.0294  -0.0133   0.0012  -0.0162
        Y   -0.0200   0.0065   0.0130  -0.0213  -0.0053  -0.0080
        Z   -0.0172   0.0065  -0.0005   0.0109  -0.0052  -0.0101
AT.  8 CA X   -0.0086  -0.0204   0.0294   0.0133   0.0012   0.0162
        Y    0.0200  -0.0065   0.0130  -0.0213   0.0053  -0.0080
        Z    0.0172  -0.0065  -0.0005   0.0109   0.0052  -0.0101
AT.  9 CA X    0.0030  -0.0226   0.0056   0.0107  -0.0149   0.0007
        Y    0.0126   0.0023   0.0000   0.0112   0.0277  -0.0010
        Z   -0.0029  -0.0050   0.0085   0.0113   0.0029  -0.0021
AT. 10 CA X    0.0030  -0.0226  -0.0056  -0.0107  -0.0149  -0.0007
        Y   -0.0126  -0.0023   0.0000   0.0112  -0.0277  -0.0010
        Z    0.0029   0.0050   0.0085   0.0113  -0.0029  -0.0021
AT. 11 CA X   -0.0030  -0.0226   0.0056  -0.0107  -0.0149   0.0007
        Y    0.0126  -0.0023   0.0000   0.0112  -0.0277   0.0010
        Z    0.0029  -0.0050   0.0085  -0.0113   0.0029  -0.0021
AT. 12 CA X   -0.0030  -0.0226  -0.0056   0.0107  -0.0149  -0.0007
        Y   -0.0126   0.0023   0.0000   0.0112   0.0277   0.0010
        Z   -0.0029   0.0050   0.0085  -0.0113  -0.0029  -0.0021
AT. 13 SI X    0.0000   0.0107   0.0000  -0.0170   0.0166   0.0000
        Y    0.0000  -0.0103   0.0000  -0.0119  -0.0031   0.0000
        Z   -0.0129   0.0000  -0.0277   0.0000   0.0000   0.0006
AT. 14 SI X    0.0000   0.0107   0.0000   0.0170   0.0166   0.0000
        Y    0.0000   0.0103   0.0000  -0.0119   0.0031   0.0000
        Z    0.0129   0.0000  -0.0277   0.0000   0.0000   0.0006
AT. 15 SI X    0.0232  -0.0032   0.0134   0.0052  -0.0116   0.0056
        Y   -0.0019  -0.0126   0.0033  -0.0069   0.0175   0.0034
        Z   -0.0076  -0.0098   0.0050  -0.0129   0.0023  -0.0069
AT. 16 SI X    0.0232  -0.0032  -0.0134  -0.0052  -0.0116  -0.0056
        Y    0.0019   0.0126   0.0033  -0.0069  -0.0175   0.0034
        Z    0.0076   0.0098   0.0050  -0.0129  -0.0023  -0.0069
AT. 17 SI X   -0.0232  -0.0032   0.0134  -0.0052  -0.0116   0.0056
        Y   -0.0019   0.0126  -0.0033  -0.0069  -0.0175  -0.0034
        Z    0.0076  -0.0098   0.0050   0.0129   0.0023  -0.0069
AT. 18 SI X   -0.0232  -0.0032  -0.0134   0.0052  -0.0116  -0.0056
        Y    0.0019  -0.0126  -0.0033  -0.0069   0.0175  -0.0034
        Z   -0.0076   0.0098   0.0050   0.0129  -0.0023  -0.0069
AT. 19 SI X    0.0133   0.0136   0.0000   0.0000   0.0149   0.0000
        Y    0.0000   0.0000  -0.0031   0.0156   0.0000  -0.0101
        Z    0.0000   0.0000   0.0254  -0.0065   0.0000   0.0026
AT. 20 SI X   -0.0133   0.0136   0.0000   0.0000   0.0149   0.0000
        Y    0.0000   0.0000   0.0031   0.0156   0.0000   0.0101
        Z    0.0000   0.0000   0.0254   0.0065   0.0000   0.0026
AT. 21 O  X    0.0222   0.0066  -0.0072  -0.0012   0.0139  -0.0090
        Y   -0.0002  -0.0094  -0.0211  -0.0036  -0.0034   0.0033
        Z    0.0004  -0.0015  -0.0193   0.0022  -0.0007  -0.0032
AT. 22 O  X    0.0222   0.0066   0.0072   0.0012   0.0139   0.0090
        Y    0.0002   0.0094  -0.0211  -0.0036   0.0034   0.0033
        Z   -0.0004   0.0015  -0.0193   0.0022   0.0007  -0.0032
AT. 23 O  X   -0.0222   0.0066  -0.0072   0.0012   0.0139  -0.0090
        Y   -0.0002   0.0094   0.0211  -0.0036   0.0034  -0.0033
        Z   -0.0004  -0.0015  -0.0193  -0.0022  -0.0007  -0.0032
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AT. 24 O  X  -0.0222   0.0066   0.0072  -0.0012   0.0139   0.0090
         Y   0.0002  -0.0094   0.0211  -0.0036  -0.0034  -0.0033
         Z   0.0004   0.0015  -0.0193  -0.0022   0.0007  -0.0032
AT. 25 O  X   0.0000   0.0109   0.0000  -0.0068   0.0112   0.0000
         Y   0.0000  -0.0183   0.0000  -0.0229   0.0063   0.0000
         Z  -0.0292   0.0000  -0.0071   0.0000   0.0000   0.0147
AT. 26 O  X   0.0000   0.0109   0.0000   0.0068   0.0112   0.0000
         Y   0.0000   0.0183   0.0000  -0.0229  -0.0063   0.0000
         Z   0.0292   0.0000  -0.0071   0.0000   0.0000   0.0147
AT. 27 O  X   0.0000  -0.0058   0.0000  -0.0163   0.0143   0.0000
         Y   0.0000  -0.0122   0.0000  -0.0125  -0.0017   0.0000
         Z  -0.0066   0.0000  -0.0444   0.0000   0.0000   0.0114
AT. 28 O  X   0.0000  -0.0058   0.0000   0.0163   0.0143   0.0000
         Y   0.0000   0.0122   0.0000  -0.0125   0.0017   0.0000
         Z   0.0066   0.0000  -0.0444   0.0000   0.0000   0.0114
AT. 29 O  X   0.0290   0.0022   0.0311  -0.0105  -0.0257   0.0127
         Y   0.0128  -0.0091  -0.0020   0.0100   0.0170   0.0243
         Z   0.0040  -0.0041   0.0136  -0.0108  -0.0079   0.0084
AT. 30 O  X   0.0290   0.0022  -0.0311   0.0105  -0.0257  -0.0127
         Y  -0.0128   0.0091  -0.0020   0.0100  -0.0170   0.0243
         Z  -0.0040   0.0041   0.0136  -0.0108   0.0079   0.0084
AT. 31 O  X  -0.0290   0.0022   0.0311   0.0105  -0.0257   0.0127
         Y   0.0128   0.0091   0.0020   0.0100  -0.0170  -0.0243
         Z  -0.0040  -0.0041   0.0136   0.0108  -0.0079   0.0084
AT. 32 O  X  -0.0290   0.0022  -0.0311  -0.0105  -0.0257  -0.0127
         Y  -0.0128  -0.0091   0.0020   0.0100   0.0170  -0.0243
         Z   0.0040   0.0041   0.0136   0.0108   0.0079   0.0084
AT. 33 O  X  -0.0148  -0.0044   0.0108   0.0028  -0.0076   0.0023
         Y  -0.0142   0.0151  -0.0074  -0.0253  -0.0205   0.0037
         Z   0.0167  -0.0174  -0.0105   0.0029   0.0241  -0.0122
AT. 34 O  X  -0.0148  -0.0044  -0.0108  -0.0028  -0.0076  -0.0023
         Y   0.0142  -0.0151  -0.0074  -0.0253   0.0205   0.0037
         Z  -0.0167   0.0174  -0.0105   0.0029  -0.0241  -0.0122
AT. 35 O  X   0.0148  -0.0044   0.0108  -0.0028  -0.0076   0.0023
         Y  -0.0142  -0.0151   0.0074  -0.0253   0.0205  -0.0037
         Z  -0.0167  -0.0174  -0.0105  -0.0029   0.0241  -0.0122
AT. 36 O  X   0.0148  -0.0044  -0.0108   0.0028  -0.0076  -0.0023
         Y   0.0142   0.0151   0.0074  -0.0253  -0.0205  -0.0037
         Z   0.0167   0.0174  -0.0105  -0.0029  -0.0241  -0.0122
AT. 37 O  X   0.0070   0.0040  -0.0044   0.0069   0.0163  -0.0016
         Y  -0.0018  -0.0164  -0.0061   0.0079  -0.0018  -0.0122
         Z   0.0028  -0.0111   0.0235  -0.0187  -0.0078   0.0017
AT. 38 O  X   0.0070   0.0040   0.0044  -0.0069   0.0163   0.0016
         Y   0.0018   0.0164  -0.0061   0.0079   0.0018  -0.0122
         Z  -0.0028   0.0111   0.0235  -0.0187   0.0078   0.0017
AT. 39 O  X  -0.0070   0.0040  -0.0044  -0.0069   0.0163  -0.0016
         Y  -0.0018   0.0164   0.0061   0.0079   0.0018   0.0122
         Z  -0.0028  -0.0111   0.0235   0.0187  -0.0078   0.0017
AT. 40 O  X  -0.0070   0.0040   0.0044   0.0069   0.0163   0.0016
         Y   0.0018  -0.0164   0.0061   0.0079  -0.0018   0.0122
         Z   0.0028   0.0111   0.0235   0.0187   0.0078   0.0017
AT. 41 O  X   0.0217   0.0002  -0.0073   0.0206  -0.0046   0.0102
         Y  -0.0024  -0.0135   0.0011  -0.0055   0.0172   0.0034
         Z  -0.0283   0.0004   0.0031  -0.0142  -0.0118  -0.0358
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AT. 42 O  X   0.0217   0.0002   0.0073  -0.0206  -0.0046  -0.0102
        Y   0.0024   0.0135   0.0011  -0.0055  -0.0172   0.0034
        Z   0.0283  -0.0004   0.0031  -0.0142   0.0118  -0.0358
AT. 43 O  X  -0.0217   0.0002  -0.0073  -0.0206  -0.0046   0.0102
        Y  -0.0024   0.0135  -0.0011  -0.0055  -0.0172  -0.0034
        Z   0.0283   0.0004   0.0031   0.0142  -0.0118  -0.0358
AT. 44 O  X  -0.0217   0.0002   0.0073   0.0206  -0.0046  -0.0102
        Y   0.0024  -0.0135  -0.0011  -0.0055   0.0172  -0.0034
        Z  -0.0283  -0.0004   0.0031   0.0142   0.0118  -0.0358
AT. 45 O  X   0.0102   0.0123  -0.0063   0.0095   0.0139   0.0013
        Y   0.0070  -0.0203  -0.0028   0.0149  -0.0198  -0.0081
        Z  -0.0080   0.0188   0.0171   0.0037   0.0212   0.0010
AT. 46 O  X   0.0102   0.0123   0.0063  -0.0095   0.0139  -0.0013
        Y  -0.0070   0.0203  -0.0028   0.0149   0.0198  -0.0081
        Z   0.0080  -0.0188   0.0171   0.0037  -0.0212   0.0010
AT. 47 O  X  -0.0102   0.0123  -0.0063  -0.0095   0.0139   0.0013
        Y   0.0070   0.0203   0.0028   0.0149   0.0198   0.0081
        Z   0.0080   0.0188   0.0171  -0.0037   0.0212   0.0010
AT. 48 O  X  -0.0102   0.0123   0.0063   0.0095   0.0139  -0.0013
        Y  -0.0070  -0.0203   0.0028   0.0149  -0.0198   0.0081
        Z  -0.0080  -0.0188   0.0171  -0.0037  -0.0212   0.0010


FREQ(CM**-1)   220.85   221.77   224.14   231.92   234.34   241.60

AT.  1 CA X  -0.0101   0.0176   0.0000  -0.0143   0.0000   0.0158
        Y   0.0000   0.0000  -0.0001   0.0000  -0.0037   0.0000
        Z   0.0000   0.0000  -0.0125   0.0000  -0.0163   0.0000
AT.  2 CA X   0.0101   0.0176   0.0000  -0.0143   0.0000  -0.0158
        Y   0.0000   0.0000  -0.0001   0.0000   0.0037   0.0000
        Z   0.0000   0.0000   0.0125   0.0000  -0.0163   0.0000
AT.  3 CA X   0.0000   0.0146   0.0080  -0.0034   0.0000   0.0000
        Y   0.0000  -0.0087   0.0032   0.0109   0.0000   0.0000
        Z   0.0250   0.0000   0.0000   0.0000  -0.0106  -0.0299
AT.  4 CA X   0.0000   0.0146  -0.0080  -0.0034   0.0000   0.0000
        Y   0.0000   0.0087   0.0032  -0.0109   0.0000   0.0000
        Z  -0.0250   0.0000   0.0000   0.0000  -0.0106   0.0299
AT.  5 CA X  -0.0166   0.0216  -0.0019  -0.0182   0.0166   0.0096
        Y  -0.0006   0.0067   0.0048   0.0081  -0.0223   0.0021
        Z   0.0035  -0.0173   0.0010  -0.0024   0.0018  -0.0029
AT.  6 CA X  -0.0166   0.0216   0.0019  -0.0182  -0.0166   0.0096
        Y   0.0006  -0.0067   0.0048  -0.0081  -0.0223  -0.0021
        Z  -0.0035   0.0173   0.0010   0.0024   0.0018   0.0029
AT.  7 CA X   0.0166   0.0216   0.0019  -0.0182   0.0166  -0.0096
        Y  -0.0006  -0.0067   0.0048  -0.0081   0.0223   0.0021
        Z  -0.0035  -0.0173  -0.0010  -0.0024   0.0018   0.0029
AT.  8 CA X   0.0166   0.0216  -0.0019  -0.0182  -0.0166  -0.0096
        Y   0.0006   0.0067   0.0048   0.0081   0.0223  -0.0021
        Z   0.0035   0.0173  -0.0010   0.0024   0.0018  -0.0029
AT.  9 CA X   0.0331  -0.0143  -0.0066   0.0055  -0.0306   0.0144
        Y  -0.0152   0.0215  -0.0138   0.0171   0.0088  -0.0205
        Z  -0.0180   0.0114   0.0348   0.0384   0.0066  -0.0076
AT. 10 CA X   0.0331  -0.0143   0.0066   0.0055   0.0306   0.0144
        Y   0.0152  -0.0215  -0.0138  -0.0171   0.0088   0.0205
        Z   0.0180  -0.0114   0.0348  -0.0384   0.0066   0.0076
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AT.  11 CA X   -0.0331  -0.0143   0.0066   0.0055  -0.0306  -0.0144
        Y   -0.0152  -0.0215  -0.0138  -0.0171  -0.0088  -0.0205
        Z    0.0180   0.0114  -0.0348   0.0384   0.0066   0.0076
AT.  12 CA X   -0.0331  -0.0143  -0.0066   0.0055   0.0306  -0.0144
        Y    0.0152   0.0215  -0.0138   0.0171  -0.0088   0.0205
        Z   -0.0180  -0.0114  -0.0348  -0.0384   0.0066  -0.0076
AT.  13 SI X    0.0000  -0.0244   0.0018   0.0037   0.0000   0.0000
        Y    0.0000  -0.0119   0.0009   0.0019   0.0000   0.0000
        Z   -0.0014   0.0000   0.0000   0.0000   0.0183   0.0134
AT.  14 SI X    0.0000  -0.0244  -0.0018   0.0037   0.0000   0.0000
        Y    0.0000   0.0119   0.0009  -0.0019   0.0000   0.0000
        Z    0.0014   0.0000   0.0000   0.0000   0.0183  -0.0134
AT.  15 SI X   -0.0051  -0.0021  -0.0104   0.0094   0.0027   0.0068
        Y    0.0024  -0.0062   0.0083   0.0028   0.0024  -0.0003
        Z    0.0039   0.0073  -0.0030  -0.0058  -0.0107  -0.0038
AT.  16 SI X   -0.0051  -0.0021   0.0104   0.0094  -0.0027   0.0068
        Y   -0.0024   0.0062   0.0083  -0.0028   0.0024   0.0003
        Z   -0.0039  -0.0073  -0.0030   0.0058  -0.0107   0.0038
AT.  17 SI X    0.0051  -0.0021   0.0104   0.0094   0.0027  -0.0068
        Y    0.0024   0.0062   0.0083  -0.0028  -0.0024  -0.0003
        Z   -0.0039   0.0073   0.0030  -0.0058  -0.0107   0.0038
AT.  18 SI X    0.0051  -0.0021  -0.0104   0.0094  -0.0027  -0.0068
        Y   -0.0024  -0.0062   0.0083   0.0028  -0.0024   0.0003
        Z    0.0039  -0.0073   0.0030   0.0058  -0.0107  -0.0038
AT.  19 SI X    0.0030   0.0042   0.0000  -0.0137   0.0000   0.0148
        Y    0.0000   0.0000  -0.0114   0.0000  -0.0097   0.0000
        Z    0.0000   0.0000   0.0014   0.0000   0.0083   0.0000
AT.  20 SI X   -0.0030   0.0042   0.0000  -0.0137   0.0000  -0.0148
        Y    0.0000   0.0000  -0.0114   0.0000   0.0097   0.0000
        Z    0.0000   0.0000  -0.0014   0.0000   0.0083   0.0000
AT.  21 O  X   -0.0166  -0.0177  -0.0020   0.0009  -0.0107   0.0212
        Y    0.0144  -0.0041  -0.0134  -0.0076   0.0019   0.0080
        Z   -0.0145  -0.0013   0.0062   0.0041   0.0091   0.0178
AT.  22 O  X   -0.0166  -0.0177   0.0020   0.0009   0.0107   0.0212
        Y   -0.0144   0.0041  -0.0134   0.0076   0.0019  -0.0080
        Z    0.0145   0.0013   0.0062  -0.0041   0.0091  -0.0178
AT.  23 O  X    0.0166  -0.0177   0.0020   0.0009  -0.0107  -0.0212
        Y    0.0144   0.0041  -0.0134   0.0076  -0.0019   0.0080
        Z    0.0145  -0.0013  -0.0062   0.0041   0.0091  -0.0178
AT.  24 O  X    0.0166  -0.0177  -0.0020   0.0009   0.0107  -0.0212
        Y   -0.0144  -0.0041  -0.0134  -0.0076  -0.0019  -0.0080
        Z   -0.0145   0.0013  -0.0062  -0.0041   0.0091   0.0178
AT.  25 O  X    0.0000  -0.0169  -0.0023   0.0016   0.0000   0.0000
        Y    0.0000  -0.0237   0.0156   0.0080   0.0000   0.0000
        Z    0.0170   0.0000   0.0000   0.0000   0.0226  -0.0089
AT.  26 O  X    0.0000  -0.0169   0.0023   0.0016   0.0000   0.0000
        Y    0.0000   0.0237   0.0156  -0.0080   0.0000   0.0000
        Z   -0.0170   0.0000   0.0000   0.0000   0.0226   0.0089
AT.  27 O  X    0.0000  -0.0255   0.0305   0.0258   0.0000   0.0000
        Y    0.0000  -0.0132  -0.0008   0.0009   0.0000   0.0000
        Z    0.0345   0.0000   0.0000   0.0000   0.0038   0.0190
AT.  28 O  X    0.0000  -0.0255  -0.0305   0.0258   0.0000   0.0000
        Y    0.0000   0.0132  -0.0008  -0.0009   0.0000   0.0000
        Z   -0.0345   0.0000   0.0000   0.0000   0.0038  -0.0190
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AT. 29 O  X   -0.0140   0.0032  -0.0297   0.0266   0.0147   0.0019
        Y    0.0130  -0.0101   0.0118   0.0051   0.0075  -0.0030
        Z    0.0011   0.0075  -0.0128   0.0085  -0.0002  -0.0090
AT. 30 O  X   -0.0140   0.0032   0.0297   0.0266  -0.0147   0.0019
        Y   -0.0130   0.0101   0.0118  -0.0051   0.0075   0.0030
        Z   -0.0011  -0.0075  -0.0128  -0.0085  -0.0002   0.0090
AT. 31 O  X    0.0140   0.0032   0.0297   0.0266   0.0147  -0.0019
        Y    0.0130   0.0101   0.0118  -0.0051  -0.0075  -0.0030
        Z   -0.0011   0.0075   0.0128   0.0085  -0.0002   0.0090
AT. 32 O  X    0.0140   0.0032  -0.0297   0.0266  -0.0147  -0.0019
        Y   -0.0130  -0.0101   0.0118   0.0051  -0.0075   0.0030
        Z    0.0011  -0.0075   0.0128  -0.0085  -0.0002  -0.0090
AT. 33 O  X    0.0059  -0.0059   0.0045   0.0056  -0.0024  -0.0013
        Y   -0.0033   0.0140   0.0135   0.0034   0.0070  -0.0022
        Z   -0.0142  -0.0115  -0.0214  -0.0097  -0.0274   0.0092
AT. 34 O  X    0.0059  -0.0059  -0.0045   0.0056   0.0024  -0.0013
        Y    0.0033  -0.0140   0.0135  -0.0034   0.0070   0.0022
        Z    0.0142   0.0115  -0.0214   0.0097  -0.0274  -0.0092
AT. 35 O  X   -0.0059  -0.0059  -0.0045   0.0056  -0.0024   0.0013
        Y   -0.0033  -0.0140   0.0135  -0.0034  -0.0070  -0.0022
        Z    0.0142  -0.0115   0.0214  -0.0097  -0.0274  -0.0092
AT. 36 O  X   -0.0059  -0.0059   0.0045   0.0056   0.0024   0.0013
        Y    0.0033   0.0140   0.0135   0.0034  -0.0070   0.0022
        Z   -0.0142   0.0115   0.0214   0.0097  -0.0274   0.0092
AT. 37 O  X    0.0084  -0.0060   0.0211  -0.0064  -0.0060   0.0108
        Y    0.0002   0.0031  -0.0032   0.0052  -0.0141   0.0020
        Z   -0.0040   0.0103  -0.0174   0.0058   0.0045  -0.0003
AT. 38 O  X    0.0084  -0.0060  -0.0211  -0.0064   0.0060   0.0108
        Y   -0.0002  -0.0031  -0.0032  -0.0052  -0.0141  -0.0020
        Z    0.0040  -0.0103  -0.0174  -0.0058   0.0045   0.0003
AT. 39 O  X   -0.0084  -0.0060  -0.0211  -0.0064  -0.0060  -0.0108
        Y    0.0002  -0.0031  -0.0032  -0.0052   0.0141   0.0020
        Z    0.0040   0.0103   0.0174   0.0058   0.0045   0.0003
AT. 40 O  X   -0.0084  -0.0060   0.0211  -0.0064   0.0060  -0.0108
        Y   -0.0002   0.0031  -0.0032   0.0052   0.0141  -0.0020
        Z   -0.0040  -0.0103   0.0174  -0.0058   0.0045  -0.0003
AT. 41 O  X    0.0175   0.0024  -0.0095   0.0046   0.0100  -0.0081
        Y    0.0027  -0.0074   0.0092   0.0031   0.0018  -0.0014
        Z   -0.0141   0.0162  -0.0040   0.0034  -0.0056   0.0010
AT. 42 O  X    0.0175   0.0024   0.0095   0.0046  -0.0100  -0.0081
        Y   -0.0027   0.0074   0.0092  -0.0031   0.0018   0.0014
        Z    0.0141  -0.0162  -0.0040  -0.0034  -0.0056  -0.0010
AT. 43 O  X   -0.0175   0.0024   0.0095   0.0046   0.0100   0.0081
        Y    0.0027   0.0074   0.0092  -0.0031  -0.0018  -0.0014
        Z    0.0141   0.0162   0.0040   0.0034  -0.0056  -0.0010
AT. 44 O  X   -0.0175   0.0024  -0.0095   0.0046  -0.0100   0.0081
        Y   -0.0027  -0.0074   0.0092   0.0031  -0.0018   0.0014
        Z   -0.0141  -0.0162   0.0040  -0.0034  -0.0056   0.0010
AT. 45 O  X    0.0029   0.0080   0.0103   0.0007   0.0043   0.0128
        Y   -0.0048   0.0207  -0.0118  -0.0003  -0.0117   0.0313
        Z    0.0017  -0.0149   0.0114   0.0162   0.0144  -0.0370
AT. 46 O  X    0.0029   0.0080  -0.0103   0.0007  -0.0043   0.0128
        Y    0.0048  -0.0207  -0.0118   0.0003  -0.0117  -0.0313
        Z   -0.0017   0.0149   0.0114  -0.0162   0.0144   0.0370
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AT. 47 O  X  -0.0029   0.0080  -0.0103   0.0007   0.0043  -0.0128
        Y  -0.0048  -0.0207  -0.0118   0.0003   0.0117   0.0313
        Z  -0.0017  -0.0149  -0.0114   0.0162   0.0144   0.0370
AT. 48 O  X  -0.0029   0.0080   0.0103   0.0007  -0.0043  -0.0128
        Y   0.0048   0.0207  -0.0118  -0.0003   0.0117  -0.0313
        Z   0.0017   0.0149  -0.0114  -0.0162   0.0144  -0.0370


FREQ(CM**-1)   244.17   246.05   246.17   247.54   252.51   253.67


AT.  1 CA X   0.0000   0.0157   0.0000   0.0266  -0.0421  -0.0137
        Y  -0.0006   0.0000   0.0034   0.0000   0.0000   0.0000
        Z  -0.0077   0.0000  -0.0027   0.0000   0.0000   0.0000
AT.  2 CA X   0.0000   0.0157   0.0000  -0.0266  -0.0421   0.0137
        Y  -0.0006   0.0000   0.0034   0.0000   0.0000   0.0000
        Z   0.0077   0.0000   0.0027   0.0000   0.0000   0.0000
AT.  3 CA X   0.0129  -0.0355  -0.0381   0.0000   0.0083   0.0000
        Y   0.0242   0.0004   0.0016   0.0000  -0.0114   0.0000
        Z   0.0000   0.0000   0.0000  -0.0149   0.0000  -0.0188
AT.  4 CA X  -0.0129  -0.0355   0.0381   0.0000   0.0083   0.0000
        Y   0.0242  -0.0004   0.0016   0.0000   0.0114   0.0000
        Z   0.0000   0.0000   0.0000   0.0149   0.0000   0.0188
AT.  5 CA X  -0.0130   0.0119  -0.0074  -0.0074   0.0117  -0.0026
        Y  -0.0127  -0.0194  -0.0131  -0.0141  -0.0102  -0.0162
        Z   0.0070   0.0057   0.0177  -0.0016   0.0206   0.0081
AT.  6 CA X   0.0130   0.0119   0.0074  -0.0074   0.0117  -0.0026
        Y  -0.0127   0.0194  -0.0131   0.0141   0.0102   0.0162
        Z   0.0070  -0.0057   0.0177   0.0016  -0.0206  -0.0081
AT.  7 CA X   0.0130   0.0119   0.0074   0.0074   0.0117   0.0026
        Y  -0.0127   0.0194  -0.0131  -0.0141   0.0102  -0.0162
        Z  -0.0070   0.0057  -0.0177   0.0016   0.0206  -0.0081
AT.  8 CA X  -0.0130   0.0119  -0.0074   0.0074   0.0117   0.0026
        Y  -0.0127  -0.0194  -0.0131   0.0141  -0.0102   0.0162
        Z  -0.0070  -0.0057  -0.0177  -0.0016  -0.0206   0.0081
AT.  9 CA X   0.0196  -0.0039   0.0040   0.0036  -0.0143   0.0233
        Y  -0.0102   0.0101   0.0119  -0.0064   0.0059   0.0300
        Z  -0.0149  -0.0104   0.0029   0.0075   0.0006   0.0072
AT. 10 CA X  -0.0196  -0.0039  -0.0040   0.0036  -0.0143   0.0233
        Y  -0.0102  -0.0101   0.0119   0.0064  -0.0059  -0.0300
        Z  -0.0149   0.0104   0.0029  -0.0075  -0.0006  -0.0072
AT. 11 CA X  -0.0196  -0.0039  -0.0040  -0.0036  -0.0143  -0.0233
        Y  -0.0102  -0.0101   0.0119  -0.0064  -0.0059   0.0300
        Z   0.0149  -0.0104  -0.0029  -0.0075   0.0006  -0.0072
AT. 12 CA X   0.0196  -0.0039   0.0040  -0.0036  -0.0143  -0.0233
        Y  -0.0102   0.0101   0.0119   0.0064   0.0059  -0.0300
        Z   0.0149   0.0104  -0.0029   0.0075  -0.0006   0.0072
AT. 13 SI X   0.0265   0.0022   0.0175   0.0000  -0.0125   0.0000
        Y  -0.0099   0.0015   0.0042   0.0000   0.0039   0.0000
        Z   0.0000   0.0000   0.0000  -0.0231   0.0000   0.0021
AT. 14 SI X  -0.0265   0.0022  -0.0175   0.0000  -0.0125   0.0000
        Y  -0.0099  -0.0015   0.0042   0.0000  -0.0039   0.0000
        Z   0.0000   0.0000   0.0000   0.0231   0.0000  -0.0021
AT. 15 SI X   0.0043  -0.0031  -0.0121  -0.0145   0.0124  -0.0093
        Y   0.0069   0.0005   0.0003   0.0097  -0.0039  -0.0011
        Z   0.0159   0.0047   0.0043  -0.0087   0.0021   0.0036
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AT. 16 SI X  -0.0043 -0.0031  0.0121 -0.0145  0.0124 -0.0093
         Y   0.0069 -0.0005  0.0003 -0.0097  0.0039  0.0011
         Z   0.0159 -0.0047  0.0043  0.0087 -0.0021 -0.0036
AT. 17 SI X  -0.0043 -0.0031  0.0121  0.0145  0.0124  0.0093
         Y   0.0069 -0.0005  0.0003  0.0097  0.0039 -0.0011
         Z  -0.0159  0.0047 -0.0043  0.0087  0.0021 -0.0036
AT. 18 SI X   0.0043 -0.0031 -0.0121  0.0145  0.0124  0.0093
         Y   0.0069  0.0005  0.0003 -0.0097 -0.0039  0.0011
         Z  -0.0159 -0.0047 -0.0043 -0.0087 -0.0021  0.0036
AT. 19 SI X   0.0000 -0.0018  0.0000 -0.0111  0.0036 -0.0098
         Y   0.0036  0.0000 -0.0096  0.0000  0.0000  0.0000
         Z   0.0004  0.0000  0.0174  0.0000  0.0000  0.0000
AT. 20 SI X   0.0000 -0.0018  0.0000  0.0111  0.0036  0.0098
         Y   0.0036  0.0000 -0.0096  0.0000  0.0000  0.0000
         Z  -0.0004  0.0000 -0.0174  0.0000  0.0000  0.0000
AT. 21 O  X   0.0158 -0.0065  0.0103  0.0107 -0.0087  0.0204
         Y  -0.0141  0.0006  0.0064 -0.0164  0.0093  0.0107
         Z  -0.0055 -0.0050 -0.0003 -0.0074  0.0023  0.0098
AT. 22 O  X  -0.0158 -0.0065 -0.0103  0.0107 -0.0087  0.0204
         Y  -0.0141 -0.0006  0.0064  0.0164 -0.0093 -0.0107
         Z  -0.0055  0.0050 -0.0003  0.0074 -0.0023 -0.0098
AT. 23 O  X  -0.0158 -0.0065 -0.0103 -0.0107 -0.0087 -0.0204
         Y  -0.0141 -0.0006  0.0064 -0.0164 -0.0093  0.0107
         Z   0.0055 -0.0050  0.0003  0.0074  0.0023 -0.0098
AT. 24 O  X   0.0158 -0.0065  0.0103 -0.0107 -0.0087 -0.0204
         Y  -0.0141  0.0006  0.0064  0.0164  0.0093 -0.0107
         Z   0.0055  0.0050  0.0003 -0.0074 -0.0023  0.0098
AT. 25 O  X   0.0129 -0.0017  0.0167  0.0000 -0.0108  0.0000
         Y   0.0097  0.0192  0.0050  0.0000  0.0033  0.0000
         Z   0.0000  0.0000  0.0000 -0.0161  0.0000 -0.0180
AT. 26 O  X  -0.0129 -0.0017 -0.0167  0.0000 -0.0108  0.0000
         Y   0.0097 -0.0192  0.0050  0.0000 -0.0033  0.0000
         Z   0.0000  0.0000  0.0000  0.0161  0.0000  0.0180
AT. 27 O  X   0.0300  0.0460  0.0022  0.0000 -0.0173  0.0000
         Y  -0.0097  0.0041  0.0046  0.0000  0.0044  0.0000
         Z   0.0000  0.0000  0.0000 -0.0377  0.0000  0.0159
AT. 28 O  X  -0.0300  0.0460 -0.0022  0.0000 -0.0173  0.0000
         Y  -0.0097 -0.0041  0.0046  0.0000 -0.0044  0.0000
         Z   0.0000  0.0000  0.0000  0.0377  0.0000 -0.0159
AT. 29 O  X   0.0010  0.0175 -0.0124 -0.0241  0.0038 -0.0132
         Y   0.0048 -0.0120  0.0148  0.0252 -0.0022 -0.0055
         Z   0.0073  0.0091  0.0087 -0.0075 -0.0002 -0.0015
AT. 30 O  X  -0.0010  0.0175  0.0124 -0.0241  0.0038 -0.0132
         Y   0.0048  0.0120  0.0148 -0.0252  0.0022  0.0055
         Z   0.0073 -0.0091  0.0087  0.0075  0.0002  0.0015
AT. 31 O  X  -0.0010  0.0175  0.0124  0.0241  0.0038  0.0132
         Y   0.0048  0.0120  0.0148  0.0252  0.0022 -0.0055
         Z  -0.0073  0.0091 -0.0087  0.0075 -0.0002  0.0015
AT. 32 O  X   0.0010  0.0175 -0.0124  0.0241  0.0038  0.0132
         Y   0.0048 -0.0120  0.0148 -0.0252 -0.0022  0.0055
         Z  -0.0073 -0.0091 -0.0087 -0.0075  0.0002 -0.0015
AT. 33 O  X  -0.0039 -0.0056  0.0103  0.0158  0.0077  0.0092
         Y   0.0047  0.0003  0.0034  0.0029  0.0149 -0.0001
         Z  -0.0242 -0.0278 -0.0008 -0.0117  0.0069 -0.0040
```

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AT. 34 O  X    0.0039  -0.0056  -0.0103   0.0158   0.0077   0.0092
        Y    0.0047  -0.0003   0.0034  -0.0029  -0.0149   0.0001
        Z   -0.0242   0.0278  -0.0008   0.0117  -0.0069   0.0040
AT. 35 O  X    0.0039  -0.0056  -0.0103  -0.0158   0.0077  -0.0092
        Y    0.0047  -0.0003   0.0034   0.0029  -0.0149  -0.0001
        Z    0.0242  -0.0278   0.0008   0.0117   0.0069   0.0040
AT. 36 O  X   -0.0039  -0.0056   0.0103  -0.0158   0.0077  -0.0092
        Y    0.0047   0.0003   0.0034  -0.0029   0.0149   0.0001
        Z    0.0242   0.0278   0.0008  -0.0117  -0.0069  -0.0040
AT. 37 O  X    0.0125  -0.0112  -0.0165  -0.0114   0.0148   0.0007
        Y    0.0190  -0.0001  -0.0250   0.0002  -0.0025   0.0047
        Z    0.0046   0.0060   0.0170  -0.0031  -0.0062  -0.0020
AT. 38 O  X   -0.0125  -0.0112   0.0165  -0.0114   0.0148   0.0007
        Y    0.0190   0.0001  -0.0250  -0.0002   0.0025  -0.0047
        Z    0.0046  -0.0060   0.0170   0.0031   0.0062   0.0020
AT. 39 O  X   -0.0125  -0.0112   0.0165   0.0114   0.0148  -0.0007
        Y    0.0190   0.0001  -0.0250   0.0002   0.0025   0.0047
        Z   -0.0046   0.0060  -0.0170   0.0031  -0.0062   0.0020
AT. 40 O  X    0.0125  -0.0112  -0.0165   0.0114   0.0148  -0.0007
        Y    0.0190  -0.0001  -0.0250  -0.0002  -0.0025  -0.0047
        Z   -0.0046  -0.0060  -0.0170  -0.0031   0.0062  -0.0020
AT. 41 O  X    0.0129  -0.0062  -0.0040   0.0007   0.0237  -0.0024
        Y    0.0077   0.0000  -0.0008   0.0117  -0.0041  -0.0012
        Z    0.0057   0.0218  -0.0294  -0.0315   0.0073   0.0226
AT. 42 O  X   -0.0129  -0.0062   0.0040   0.0007   0.0237  -0.0024
        Y    0.0077   0.0000  -0.0008  -0.0117   0.0041   0.0012
        Z    0.0057  -0.0218  -0.0294   0.0315  -0.0073  -0.0226
AT. 43 O  X   -0.0129  -0.0062   0.0040  -0.0007   0.0237   0.0024
        Y    0.0077   0.0000  -0.0008   0.0117   0.0041  -0.0012
        Z   -0.0057   0.0218   0.0294   0.0315   0.0073  -0.0226
AT. 44 O  X    0.0129  -0.0062  -0.0040  -0.0007   0.0237   0.0024
        Y    0.0077   0.0000  -0.0008  -0.0117  -0.0041   0.0012
        Z   -0.0057  -0.0218   0.0294  -0.0315  -0.0073   0.0226
AT. 45 O  X   -0.0093   0.0000   0.0040  -0.0072   0.0071   0.0059
        Y   -0.0011  -0.0134  -0.0024   0.0036  -0.0160   0.0049
        Z   -0.0047   0.0157   0.0128  -0.0011   0.0179   0.0090
AT. 46 O  X    0.0093   0.0000  -0.0040  -0.0072   0.0071   0.0059
        Y   -0.0011   0.0134  -0.0024  -0.0036   0.0160  -0.0049
        Z   -0.0047  -0.0157   0.0128   0.0011  -0.0179  -0.0090
AT. 47 O  X    0.0093   0.0000  -0.0040   0.0072   0.0071  -0.0059
        Y   -0.0011   0.0134  -0.0024   0.0036   0.0160   0.0049
        Z    0.0047   0.0157  -0.0128   0.0011   0.0179  -0.0090
AT. 48 O  X   -0.0093   0.0000   0.0040   0.0072   0.0071  -0.0059
        Y   -0.0011  -0.0134  -0.0024  -0.0036  -0.0160  -0.0049
        Z    0.0047  -0.0157  -0.0128  -0.0011  -0.0179   0.0090


FREQ(CM**-1)   253.74   254.91   257.72   258.77   263.63   270.40

AT.  1 CA X    0.0000   0.0000   0.0140   0.0250   0.0368   0.0000
        Y    0.0003  -0.0037   0.0000   0.0000   0.0000   0.0104
        Z    0.0091  -0.0034   0.0000   0.0000   0.0000   0.0168
AT.  2 CA X    0.0000   0.0000   0.0140  -0.0250  -0.0368   0.0000
        Y    0.0003   0.0037   0.0000   0.0000   0.0000  -0.0104
        Z   -0.0091  -0.0034   0.0000   0.0000   0.0000   0.0168
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AT.  3 CA X    0.0074   0.0000   0.0276   0.0000   0.0000   0.0000
        Y   -0.0003   0.0000  -0.0242   0.0000   0.0000   0.0000
        Z    0.0000  -0.0098   0.0000   0.0022   0.0083  -0.0246
AT.  4 CA X   -0.0074   0.0000   0.0276   0.0000   0.0000   0.0000
        Y   -0.0003   0.0000   0.0242   0.0000   0.0000   0.0000
        Z    0.0000  -0.0098   0.0000  -0.0022  -0.0083  -0.0246
AT.  5 CA X    0.0112  -0.0062  -0.0098   0.0115  -0.0106  -0.0042
        Y    0.0006   0.0028  -0.0023  -0.0049   0.0159   0.0165
        Z   -0.0036   0.0101   0.0136  -0.0145   0.0028  -0.0124
AT.  6 CA X   -0.0112   0.0062  -0.0098   0.0115  -0.0106   0.0042
        Y    0.0006   0.0028   0.0023   0.0049  -0.0159   0.0165
        Z   -0.0036   0.0101  -0.0136   0.0145  -0.0028  -0.0124
AT.  7 CA X   -0.0112  -0.0062  -0.0098  -0.0115   0.0106  -0.0042
        Y    0.0006  -0.0028   0.0023  -0.0049   0.0159  -0.0165
        Z    0.0036   0.0101   0.0136   0.0145  -0.0028  -0.0124
AT.  8 CA X    0.0112   0.0062  -0.0098  -0.0115   0.0106   0.0042
        Y    0.0006  -0.0028  -0.0023   0.0049  -0.0159  -0.0165
        Z    0.0036   0.0101  -0.0136  -0.0145   0.0028  -0.0124
AT.  9 CA X   -0.0012  -0.0076   0.0178   0.0091   0.0009  -0.0056
        Y   -0.0199   0.0003   0.0100   0.0170   0.0069  -0.0170
        Z    0.0000  -0.0097  -0.0036   0.0091  -0.0168  -0.0005
AT. 10 CA X    0.0012   0.0076   0.0178   0.0091   0.0009   0.0056
        Y   -0.0199   0.0003  -0.0100  -0.0170  -0.0069  -0.0170
        Z    0.0000  -0.0097   0.0036  -0.0091   0.0168  -0.0005
AT. 11 CA X    0.0012  -0.0076   0.0178  -0.0091  -0.0009  -0.0056
        Y   -0.0199  -0.0003  -0.0100   0.0170   0.0069   0.0170
        Z    0.0000  -0.0097  -0.0036  -0.0091   0.0168  -0.0005
AT. 12 CA X   -0.0012   0.0076   0.0178  -0.0091  -0.0009   0.0056
        Y   -0.0199  -0.0003   0.0100  -0.0170  -0.0069   0.0170
        Z    0.0000  -0.0097   0.0036   0.0091  -0.0168  -0.0005
AT. 13 SI X   -0.0141   0.0000  -0.0055   0.0000   0.0000   0.0000
        Y   -0.0164   0.0000   0.0098   0.0000   0.0000   0.0000
        Z    0.0000   0.0025   0.0000   0.0049  -0.0140   0.0255
AT. 14 SI X    0.0141   0.0000  -0.0055   0.0000   0.0000   0.0000
        Y   -0.0164   0.0000  -0.0098   0.0000   0.0000   0.0000
        Z    0.0000   0.0025   0.0000  -0.0049   0.0140   0.0255
AT. 15 SI X    0.0045   0.0010  -0.0027   0.0005  -0.0121   0.0037
        Y    0.0196   0.0041   0.0068  -0.0085  -0.0087   0.0137
        Z   -0.0028   0.0021   0.0009  -0.0077   0.0002  -0.0032
AT. 16 SI X   -0.0045  -0.0010  -0.0027   0.0005  -0.0121  -0.0037
        Y    0.0196   0.0041  -0.0068   0.0085   0.0087   0.0137
        Z   -0.0028   0.0021  -0.0009   0.0077  -0.0002  -0.0032
AT. 17 SI X   -0.0045   0.0010  -0.0027  -0.0005   0.0121   0.0037
        Y    0.0196  -0.0041  -0.0068  -0.0085  -0.0087  -0.0137
        Z    0.0028   0.0021   0.0009   0.0077  -0.0002  -0.0032
AT. 18 SI X    0.0045  -0.0010  -0.0027  -0.0005   0.0121  -0.0037
        Y    0.0196  -0.0041   0.0068   0.0085   0.0087  -0.0137
        Z    0.0028   0.0021  -0.0009  -0.0077   0.0002  -0.0032
AT. 19 SI X    0.0000   0.0000  -0.0096  -0.0063   0.0008   0.0000
        Y   -0.0054  -0.0014   0.0000   0.0000   0.0000   0.0057
        Z    0.0059   0.0054   0.0000   0.0000   0.0000  -0.0036
AT. 20 SI X    0.0000   0.0000  -0.0096   0.0063  -0.0008   0.0000
        Y   -0.0054   0.0014   0.0000   0.0000   0.0000  -0.0057
        Z   -0.0059   0.0054   0.0000   0.0000   0.0000  -0.0036
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AT. 21 O  X    0.0004   0.0511   0.0000  -0.0367   0.0152  -0.0170
        Y   -0.0104   0.0057   0.0223   0.0049   0.0110   0.0094
        Z    0.0034   0.0279  -0.0004  -0.0188  -0.0078   0.0059
AT. 22 O  X   -0.0004  -0.0511   0.0000  -0.0367   0.0152   0.0170
        Y   -0.0104   0.0057  -0.0223  -0.0049  -0.0110   0.0094
        Z    0.0034   0.0279   0.0004   0.0188   0.0078   0.0059
AT. 23 O  X   -0.0004   0.0511   0.0000   0.0367  -0.0152  -0.0170
        Y   -0.0104  -0.0057  -0.0223   0.0049   0.0110  -0.0094
        Z   -0.0034   0.0279  -0.0004   0.0188   0.0078   0.0059
AT. 24 O  X    0.0004  -0.0511   0.0000   0.0367  -0.0152   0.0170
        Y   -0.0104  -0.0057   0.0223  -0.0049  -0.0110  -0.0094
        Z   -0.0034   0.0279   0.0004  -0.0188  -0.0078   0.0059
AT. 25 O  X   -0.0090   0.0000  -0.0029   0.0000   0.0000   0.0000
        Y   -0.0212   0.0000  -0.0018   0.0000   0.0000   0.0000
        Z    0.0000  -0.0511   0.0000   0.0436  -0.0291   0.0236
AT. 26 O  X    0.0090   0.0000  -0.0029   0.0000   0.0000   0.0000
        Y   -0.0212   0.0000   0.0018   0.0000   0.0000   0.0000
        Z    0.0000  -0.0511   0.0000  -0.0436   0.0291   0.0236
AT. 27 O  X   -0.0262   0.0000  -0.0424   0.0000   0.0000   0.0000
        Y   -0.0189   0.0000   0.0119   0.0000   0.0000   0.0000
        Z    0.0000   0.0083   0.0000   0.0096   0.0162   0.0205
AT. 28 O  X    0.0262   0.0000  -0.0424   0.0000   0.0000   0.0000
        Y   -0.0189   0.0000  -0.0119   0.0000   0.0000   0.0000
        Z    0.0000   0.0083   0.0000  -0.0096  -0.0162   0.0205
AT. 29 O  X    0.0139   0.0078   0.0107  -0.0026   0.0042   0.0170
        Y    0.0357   0.0094  -0.0032  -0.0069  -0.0150   0.0161
        Z    0.0116   0.0078   0.0048  -0.0068   0.0041   0.0041
AT. 30 O  X   -0.0139  -0.0078   0.0107  -0.0026   0.0042  -0.0170
        Y    0.0357   0.0094   0.0032   0.0069   0.0150   0.0161
        Z    0.0116   0.0078  -0.0048   0.0068  -0.0041   0.0041
AT. 31 O  X   -0.0139   0.0078   0.0107   0.0026  -0.0042   0.0170
        Y    0.0357  -0.0094   0.0032  -0.0069  -0.0150  -0.0161
        Z   -0.0116   0.0078   0.0048   0.0068  -0.0041   0.0041
AT. 32 O  X    0.0139  -0.0078   0.0107   0.0026  -0.0042  -0.0170
        Y    0.0357  -0.0094  -0.0032   0.0069   0.0150  -0.0161
        Z   -0.0116   0.0078  -0.0048  -0.0068   0.0041   0.0041
AT. 33 O  X    0.0007  -0.0004  -0.0038   0.0058   0.0129   0.0052
        Y    0.0119  -0.0006  -0.0112  -0.0160  -0.0048  -0.0194
        Z    0.0026   0.0019  -0.0126   0.0158   0.0209  -0.0047
AT. 34 O  X   -0.0007   0.0004  -0.0038   0.0058   0.0129  -0.0052
        Y    0.0119  -0.0006   0.0112   0.0160   0.0048  -0.0194
        Z    0.0026   0.0019   0.0126  -0.0158  -0.0209  -0.0047
AT. 35 O  X   -0.0007  -0.0004  -0.0038  -0.0058  -0.0129   0.0052
        Y    0.0119   0.0006   0.0112  -0.0160  -0.0048   0.0194
        Z   -0.0026   0.0019  -0.0126  -0.0158  -0.0209  -0.0047
AT. 36 O  X    0.0007   0.0004  -0.0038  -0.0058  -0.0129  -0.0052
        Y    0.0119   0.0006  -0.0112   0.0160   0.0048   0.0194
        Z   -0.0026   0.0019   0.0126   0.0158   0.0209  -0.0047
AT. 37 O  X   -0.0124  -0.0172  -0.0092  -0.0117  -0.0139  -0.0084
        Y   -0.0011  -0.0075   0.0044  -0.0021  -0.0127   0.0134
        Z    0.0196   0.0181   0.0034   0.0000  -0.0021   0.0132
AT. 38 O  X    0.0124   0.0172  -0.0092  -0.0117  -0.0139   0.0084
        Y   -0.0011  -0.0075  -0.0044   0.0021   0.0127   0.0134
        Z    0.0196   0.0181  -0.0034   0.0000   0.0021   0.0132
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AT. 39 O  X   0.0124 -0.0172 -0.0092  0.0117  0.0139 -0.0084
         Y  -0.0011  0.0075 -0.0044 -0.0021 -0.0127 -0.0134
         Z  -0.0196  0.0181  0.0034  0.0000  0.0021  0.0132
AT. 40 O  X  -0.0124  0.0172 -0.0092  0.0117  0.0139  0.0084
         Y  -0.0011  0.0075  0.0044  0.0021  0.0127 -0.0134
         Z  -0.0196  0.0181 -0.0034  0.0000 -0.0021  0.0132
AT. 41 O  X   0.0033  0.0097 -0.0226  0.0057 -0.0222 -0.0059
         Y   0.0206  0.0035  0.0063 -0.0090 -0.0100  0.0159
         Z  -0.0311 -0.0229  0.0189 -0.0075  0.0027 -0.0067
AT. 42 O  X  -0.0033 -0.0097 -0.0226  0.0057 -0.0222  0.0059
         Y   0.0206  0.0035 -0.0063  0.0090  0.0100  0.0159
         Z  -0.0311 -0.0229 -0.0189  0.0075 -0.0027 -0.0067
AT. 43 O  X  -0.0033  0.0097 -0.0226 -0.0057  0.0222 -0.0059
         Y   0.0206 -0.0035 -0.0063 -0.0090 -0.0100 -0.0159
         Z   0.0311 -0.0229  0.0189  0.0075 -0.0027 -0.0067
AT. 44 O  X   0.0033 -0.0097 -0.0226 -0.0057  0.0222  0.0059
         Y   0.0206 -0.0035  0.0063  0.0090  0.0100 -0.0159
         Z   0.0311 -0.0229 -0.0189 -0.0075  0.0027 -0.0067
AT. 45 O  X  -0.0098 -0.0082 -0.0065 -0.0004  0.0011 -0.0119
         Y  -0.0037  0.0023 -0.0105  0.0182 -0.0115  0.0005
         Z  -0.0031 -0.0064  0.0143 -0.0121  0.0098 -0.0055
AT. 46 O  X   0.0098  0.0082 -0.0065 -0.0004  0.0011  0.0119
         Y  -0.0037  0.0023  0.0105 -0.0182  0.0115  0.0005
         Z  -0.0031 -0.0064 -0.0143  0.0121 -0.0098 -0.0055
AT. 47 O  X   0.0098 -0.0082 -0.0065  0.0004 -0.0011 -0.0119
         Y  -0.0037 -0.0023  0.0105  0.0182 -0.0115 -0.0005
         Z   0.0031 -0.0064  0.0143  0.0121 -0.0098 -0.0055
AT. 48 O  X  -0.0098  0.0082 -0.0065  0.0004 -0.0011  0.0119
         Y  -0.0037 -0.0023 -0.0105 -0.0182  0.0115 -0.0005
         Z   0.0031 -0.0064 -0.0143 -0.0121  0.0098 -0.0055


FREQ(CM**-1)   270.87   272.87   278.72   280.80   284.59   284.86

AT.  1 CA X   0.0161  0.0000  0.0000  0.0208  0.0000 -0.0048
         Y   0.0000  0.0032 -0.0026  0.0000  0.0088  0.0000
         Z   0.0000 -0.0072 -0.0010  0.0000  0.0086  0.0000
AT.  2 CA X   0.0161  0.0000  0.0000  0.0208  0.0000  0.0048
         Y   0.0000  0.0032  0.0026  0.0000 -0.0088  0.0000
         Z   0.0000  0.0072 -0.0010  0.0000  0.0086  0.0000
AT.  3 CA X   0.0153  0.0204  0.0000 -0.0004  0.0000  0.0000
         Y  -0.0112 -0.0297  0.0000 -0.0060  0.0000  0.0000
         Z   0.0000  0.0000 -0.0128  0.0000  0.0176  0.0041
AT.  4 CA X   0.0153 -0.0204  0.0000 -0.0004  0.0000  0.0000
         Y   0.0112 -0.0297  0.0000  0.0060  0.0000  0.0000
         Z   0.0000  0.0000 -0.0128  0.0000  0.0176 -0.0041
AT.  5 CA X   0.0010  0.0049 -0.0051  0.0071 -0.0111  0.0157
         Y  -0.0015 -0.0174 -0.0053 -0.0129 -0.0084  0.0040
         Z  -0.0020  0.0089  0.0012  0.0122 -0.0093  0.0137
AT.  6 CA X   0.0010 -0.0049  0.0051  0.0071  0.0111  0.0157
         Y   0.0015 -0.0174 -0.0053  0.0129 -0.0084 -0.0040
         Z   0.0020  0.0089  0.0012 -0.0122 -0.0093 -0.0137
AT.  7 CA X   0.0010 -0.0049 -0.0051  0.0071 -0.0111 -0.0157
         Y   0.0015 -0.0174  0.0053  0.0129  0.0084  0.0040
         Z  -0.0020 -0.0089  0.0012  0.0122 -0.0093 -0.0137
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AT.  8 CA X    0.0010   0.0049   0.0051   0.0071   0.0111  -0.0157
        Y   -0.0015  -0.0174   0.0053  -0.0129   0.0084  -0.0040
        Z    0.0020  -0.0089   0.0012  -0.0122  -0.0093   0.0137
AT.  9 CA X   -0.0257   0.0067   0.0262   0.0064  -0.0046   0.0194
        Y   -0.0221  -0.0071   0.0129   0.0002   0.0046  -0.0046
        Z    0.0086   0.0045   0.0031   0.0159  -0.0039   0.0012
AT. 10 CA X   -0.0257  -0.0067  -0.0262   0.0064   0.0046   0.0194
        Y    0.0221  -0.0071   0.0129  -0.0002   0.0046   0.0046
        Z   -0.0086   0.0045   0.0031  -0.0159  -0.0039  -0.0012
AT. 11 CA X   -0.0257  -0.0067   0.0262   0.0064  -0.0046  -0.0194
        Y    0.0221  -0.0071  -0.0129  -0.0002  -0.0046  -0.0046
        Z    0.0086  -0.0045   0.0031   0.0159  -0.0039  -0.0012
AT. 12 CA X   -0.0257   0.0067  -0.0262   0.0064   0.0046  -0.0194
        Y   -0.0221  -0.0071  -0.0129   0.0002  -0.0046   0.0046
        Z   -0.0086  -0.0045   0.0031  -0.0159  -0.0039   0.0012
AT. 13 SI X   -0.0047  -0.0130   0.0000   0.0028   0.0000   0.0000
        Y    0.0210   0.0243   0.0000   0.0080   0.0000   0.0000
        Z    0.0000   0.0000   0.0122   0.0000   0.0086  -0.0160
AT. 14 SI X   -0.0047   0.0130   0.0000   0.0028   0.0000   0.0000
        Y   -0.0210   0.0243   0.0000  -0.0080   0.0000   0.0000
        Z    0.0000   0.0000   0.0122   0.0000   0.0086   0.0160
AT. 15 SI X    0.0027   0.0027  -0.0151  -0.0088   0.0008  -0.0060
        Y    0.0116  -0.0016   0.0012  -0.0046  -0.0005   0.0071
        Z    0.0009   0.0043  -0.0100  -0.0163  -0.0044  -0.0084
AT. 16 SI X    0.0027  -0.0027   0.0151  -0.0088  -0.0008  -0.0060
        Y   -0.0116  -0.0016   0.0012   0.0046  -0.0005  -0.0071
        Z   -0.0009   0.0043  -0.0100   0.0163  -0.0044   0.0084
AT. 17 SI X    0.0027  -0.0027  -0.0151  -0.0088   0.0008   0.0060
        Y   -0.0116  -0.0016  -0.0012   0.0046   0.0005   0.0071
        Z    0.0009  -0.0043  -0.0100  -0.0163  -0.0044   0.0084
AT. 18 SI X    0.0027   0.0027   0.0151  -0.0088  -0.0008   0.0060
        Y    0.0116  -0.0016  -0.0012  -0.0046   0.0005  -0.0071
        Z   -0.0009  -0.0043  -0.0100   0.0163  -0.0044  -0.0084
AT. 19 SI X    0.0057   0.0000   0.0000  -0.0144   0.0000   0.0029
        Y    0.0000   0.0087  -0.0093   0.0000   0.0041   0.0000
        Z    0.0000   0.0041   0.0016   0.0000  -0.0099   0.0000
AT. 20 SI X    0.0057   0.0000   0.0000  -0.0144   0.0000  -0.0029
        Y    0.0000   0.0087   0.0093   0.0000  -0.0041   0.0000
        Z    0.0000  -0.0041   0.0016   0.0000  -0.0099   0.0000
AT. 21 O  X   -0.0085  -0.0044  -0.0043   0.0057   0.0188  -0.0087
        Y    0.0148   0.0330   0.0176   0.0077   0.0071  -0.0144
        Z    0.0027   0.0022   0.0013   0.0049   0.0174  -0.0141
AT. 22 O  X   -0.0085   0.0044   0.0043   0.0057  -0.0188  -0.0087
        Y   -0.0148   0.0330   0.0176  -0.0077   0.0071   0.0144
        Z   -0.0027   0.0022   0.0013  -0.0049   0.0174   0.0141
AT. 23 O  X   -0.0085   0.0044  -0.0043   0.0057   0.0188   0.0087
        Y   -0.0148   0.0330  -0.0176  -0.0077  -0.0071  -0.0144
        Z    0.0027  -0.0022   0.0013   0.0049   0.0174   0.0141
AT. 24 O  X   -0.0085  -0.0044   0.0043   0.0057  -0.0188   0.0087
        Y    0.0148   0.0330  -0.0176   0.0077  -0.0071   0.0144
        Z   -0.0027  -0.0022   0.0013  -0.0049   0.0174  -0.0141
AT. 25 O  X   -0.0027  -0.0068   0.0000   0.0018   0.0000   0.0000
        Y    0.0217   0.0166   0.0000   0.0154   0.0000   0.0000
        Z    0.0000   0.0000   0.0015   0.0000  -0.0135   0.0184
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AT. 26 O  X  -0.0027   0.0068   0.0000   0.0018   0.0000   0.0000
        Y  -0.0217   0.0166   0.0000  -0.0154   0.0000   0.0000
        Z   0.0000   0.0000   0.0015   0.0000  -0.0135  -0.0184
AT. 27 O  X   0.0119  -0.0157   0.0000  -0.0006   0.0000   0.0000
        Y   0.0223   0.0284   0.0000   0.0094   0.0000   0.0000
        Z   0.0000   0.0000   0.0306   0.0000   0.0215  -0.0403
AT. 28 O  X   0.0119   0.0157   0.0000  -0.0006   0.0000   0.0000
        Y  -0.0223   0.0284   0.0000  -0.0094   0.0000   0.0000
        Z   0.0000   0.0000   0.0306   0.0000   0.0215   0.0403
AT. 29 O  X   0.0194  -0.0090  -0.0062  -0.0303   0.0227   0.0165
        Y   0.0160   0.0095   0.0056   0.0125  -0.0274  -0.0107
        Z   0.0120   0.0032  -0.0012  -0.0149  -0.0060  -0.0061
AT. 30 O  X   0.0194   0.0090   0.0062  -0.0303  -0.0227   0.0165
        Y  -0.0160   0.0095   0.0056  -0.0125  -0.0274   0.0107
        Z  -0.0120   0.0032  -0.0012   0.0149  -0.0060   0.0061
AT. 31 O  X   0.0194   0.0090  -0.0062  -0.0303   0.0227  -0.0165
        Y  -0.0160   0.0095  -0.0056  -0.0125   0.0274  -0.0107
        Z   0.0120  -0.0032  -0.0012  -0.0149  -0.0060   0.0061
AT. 32 O  X   0.0194  -0.0090   0.0062  -0.0303  -0.0227  -0.0165
        Y   0.0160   0.0095  -0.0056   0.0125   0.0274   0.0107
        Z  -0.0120  -0.0032  -0.0012   0.0149  -0.0060  -0.0061
AT. 33 O  X   0.0025   0.0021  -0.0140  -0.0148   0.0058  -0.0002
        Y  -0.0116  -0.0127  -0.0075   0.0253  -0.0139   0.0238
        Z  -0.0054  -0.0176  -0.0131  -0.0026  -0.0236   0.0138
AT. 34 O  X   0.0025  -0.0021   0.0140  -0.0148  -0.0058  -0.0002
        Y   0.0116  -0.0127  -0.0075  -0.0253  -0.0139  -0.0238
        Z   0.0054  -0.0176  -0.0131   0.0026  -0.0236  -0.0138
AT. 35 O  X   0.0025  -0.0021  -0.0140  -0.0148   0.0058   0.0002
        Y   0.0116  -0.0127   0.0075  -0.0253   0.0139   0.0238
        Z  -0.0054   0.0176  -0.0131  -0.0026  -0.0236  -0.0138
AT. 36 O  X   0.0025   0.0021   0.0140  -0.0148  -0.0058   0.0002
        Y  -0.0116  -0.0127   0.0075   0.0253   0.0139  -0.0238
        Z   0.0054   0.0176  -0.0131   0.0026  -0.0236   0.0138
AT. 37 O  X  -0.0072   0.0020  -0.0194  -0.0157   0.0129   0.0104
        Y   0.0054   0.0089  -0.0263  -0.0024   0.0142  -0.0020
        Z   0.0140   0.0048   0.0058  -0.0059  -0.0147  -0.0095
AT. 38 O  X  -0.0072  -0.0020   0.0194  -0.0157  -0.0129   0.0104
        Y  -0.0054   0.0089  -0.0263   0.0024   0.0142   0.0020
        Z  -0.0140   0.0048   0.0058   0.0059  -0.0147   0.0095
AT. 39 O  X  -0.0072  -0.0020  -0.0194  -0.0157   0.0129  -0.0104
        Y  -0.0054   0.0089   0.0263   0.0024  -0.0142  -0.0020
        Z   0.0140  -0.0048   0.0058  -0.0059  -0.0147   0.0095
AT. 40 O  X  -0.0072   0.0020   0.0194  -0.0157  -0.0129  -0.0104
        Y   0.0054   0.0089   0.0263  -0.0024  -0.0142   0.0020
        Z  -0.0140  -0.0048   0.0058   0.0059  -0.0147  -0.0095
AT. 41 O  X   0.0061   0.0206  -0.0270   0.0253  -0.0215  -0.0275
        Y   0.0125  -0.0017   0.0009  -0.0031  -0.0002   0.0073
        Z  -0.0115  -0.0059  -0.0066  -0.0081   0.0271   0.0081
AT. 42 O  X   0.0061  -0.0206   0.0270   0.0253   0.0215  -0.0275
        Y  -0.0125  -0.0017   0.0009   0.0031  -0.0002  -0.0073
        Z   0.0115  -0.0059  -0.0066   0.0081   0.0271  -0.0081
AT. 43 O  X   0.0061  -0.0206  -0.0270   0.0253  -0.0215   0.0275
        Y  -0.0125  -0.0017  -0.0009   0.0031   0.0002   0.0073
        Z  -0.0115   0.0059  -0.0066  -0.0081   0.0271  -0.0081
```

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AT. 44 O  X    0.0061   0.0206   0.0270   0.0253   0.0215   0.0275
         Y    0.0125  -0.0017  -0.0009  -0.0031   0.0002  -0.0073
         Z    0.0115   0.0059  -0.0066   0.0081   0.0271   0.0081
AT. 45 O  X   -0.0002  -0.0026   0.0140  -0.0046  -0.0004   0.0110
         Y   -0.0018   0.0082  -0.0028   0.0107  -0.0087  -0.0045
         Z   -0.0033   0.0018   0.0095  -0.0014   0.0047   0.0082
AT. 46 O  X   -0.0002   0.0026  -0.0140  -0.0046   0.0004   0.0110
         Y    0.0018   0.0082  -0.0028  -0.0107  -0.0087   0.0045
         Z    0.0033   0.0018   0.0095   0.0014   0.0047  -0.0082
AT. 47 O  X   -0.0002   0.0026   0.0140  -0.0046  -0.0004  -0.0110
         Y    0.0018   0.0082   0.0028  -0.0107   0.0087  -0.0045
         Z   -0.0033  -0.0018   0.0095  -0.0014   0.0047  -0.0082
AT. 48 O  X   -0.0002  -0.0026  -0.0140  -0.0046   0.0004  -0.0110
         Y   -0.0018   0.0082   0.0028   0.0107   0.0087   0.0045
         Z    0.0033  -0.0018   0.0095   0.0014   0.0047   0.0082


FREQ(CM**-1)   285.21   296.61   299.14   299.25   304.40   308.73


AT.  1 CA X    0.0000   0.0000  -0.0081   0.0070   0.0000   0.0000
         Y   -0.0052   0.0042   0.0000   0.0000  -0.0074   0.0011
         Z   -0.0184   0.0001   0.0000   0.0000  -0.0120  -0.0007
AT.  2 CA X    0.0000   0.0000   0.0081   0.0070   0.0000   0.0000
         Y   -0.0052   0.0042   0.0000   0.0000  -0.0074  -0.0011
         Z    0.0184  -0.0001   0.0000   0.0000   0.0120  -0.0007
AT.  3 CA X    0.0218   0.0248   0.0000  -0.0180  -0.0099   0.0000
         Y   -0.0017  -0.0064   0.0000  -0.0017  -0.0067   0.0000
         Z    0.0000   0.0000   0.0210   0.0000   0.0000   0.0042
AT.  4 CA X   -0.0218  -0.0248   0.0000  -0.0180   0.0099   0.0000
         Y   -0.0017  -0.0064   0.0000   0.0017  -0.0067   0.0000
         Z    0.0000   0.0000  -0.0210   0.0000   0.0000   0.0042
AT.  5 CA X    0.0013  -0.0057  -0.0048   0.0032   0.0084   0.0099
         Y    0.0063   0.0068   0.0160   0.0120  -0.0146   0.0148
         Z    0.0118  -0.0116   0.0063   0.0081   0.0023   0.0163
AT.  6 CA X   -0.0013   0.0057  -0.0048   0.0032  -0.0084  -0.0099
         Y    0.0063   0.0068  -0.0160  -0.0120  -0.0146   0.0148
         Z    0.0118  -0.0116  -0.0063  -0.0081   0.0023   0.0163
AT.  7 CA X   -0.0013   0.0057   0.0048   0.0032  -0.0084   0.0099
         Y    0.0063   0.0068   0.0160  -0.0120  -0.0146  -0.0148
         Z   -0.0118   0.0116  -0.0063   0.0081  -0.0023   0.0163
AT.  8 CA X    0.0013  -0.0057   0.0048   0.0032   0.0084  -0.0099
         Y    0.0063   0.0068  -0.0160   0.0120  -0.0146  -0.0148
         Z   -0.0118   0.0116   0.0063  -0.0081  -0.0023   0.0163
AT.  9 CA X    0.0184   0.0098  -0.0034   0.0005   0.0159   0.0022
         Y    0.0078   0.0181   0.0057  -0.0045   0.0017   0.0125
         Z    0.0008  -0.0072   0.0038  -0.0027  -0.0057  -0.0058
AT. 10 CA X   -0.0184  -0.0098  -0.0034   0.0005  -0.0159  -0.0022
         Y    0.0078   0.0181  -0.0057   0.0045   0.0017   0.0125
         Z    0.0008  -0.0072  -0.0038   0.0027  -0.0057  -0.0058
AT. 11 CA X   -0.0184  -0.0098   0.0034   0.0005  -0.0159   0.0022
         Y    0.0078   0.0181   0.0057   0.0045   0.0017  -0.0125
         Z   -0.0008   0.0072  -0.0038  -0.0027   0.0057  -0.0058
AT. 12 CA X    0.0184   0.0098   0.0034   0.0005   0.0159  -0.0022
         Y    0.0078   0.0181  -0.0057  -0.0045   0.0017  -0.0125
         Z   -0.0008   0.0072   0.0038   0.0027   0.0057  -0.0058
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AT. 13 SI X  -0.0004 -0.0091  0.0000  0.0032 -0.0183  0.0000
        Y  -0.0079 -0.0078  0.0000 -0.0117  0.0009  0.0000
        Z   0.0000  0.0000 -0.0071  0.0000  0.0000  0.0027
AT. 14 SI X   0.0004  0.0091  0.0000  0.0032  0.0183  0.0000
        Y  -0.0079 -0.0078  0.0000  0.0117  0.0009  0.0000
        Z   0.0000  0.0000  0.0071  0.0000  0.0000  0.0027
AT. 15 SI X  -0.0126 -0.0067 -0.0042 -0.0010 -0.0035 -0.0006
        Y   0.0043 -0.0022 -0.0102 -0.0014  0.0081  0.0046
        Z  -0.0019 -0.0012 -0.0110  0.0136 -0.0049 -0.0040
AT. 16 SI X   0.0126  0.0067 -0.0042 -0.0010  0.0035  0.0006
        Y   0.0043 -0.0022  0.0102  0.0014  0.0081  0.0046
        Z  -0.0019 -0.0012  0.0110 -0.0136 -0.0049 -0.0040
AT. 17 SI X   0.0126  0.0067  0.0042 -0.0010  0.0035 -0.0006
        Y   0.0043 -0.0022 -0.0102  0.0014  0.0081 -0.0046
        Z   0.0019  0.0012  0.0110  0.0136  0.0049 -0.0040
AT. 18 SI X  -0.0126 -0.0067  0.0042 -0.0010 -0.0035  0.0006
        Y   0.0043 -0.0022  0.0102 -0.0014  0.0081 -0.0046
        Z   0.0019  0.0012 -0.0110 -0.0136  0.0049 -0.0040
AT. 19 SI X   0.0000  0.0000  0.0012 -0.0034  0.0000  0.0000
        Y  -0.0080 -0.0178  0.0000  0.0000  0.0005 -0.0096
        Z  -0.0045 -0.0076  0.0000  0.0000 -0.0027 -0.0103
AT. 20 SI X   0.0000  0.0000 -0.0012 -0.0034  0.0000  0.0000
        Y  -0.0080 -0.0178  0.0000  0.0000  0.0005  0.0096
        Z   0.0045  0.0076  0.0000  0.0000  0.0027 -0.0103
AT. 21 O  X   0.0224 -0.0165  0.0071  0.0182 -0.0288  0.0063
        Y   0.0079 -0.0101 -0.0136 -0.0018 -0.0043 -0.0201
        Z   0.0047 -0.0068  0.0047  0.0031 -0.0039  0.0142
AT. 22 O  X  -0.0224  0.0165  0.0071  0.0182  0.0288 -0.0063
        Y   0.0079 -0.0101  0.0136  0.0018 -0.0043 -0.0201
        Z   0.0047 -0.0068 -0.0047 -0.0031 -0.0039  0.0142
AT. 23 O  X  -0.0224  0.0165 -0.0071  0.0182  0.0288  0.0063
        Y   0.0079 -0.0101 -0.0136  0.0018 -0.0043  0.0201
        Z  -0.0047  0.0068 -0.0047  0.0031  0.0039  0.0142
AT. 24 O  X   0.0224 -0.0165 -0.0071  0.0182 -0.0288 -0.0063
        Y   0.0079 -0.0101  0.0136 -0.0018 -0.0043  0.0201
        Z  -0.0047  0.0068  0.0047 -0.0031  0.0039  0.0142
AT. 25 O  X   0.0071 -0.0185  0.0000  0.0122 -0.0235  0.0000
        Y  -0.0323  0.0087  0.0000 -0.0345  0.0221  0.0000
        Z   0.0000  0.0000 -0.0069  0.0000  0.0000  0.0316
AT. 26 O  X  -0.0071  0.0185  0.0000  0.0122  0.0235  0.0000
        Y  -0.0323  0.0087  0.0000  0.0345  0.0221  0.0000
        Z   0.0000  0.0000  0.0069  0.0000  0.0000  0.0316
AT. 27 O  X  -0.0515  0.0225  0.0000 -0.0276  0.0306  0.0000
        Y  -0.0093 -0.0076  0.0000 -0.0142  0.0026  0.0000
        Z   0.0000  0.0000 -0.0190  0.0000  0.0000 -0.0483
AT. 28 O  X   0.0515 -0.0225  0.0000 -0.0276 -0.0306  0.0000
        Y  -0.0093 -0.0076  0.0000  0.0142  0.0026  0.0000
        Z   0.0000  0.0000  0.0190  0.0000  0.0000 -0.0483
AT. 29 O  X   0.0020 -0.0064 -0.0316  0.0078  0.0168  0.0153
        Y  -0.0058  0.0082 -0.0145  0.0163  0.0044  0.0019
        Z  -0.0001  0.0044 -0.0271  0.0265  0.0031  0.0026
AT. 30 O  X  -0.0020  0.0064 -0.0316  0.0078 -0.0168 -0.0153
        Y  -0.0058  0.0082  0.0145 -0.0163  0.0044  0.0019
        Z  -0.0001  0.0044  0.0271 -0.0265  0.0031  0.0026
```

```
AT. 31 O  X   -0.0020   0.0064   0.0316   0.0078  -0.0168   0.0153
       Y   -0.0058   0.0082  -0.0145  -0.0163   0.0044  -0.0019
       Z    0.0001  -0.0044   0.0271   0.0265  -0.0031   0.0026
AT. 32 O  X    0.0020  -0.0064   0.0316   0.0078   0.0168  -0.0153
       Y   -0.0058   0.0082   0.0145   0.0163   0.0044  -0.0019
       Z    0.0001  -0.0044  -0.0271  -0.0265  -0.0031   0.0026
AT. 33 O  X    0.0094   0.0055  -0.0013  -0.0065   0.0021   0.0053
       Y    0.0107  -0.0041  -0.0082   0.0115   0.0167  -0.0187
       Z    0.0044  -0.0210  -0.0051   0.0046   0.0192  -0.0036
AT. 34 O  X   -0.0094  -0.0055  -0.0013  -0.0065  -0.0021  -0.0053
       Y    0.0107  -0.0041   0.0082  -0.0115   0.0167  -0.0187
       Z    0.0044  -0.0210   0.0051  -0.0046   0.0192  -0.0036
AT. 35 O  X   -0.0094  -0.0055   0.0013  -0.0065  -0.0021   0.0053
       Y    0.0107  -0.0041  -0.0082  -0.0115   0.0167   0.0187
       Z   -0.0044   0.0210   0.0051   0.0046  -0.0192  -0.0036
AT. 36 O  X    0.0094   0.0055   0.0013  -0.0065   0.0021  -0.0053
       Y    0.0107  -0.0041   0.0082   0.0115   0.0167   0.0187
       Z   -0.0044   0.0210  -0.0051  -0.0046  -0.0192  -0.0036
AT. 37 O  X    0.0049  -0.0124   0.0163  -0.0221   0.0042   0.0017
       Y   -0.0059  -0.0268  -0.0043  -0.0009   0.0044  -0.0070
       Z   -0.0056   0.0056  -0.0220   0.0214  -0.0035  -0.0061
AT. 38 O  X   -0.0049   0.0124   0.0163  -0.0221  -0.0042  -0.0017
       Y   -0.0059  -0.0268   0.0043   0.0009   0.0044  -0.0070
       Z   -0.0056   0.0056   0.0220  -0.0214  -0.0035  -0.0061
AT. 39 O  X   -0.0049   0.0124  -0.0163  -0.0221  -0.0042   0.0017
       Y   -0.0059  -0.0268  -0.0043   0.0009   0.0044   0.0070
       Z    0.0056  -0.0056   0.0220   0.0214   0.0035  -0.0061
AT. 40 O  X    0.0049  -0.0124  -0.0163  -0.0221   0.0042  -0.0017
       Y   -0.0059  -0.0268   0.0043  -0.0009   0.0044   0.0070
       Z    0.0056  -0.0056  -0.0220  -0.0214   0.0035  -0.0061
AT. 41 O  X   -0.0122   0.0126   0.0117   0.0180  -0.0217  -0.0248
       Y    0.0043  -0.0033  -0.0102  -0.0015   0.0095   0.0048
       Z    0.0126  -0.0150   0.0057  -0.0145   0.0116  -0.0039
AT. 42 O  X    0.0122  -0.0126   0.0117   0.0180   0.0217   0.0248
       Y    0.0043  -0.0033   0.0102   0.0015   0.0095   0.0048
       Z    0.0126  -0.0150  -0.0057   0.0145   0.0116  -0.0039
AT. 43 O  X    0.0122  -0.0126  -0.0117   0.0180   0.0217  -0.0248
       Y    0.0043  -0.0033  -0.0102   0.0015   0.0095  -0.0048
       Z   -0.0126   0.0150  -0.0057  -0.0145  -0.0116  -0.0039
AT. 44 O  X   -0.0122   0.0126  -0.0117   0.0180  -0.0217   0.0248
       Y    0.0043  -0.0033   0.0102  -0.0015   0.0095  -0.0048
       Z   -0.0126   0.0150   0.0057   0.0145  -0.0116  -0.0039
AT. 45 O  X    0.0157   0.0171  -0.0014  -0.0017   0.0076  -0.0006
       Y   -0.0102   0.0023   0.0175  -0.0146  -0.0086  -0.0075
       Z    0.0108  -0.0108  -0.0201   0.0175   0.0120  -0.0121
AT. 46 O  X   -0.0157  -0.0171  -0.0014  -0.0017  -0.0076   0.0006
       Y   -0.0102   0.0023  -0.0175   0.0146  -0.0086  -0.0075
       Z    0.0108  -0.0108   0.0201  -0.0175   0.0120  -0.0121
AT. 47 O  X   -0.0157  -0.0171   0.0014  -0.0017  -0.0076  -0.0006
       Y   -0.0102   0.0023   0.0175   0.0146  -0.0086   0.0075
       Z   -0.0108   0.0108   0.0201   0.0175  -0.0120  -0.0121
AT. 48 O  X    0.0157   0.0171   0.0014  -0.0017   0.0076   0.0006
       Y   -0.0102   0.0023  -0.0175  -0.0146  -0.0086   0.0075
       Z   -0.0108   0.0108  -0.0201  -0.0175  -0.0120  -0.0121
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FREQ(CM**-1)   319.98   320.29   321.29   328.59   330.09   336.66

AT.  1 CA X    0.0000   0.0046  -0.0018  -0.0064   0.0000   0.0000
       Y    0.0025   0.0000   0.0000   0.0000   0.0014   0.0035
       Z   -0.0032   0.0000   0.0000   0.0000  -0.0043   0.0002
AT.  2 CA X    0.0000   0.0046   0.0018   0.0064   0.0000   0.0000
       Y    0.0025   0.0000   0.0000   0.0000  -0.0014  -0.0035
       Z    0.0032   0.0000   0.0000   0.0000  -0.0043   0.0002
AT.  3 CA X   -0.0017   0.0213   0.0000   0.0000   0.0000   0.0000
       Y    0.0023   0.0030   0.0000   0.0000   0.0000   0.0000
       Z    0.0000   0.0000   0.0098   0.0092  -0.0036   0.0009
AT.  4 CA X    0.0017   0.0213   0.0000   0.0000   0.0000   0.0000
       Y    0.0023  -0.0030   0.0000   0.0000   0.0000   0.0000
       Z    0.0000   0.0000  -0.0098  -0.0092  -0.0036   0.0009
AT.  5 CA X   -0.0036   0.0037  -0.0061  -0.0115  -0.0085  -0.0024
       Y   -0.0112   0.0081  -0.0118  -0.0066   0.0025  -0.0063
       Z   -0.0137   0.0110  -0.0098  -0.0164  -0.0095  -0.0040
AT.  6 CA X    0.0036   0.0037  -0.0061  -0.0115   0.0085   0.0024
       Y   -0.0112  -0.0081   0.0118   0.0066   0.0025  -0.0063
       Z   -0.0137  -0.0110   0.0098   0.0164  -0.0095  -0.0040
AT.  7 CA X    0.0036   0.0037   0.0061   0.0115  -0.0085  -0.0024
       Y   -0.0112  -0.0081  -0.0118  -0.0066  -0.0025   0.0063
       Z    0.0137   0.0110   0.0098   0.0164  -0.0095  -0.0040
AT.  8 CA X   -0.0036   0.0037   0.0061   0.0115   0.0085   0.0024
       Y   -0.0112   0.0081   0.0118   0.0066  -0.0025   0.0063
       Z    0.0137  -0.0110  -0.0098  -0.0164  -0.0095  -0.0040
AT.  9 CA X    0.0029   0.0096  -0.0055   0.0049   0.0052   0.0081
       Y   -0.0001   0.0047  -0.0067   0.0080   0.0027  -0.0084
       Z    0.0079  -0.0073   0.0140  -0.0046  -0.0045  -0.0173
AT. 10 CA X   -0.0029   0.0096  -0.0055   0.0049  -0.0052  -0.0081
       Y   -0.0001  -0.0047   0.0067  -0.0080   0.0027  -0.0084
       Z    0.0079   0.0073  -0.0140   0.0046  -0.0045  -0.0173
AT. 11 CA X   -0.0029   0.0096   0.0055  -0.0049   0.0052   0.0081
       Y   -0.0001  -0.0047  -0.0067   0.0080  -0.0027   0.0084
       Z   -0.0079  -0.0073  -0.0140   0.0046  -0.0045  -0.0173
AT. 12 CA X    0.0029   0.0096   0.0055  -0.0049  -0.0052  -0.0081
       Y   -0.0001   0.0047   0.0067  -0.0080  -0.0027   0.0084
       Z   -0.0079   0.0073   0.0140  -0.0046  -0.0045  -0.0173
AT. 13 SI X    0.0039  -0.0111   0.0000   0.0000   0.0000   0.0000
       Y    0.0074  -0.0050   0.0000   0.0000   0.0000   0.0000
       Z    0.0000   0.0000  -0.0092   0.0125   0.0046   0.0121
AT. 14 SI X   -0.0039  -0.0111   0.0000   0.0000   0.0000   0.0000
       Y    0.0074   0.0050   0.0000   0.0000   0.0000   0.0000
       Z    0.0000   0.0000   0.0092  -0.0125   0.0046   0.0121
AT. 15 SI X    0.0116  -0.0030   0.0023  -0.0012  -0.0004  -0.0061
       Y   -0.0017  -0.0020   0.0040  -0.0051   0.0078  -0.0061
       Z   -0.0031   0.0023  -0.0137  -0.0044   0.0061  -0.0035
AT. 16 SI X   -0.0116  -0.0030   0.0023  -0.0012   0.0004   0.0061
       Y   -0.0017   0.0020  -0.0040   0.0051   0.0078  -0.0061
       Z   -0.0031  -0.0023   0.0137   0.0044   0.0061  -0.0035
AT. 17 SI X   -0.0116  -0.0030  -0.0023   0.0012  -0.0004  -0.0061
       Y   -0.0017   0.0020   0.0040  -0.0051  -0.0078   0.0061
       Z    0.0031   0.0023   0.0137   0.0044   0.0061  -0.0035
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AT. 18 SI X    0.0116  -0.0030  -0.0023   0.0012   0.0004   0.0061
        Y   -0.0017  -0.0020  -0.0040   0.0051  -0.0078   0.0061
        Z    0.0031  -0.0023  -0.0137  -0.0044   0.0061  -0.0035
AT. 19 SI X    0.0000  -0.0031  -0.0038  -0.0016   0.0000   0.0000
        Y   -0.0095   0.0000   0.0000   0.0000  -0.0193   0.0258
        Z   -0.0041   0.0000   0.0000   0.0000  -0.0144   0.0154
AT. 20 SI X    0.0000  -0.0031   0.0038   0.0016   0.0000   0.0000
        Y   -0.0095   0.0000   0.0000   0.0000   0.0193  -0.0258
        Z    0.0041   0.0000   0.0000   0.0000  -0.0144   0.0154
AT. 21 O  X    0.0113  -0.0362  -0.0087   0.0095   0.0105   0.0057
        Y    0.0152  -0.0180   0.0155  -0.0075  -0.0048  -0.0153
        Z    0.0004  -0.0081  -0.0187   0.0219   0.0132   0.0220
AT. 22 O  X   -0.0113  -0.0362  -0.0087   0.0095  -0.0105  -0.0057
        Y    0.0152   0.0180  -0.0155   0.0075  -0.0048  -0.0153
        Z    0.0004   0.0081   0.0187  -0.0219   0.0132   0.0220
AT. 23 O  X   -0.0113  -0.0362   0.0087  -0.0095   0.0105   0.0057
        Y    0.0152   0.0180   0.0155  -0.0075   0.0048   0.0153
        Z   -0.0004  -0.0081   0.0187  -0.0219   0.0132   0.0220
AT. 24 O  X    0.0113  -0.0362   0.0087  -0.0095  -0.0105  -0.0057
        Y    0.0152  -0.0180  -0.0155   0.0075   0.0048   0.0153
        Z   -0.0004   0.0081  -0.0187   0.0219   0.0132   0.0220
AT. 25 O  X    0.0095  -0.0222   0.0000   0.0000   0.0000   0.0000
        Y    0.0008   0.0139   0.0000   0.0000   0.0000   0.0000
        Z    0.0000   0.0000  -0.0377   0.0168   0.0160   0.0312
AT. 26 O  X   -0.0095  -0.0222   0.0000   0.0000   0.0000   0.0000
        Y    0.0008  -0.0139   0.0000   0.0000   0.0000   0.0000
        Z    0.0000   0.0000   0.0377  -0.0168   0.0160   0.0312
AT. 27 O  X   -0.0080   0.0402   0.0000   0.0000   0.0000   0.0000
        Y    0.0095  -0.0067   0.0000   0.0000   0.0000   0.0000
        Z    0.0000   0.0000   0.0398  -0.0062  -0.0182  -0.0216
AT. 28 O  X    0.0080   0.0402   0.0000   0.0000   0.0000   0.0000
        Y    0.0095   0.0067   0.0000   0.0000   0.0000   0.0000
        Z    0.0000   0.0000  -0.0398   0.0062  -0.0182  -0.0216
AT. 29 O  X    0.0270   0.0000   0.0019   0.0139  -0.0110  -0.0131
        Y   -0.0115   0.0065   0.0016  -0.0181   0.0188  -0.0012
        Z    0.0013   0.0092  -0.0147  -0.0013   0.0041  -0.0046
AT. 30 O  X   -0.0270   0.0000   0.0019   0.0139   0.0110   0.0131
        Y   -0.0115  -0.0065  -0.0016   0.0181   0.0188  -0.0012
        Z    0.0013  -0.0092   0.0147   0.0013   0.0041  -0.0046
AT. 31 O  X   -0.0270   0.0000  -0.0019  -0.0139  -0.0110  -0.0131
        Y   -0.0115  -0.0065   0.0016  -0.0181  -0.0188   0.0012
        Z   -0.0013   0.0092   0.0147   0.0013   0.0041  -0.0046
AT. 32 O  X    0.0270   0.0000  -0.0019  -0.0139   0.0110   0.0131
        Y   -0.0115   0.0065  -0.0016   0.0181  -0.0188   0.0012
        Z   -0.0013  -0.0092  -0.0147  -0.0013   0.0041  -0.0046
AT. 33 O  X   -0.0227  -0.0035  -0.0108  -0.0122  -0.0080  -0.0104
        Y    0.0240   0.0052   0.0206   0.0183   0.0043   0.0144
        Z   -0.0183   0.0160   0.0103  -0.0159  -0.0116  -0.0075
AT. 34 O  X    0.0227  -0.0035  -0.0108  -0.0122   0.0080   0.0104
        Y    0.0240  -0.0052  -0.0206  -0.0183   0.0043   0.0144
        Z   -0.0183  -0.0160  -0.0103   0.0159  -0.0116  -0.0075
AT. 35 O  X    0.0227  -0.0035   0.0108   0.0122  -0.0080  -0.0104
        Y    0.0240  -0.0052   0.0206   0.0183  -0.0043  -0.0144
        Z    0.0183   0.0160  -0.0103   0.0159  -0.0116  -0.0075
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AT. 36 O  X  -0.0227  -0.0035   0.0108   0.0122   0.0080   0.0104
          Y   0.0240   0.0052  -0.0206  -0.0183  -0.0043  -0.0144
          Z   0.0183  -0.0160   0.0103  -0.0159  -0.0116  -0.0075
AT. 37 O  X   0.0074  -0.0104   0.0116  -0.0002  -0.0035  -0.0046
          Y  -0.0142  -0.0057   0.0008  -0.0110  -0.0011   0.0115
          Z  -0.0054   0.0056  -0.0161  -0.0045   0.0062   0.0003
AT. 38 O  X  -0.0074  -0.0104   0.0116  -0.0002   0.0035   0.0046
          Y  -0.0142   0.0057  -0.0008   0.0110  -0.0011   0.0115
          Z  -0.0054  -0.0056   0.0161   0.0045   0.0062   0.0003
AT. 39 O  X  -0.0074  -0.0104  -0.0116   0.0002  -0.0035  -0.0046
          Y  -0.0142   0.0057   0.0008  -0.0110   0.0011  -0.0115
          Z   0.0054   0.0056   0.0161   0.0045   0.0062   0.0003
AT. 40 O  X   0.0074  -0.0104  -0.0116   0.0002   0.0035   0.0046
          Y  -0.0142  -0.0057  -0.0008   0.0110   0.0011  -0.0115
          Z   0.0054  -0.0056  -0.0161  -0.0045   0.0062   0.0003
AT. 41 O  X  -0.0243  -0.0038  -0.0160  -0.0268   0.0308  -0.0013
          Y  -0.0031  -0.0024   0.0061  -0.0059   0.0091  -0.0051
          Z  -0.0160  -0.0245   0.0111  -0.0309   0.0367  -0.0100
AT. 42 O  X   0.0243  -0.0038  -0.0160  -0.0268  -0.0308   0.0013
          Y  -0.0031   0.0024  -0.0061   0.0059   0.0091  -0.0051
          Z  -0.0160   0.0245  -0.0111   0.0309   0.0367  -0.0100
AT. 43 O  X   0.0243  -0.0038   0.0160   0.0268   0.0308  -0.0013
          Y  -0.0031   0.0024   0.0061  -0.0059  -0.0091   0.0051
          Z   0.0160  -0.0245  -0.0111   0.0309   0.0367  -0.0100
AT. 44 O  X  -0.0243  -0.0038   0.0160   0.0268  -0.0308   0.0013
          Y  -0.0031  -0.0024  -0.0061   0.0059  -0.0091   0.0051
          Z   0.0160   0.0245   0.0111  -0.0309   0.0367  -0.0100
AT. 45 O  X   0.0070  -0.0033  -0.0072  -0.0066   0.0249  -0.0107
          Y   0.0115  -0.0065   0.0013   0.0025  -0.0046   0.0024
          Z  -0.0188   0.0073  -0.0039  -0.0050  -0.0045   0.0287
AT. 46 O  X  -0.0070  -0.0033  -0.0072  -0.0066  -0.0249   0.0107
          Y   0.0115   0.0065  -0.0013  -0.0025  -0.0046   0.0024
          Z  -0.0188  -0.0073   0.0039   0.0050  -0.0045   0.0287
AT. 47 O  X  -0.0070  -0.0033   0.0072   0.0066   0.0249  -0.0107
          Y   0.0115   0.0065   0.0013   0.0025   0.0046  -0.0024
          Z   0.0188   0.0073   0.0039   0.0050  -0.0045   0.0287
AT. 48 O  X   0.0070  -0.0033   0.0072   0.0066  -0.0249   0.0107
          Y   0.0115  -0.0065  -0.0013  -0.0025   0.0046  -0.0024
          Z   0.0188  -0.0073  -0.0039  -0.0050  -0.0045   0.0287

FREQ(CM**-1)   340.80   344.00   348.79   352.13   356.67   361.10

AT.  1 CA X   0.0010   0.0000   0.0169   0.0000  -0.0096   0.0000
          Y   0.0000  -0.0066   0.0000  -0.0089   0.0000  -0.0011
          Z   0.0000   0.0065   0.0000   0.0070   0.0000  -0.0066
AT.  2 CA X   0.0010   0.0000   0.0169   0.0000   0.0096   0.0000
          Y   0.0000  -0.0066   0.0000   0.0089   0.0000  -0.0011
          Z   0.0000  -0.0065   0.0000   0.0070   0.0000   0.0066
AT.  3 CA X   0.0060  -0.0040  -0.0090   0.0000   0.0000  -0.0120
          Y   0.0018  -0.0019   0.0076   0.0000   0.0000   0.0030
          Z   0.0000   0.0000   0.0000  -0.0033  -0.0102   0.0000
AT.  4 CA X   0.0060   0.0040  -0.0090   0.0000   0.0000   0.0120
          Y  -0.0018  -0.0019  -0.0076   0.0000   0.0000   0.0030
          Z   0.0000   0.0000   0.0000  -0.0033   0.0102   0.0000
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AT.  5 CA X   -0.0038  0.0006  0.0101 -0.0044  0.0061  0.0129
          Y    0.0152 -0.0110  0.0120 -0.0123  0.0124  0.0101
          Z   -0.0020 -0.0014  0.0163 -0.0136  0.0091  0.0175
AT.  6 CA X   -0.0038 -0.0006  0.0101  0.0044  0.0061 -0.0129
          Y   -0.0152 -0.0110 -0.0120 -0.0123 -0.0124  0.0101
          Z    0.0020 -0.0014 -0.0163 -0.0136 -0.0091  0.0175
AT.  7 CA X   -0.0038 -0.0006  0.0101 -0.0044 -0.0061 -0.0129
          Y   -0.0152 -0.0110 -0.0120  0.0123  0.0124  0.0101
          Z   -0.0020  0.0014  0.0163 -0.0136 -0.0091 -0.0175
AT.  8 CA X   -0.0038  0.0006  0.0101  0.0044 -0.0061  0.0129
          Y    0.0152 -0.0110  0.0120  0.0123 -0.0124  0.0101
          Z    0.0020  0.0014 -0.0163 -0.0136  0.0091 -0.0175
AT.  9 CA X    0.0009 -0.0071 -0.0101 -0.0006  0.0019  0.0017
          Y   -0.0071  0.0071  0.0030  0.0089 -0.0021 -0.0082
          Z   -0.0071  0.0075  0.0013 -0.0073  0.0158 -0.0022
AT. 10 CA X    0.0009  0.0071 -0.0101  0.0006  0.0019 -0.0017
          Y    0.0071  0.0071 -0.0030  0.0089  0.0021 -0.0082
          Z    0.0071  0.0075 -0.0013 -0.0073 -0.0158 -0.0022
AT. 11 CA X    0.0009  0.0071 -0.0101 -0.0006 -0.0019 -0.0017
          Y    0.0071  0.0071 -0.0030 -0.0089 -0.0021 -0.0082
          Z   -0.0071 -0.0075  0.0013 -0.0073 -0.0158  0.0022
AT. 12 CA X    0.0009 -0.0071 -0.0101  0.0006 -0.0019  0.0017
          Y   -0.0071  0.0071  0.0030 -0.0089  0.0021 -0.0082
          Z    0.0071 -0.0075 -0.0013 -0.0073  0.0158  0.0022
AT. 13 SI X    0.0001  0.0093 -0.0046  0.0000  0.0000 -0.0072
          Y   -0.0053  0.0014 -0.0039  0.0000  0.0000 -0.0016
          Z    0.0000  0.0000  0.0000  0.0100 -0.0075  0.0000
AT. 14 SI X    0.0001 -0.0093 -0.0046  0.0000  0.0000  0.0072
          Y    0.0053  0.0014  0.0039  0.0000  0.0000 -0.0016
          Z    0.0000  0.0000  0.0000  0.0100  0.0075  0.0000
AT. 15 SI X    0.0053  0.0085  0.0090  0.0010 -0.0061  0.0113
          Y    0.0103  0.0097  0.0019 -0.0043 -0.0099 -0.0007
          Z    0.0036  0.0048 -0.0136  0.0032  0.0013  0.0045
AT. 16 SI X    0.0053 -0.0085  0.0090 -0.0010 -0.0061 -0.0113
          Y   -0.0103  0.0097 -0.0019 -0.0043  0.0099 -0.0007
          Z   -0.0036  0.0048  0.0136  0.0032 -0.0013  0.0045
AT. 17 SI X    0.0053 -0.0085  0.0090  0.0010  0.0061 -0.0113
          Y   -0.0103  0.0097 -0.0019  0.0043 -0.0099 -0.0007
          Z    0.0036 -0.0048 -0.0136  0.0032 -0.0013 -0.0045
AT. 18 SI X    0.0053  0.0085  0.0090 -0.0010  0.0061  0.0113
          Y    0.0103  0.0097  0.0019  0.0043  0.0099 -0.0007
          Z   -0.0036 -0.0048  0.0136  0.0032  0.0013 -0.0045
AT. 19 SI X   -0.0066  0.0000 -0.0185  0.0000 -0.0008  0.0000
          Y    0.0000 -0.0281  0.0000 -0.0019  0.0000 -0.0075
          Z    0.0000 -0.0188  0.0000 -0.0084  0.0000  0.0053
AT. 20 SI X   -0.0066  0.0000 -0.0185  0.0000  0.0008  0.0000
          Y    0.0000 -0.0281  0.0000  0.0019  0.0000 -0.0075
          Z    0.0000  0.0188  0.0000 -0.0084  0.0000 -0.0053
AT. 21 O  X   -0.0104  0.0062  0.0031 -0.0037 -0.0035 -0.0109
          Y   -0.0094  0.0053 -0.0099 -0.0114  0.0191 -0.0042
          Z   -0.0045 -0.0012  0.0077  0.0116 -0.0199  0.0001
AT. 22 O  X   -0.0104 -0.0062  0.0031  0.0037 -0.0035  0.0109
          Y    0.0094  0.0053  0.0099 -0.0114 -0.0191 -0.0042
          Z    0.0045 -0.0012 -0.0077  0.0116  0.0199  0.0001
```

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AT. 23 O  X  -0.0104  -0.0062   0.0031  -0.0037   0.0035   0.0109
        Y   0.0094   0.0053   0.0099   0.0114   0.0191  -0.0042
        Z  -0.0045   0.0012   0.0077   0.0116   0.0199  -0.0001
AT. 24 O  X  -0.0104   0.0062   0.0031   0.0037   0.0035  -0.0109
        Y  -0.0094   0.0053  -0.0099   0.0114  -0.0191  -0.0042
        Z   0.0045   0.0012  -0.0077   0.0116  -0.0199  -0.0001
AT. 25 O  X  -0.0037   0.0092  -0.0037   0.0000   0.0000   0.0005
        Y  -0.0001  -0.0005  -0.0048   0.0000   0.0000  -0.0126
        Z   0.0000   0.0000   0.0000   0.0227  -0.0241   0.0000
AT. 26 O  X  -0.0037  -0.0092  -0.0037   0.0000   0.0000  -0.0005
        Y   0.0001  -0.0005   0.0048   0.0000   0.0000  -0.0126
        Z   0.0000   0.0000   0.0000   0.0227   0.0241   0.0000
AT. 27 O  X   0.0129  -0.0012  -0.0107   0.0000   0.0000   0.0073
        Y  -0.0077   0.0026  -0.0061   0.0000   0.0000  -0.0035
        Z   0.0000   0.0000   0.0000   0.0060   0.0065   0.0000
AT. 28 O  X   0.0129   0.0012  -0.0107   0.0000   0.0000  -0.0073
        Y   0.0077   0.0026   0.0061   0.0000   0.0000  -0.0035
        Z   0.0000   0.0000   0.0000   0.0060  -0.0065   0.0000
AT. 29 O  X  -0.0195  -0.0020   0.0104   0.0100   0.0101   0.0000
        Y   0.0175   0.0221  -0.0088  -0.0208  -0.0129  -0.0124
        Z  -0.0097   0.0043  -0.0163   0.0004   0.0114  -0.0070
AT. 30 O  X  -0.0195   0.0020   0.0104  -0.0100   0.0101   0.0000
        Y  -0.0175   0.0221   0.0088  -0.0208   0.0129  -0.0124
        Z   0.0097   0.0043   0.0163   0.0004  -0.0114  -0.0070
AT. 31 O  X  -0.0195   0.0020   0.0104   0.0100  -0.0101   0.0000
        Y  -0.0175   0.0221   0.0088   0.0208  -0.0129  -0.0124
        Z  -0.0097  -0.0043  -0.0163   0.0004  -0.0114   0.0070
AT. 32 O  X  -0.0195  -0.0020   0.0104  -0.0100  -0.0101   0.0000
        Y   0.0175   0.0221  -0.0088   0.0208   0.0129  -0.0124
        Z   0.0097  -0.0043   0.0163   0.0004   0.0114   0.0070
AT. 33 O  X  -0.0045  -0.0006   0.0190   0.0132  -0.0029  -0.0153
        Y   0.0043  -0.0007  -0.0181  -0.0139   0.0024   0.0140
        Z  -0.0192   0.0143   0.0101   0.0340  -0.0268  -0.0093
AT. 34 O  X  -0.0045   0.0006   0.0190  -0.0132  -0.0029   0.0153
        Y  -0.0043  -0.0007   0.0181  -0.0139  -0.0024   0.0140
        Z   0.0192   0.0143  -0.0101   0.0340   0.0268  -0.0093
AT. 35 O  X  -0.0045   0.0006   0.0190   0.0132   0.0029   0.0153
        Y  -0.0043  -0.0007   0.0181   0.0139   0.0024   0.0140
        Z  -0.0192  -0.0143   0.0101   0.0340   0.0268   0.0093
AT. 36 O  X  -0.0045  -0.0006   0.0190  -0.0132   0.0029  -0.0153
        Y   0.0043  -0.0007  -0.0181   0.0139  -0.0024   0.0140
        Z   0.0192  -0.0143  -0.0101   0.0340  -0.0268   0.0093
AT. 37 O  X   0.0045  -0.0008   0.0008  -0.0059  -0.0066   0.0012
        Y   0.0175  -0.0040   0.0065  -0.0119  -0.0086  -0.0096
        Z  -0.0026   0.0035  -0.0123   0.0053   0.0084   0.0070
AT. 38 O  X   0.0045   0.0008   0.0008   0.0059  -0.0066  -0.0012
        Y  -0.0175  -0.0040  -0.0065  -0.0119   0.0086  -0.0096
        Z   0.0026   0.0035   0.0123   0.0053  -0.0084   0.0070
AT. 39 O  X   0.0045   0.0008   0.0008  -0.0059   0.0066  -0.0012
        Y  -0.0175  -0.0040  -0.0065   0.0119  -0.0086  -0.0096
        Z  -0.0026  -0.0035  -0.0123   0.0053  -0.0084  -0.0070
AT. 40 O  X   0.0045  -0.0008   0.0008   0.0059   0.0066   0.0012
        Y   0.0175  -0.0040   0.0065   0.0119   0.0086  -0.0096
        Z   0.0026  -0.0035   0.0123   0.0053   0.0084  -0.0070
```

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AT. 41 O  X   0.0252   0.0173  -0.0037   0.0109   0.0010   0.0216
        Y   0.0133   0.0107   0.0029  -0.0067  -0.0122  -0.0023
        Z   0.0383   0.0337   0.0011  -0.0140  -0.0273   0.0053
AT. 42 O  X   0.0252  -0.0173  -0.0037  -0.0109   0.0010  -0.0216
        Y  -0.0133   0.0107  -0.0029  -0.0067   0.0122  -0.0023
        Z  -0.0383   0.0337  -0.0011  -0.0140   0.0273   0.0053
AT. 43 O  X   0.0252  -0.0173  -0.0037   0.0109  -0.0010  -0.0216
        Y  -0.0133   0.0107  -0.0029   0.0067  -0.0122  -0.0023
        Z   0.0383  -0.0337   0.0011  -0.0140   0.0273  -0.0053
AT. 44 O  X   0.0252   0.0173  -0.0037  -0.0109  -0.0010   0.0216
        Y   0.0133   0.0107   0.0029   0.0067   0.0122  -0.0023
        Z  -0.0383  -0.0337  -0.0011  -0.0140  -0.0273  -0.0053
AT. 45 O  X  -0.0048   0.0145  -0.0277   0.0148   0.0061   0.0271
        Y  -0.0072  -0.0077  -0.0020   0.0150   0.0088   0.0248
        Z   0.0077  -0.0235  -0.0037  -0.0112  -0.0033  -0.0015
AT. 46 O  X  -0.0048  -0.0145  -0.0277  -0.0148   0.0061  -0.0271
        Y   0.0072  -0.0077   0.0020   0.0150  -0.0088   0.0248
        Z  -0.0077  -0.0235   0.0037  -0.0112   0.0033  -0.0015
AT. 47 O  X  -0.0048  -0.0145  -0.0277   0.0148  -0.0061  -0.0271
        Y   0.0072  -0.0077   0.0020  -0.0150   0.0088   0.0248
        Z   0.0077   0.0235  -0.0037  -0.0112   0.0033   0.0015
AT. 48 O  X  -0.0048   0.0145  -0.0277  -0.0148  -0.0061   0.0271
        Y  -0.0072  -0.0077  -0.0020  -0.0150  -0.0088   0.0248
        Z  -0.0077   0.0235   0.0037  -0.0112  -0.0033   0.0015


FREQ(CM**-1)   362.81   374.10   387.07   387.11   397.00   398.01

AT.  1 CA X  -0.0078  -0.0210   0.0000   0.0000   0.0000   0.0000
        Y   0.0000   0.0000  -0.0026   0.0039  -0.0001  -0.0005
        Z   0.0000   0.0000  -0.0058  -0.0018   0.0015   0.0022
AT.  2 CA X  -0.0078   0.0210   0.0000   0.0000   0.0000   0.0000
        Y   0.0000   0.0000   0.0026   0.0039  -0.0001   0.0005
        Z   0.0000   0.0000  -0.0058   0.0018  -0.0015   0.0022
AT.  3 CA X  -0.0062   0.0000   0.0000  -0.0030   0.0082   0.0000
        Y  -0.0022   0.0000   0.0000   0.0017   0.0041   0.0000
        Z   0.0000  -0.0029  -0.0006   0.0000   0.0000  -0.0062
AT.  4 CA X  -0.0062   0.0000   0.0000   0.0030  -0.0082   0.0000
        Y   0.0022   0.0000   0.0000   0.0017   0.0041   0.0000
        Z   0.0000   0.0029  -0.0006   0.0000   0.0000  -0.0062
AT.  5 CA X   0.0084  -0.0042   0.0031   0.0055  -0.0063  -0.0013
        Y   0.0110   0.0009   0.0047   0.0052  -0.0091  -0.0085
        Z   0.0159  -0.0040   0.0042   0.0099  -0.0115  -0.0065
AT.  6 CA X   0.0084  -0.0042  -0.0031  -0.0055   0.0063   0.0013
        Y  -0.0110  -0.0009   0.0047   0.0052  -0.0091  -0.0085
        Z  -0.0159   0.0040   0.0042   0.0099  -0.0115  -0.0065
AT.  7 CA X   0.0084   0.0042   0.0031  -0.0055   0.0063  -0.0013
        Y  -0.0110   0.0009  -0.0047   0.0052  -0.0091   0.0085
        Z   0.0159   0.0040   0.0042  -0.0099   0.0115  -0.0065
AT.  8 CA X   0.0084   0.0042  -0.0031   0.0055  -0.0063   0.0013
        Y   0.0110  -0.0009  -0.0047   0.0052  -0.0091   0.0085
        Z  -0.0159  -0.0040   0.0042  -0.0099   0.0115  -0.0065
AT.  9 CA X  -0.0006  -0.0046  -0.0063   0.0100  -0.0008   0.0010
        Y  -0.0051   0.0046  -0.0119   0.0095  -0.0047  -0.0014
        Z   0.0043   0.0019  -0.0082   0.0112  -0.0026   0.0037
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AT. 10 CA X   -0.0006  -0.0046   0.0063  -0.0100   0.0008  -0.0010
         Y    0.0051  -0.0046  -0.0119   0.0095  -0.0047  -0.0014
         Z   -0.0043  -0.0019  -0.0082   0.0112  -0.0026   0.0037
AT. 11 CA X   -0.0006   0.0046  -0.0063  -0.0100   0.0008   0.0010
         Y    0.0051   0.0046   0.0119   0.0095  -0.0047   0.0014
         Z    0.0043  -0.0019  -0.0082  -0.0112   0.0026   0.0037
AT. 12 CA X   -0.0006   0.0046   0.0063   0.0100  -0.0008  -0.0010
         Y   -0.0051  -0.0046   0.0119   0.0095  -0.0047   0.0014
         Z   -0.0043   0.0019  -0.0082  -0.0112   0.0026   0.0037
AT. 13 SI X    0.0000   0.0000   0.0000  -0.0104  -0.0005   0.0000
         Y   -0.0019   0.0000   0.0000  -0.0006   0.0024   0.0000
         Z    0.0000  -0.0021  -0.0079   0.0000   0.0000   0.0035
AT. 14 SI X    0.0000   0.0000   0.0000   0.0104   0.0005   0.0000
         Y    0.0019   0.0000   0.0000  -0.0006   0.0024   0.0000
         Z    0.0000   0.0021  -0.0079   0.0000   0.0000   0.0035
AT. 15 SI X   -0.0054  -0.0100  -0.0046   0.0066  -0.0069  -0.0016
         Y    0.0015  -0.0032   0.0019   0.0005   0.0036  -0.0044
         Z   -0.0122  -0.0045   0.0015   0.0010  -0.0083   0.0033
AT. 16 SI X   -0.0054  -0.0100   0.0046  -0.0066   0.0069   0.0016
         Y   -0.0015   0.0032   0.0019   0.0005   0.0036  -0.0044
         Z    0.0122   0.0045   0.0015   0.0010  -0.0083   0.0033
AT. 17 SI X   -0.0054   0.0100  -0.0046  -0.0066   0.0069  -0.0016
         Y   -0.0015  -0.0032  -0.0019   0.0005   0.0036   0.0044
         Z   -0.0122   0.0045   0.0015  -0.0010   0.0083   0.0033
AT. 18 SI X   -0.0054   0.0100   0.0046   0.0066  -0.0069   0.0016
         Y    0.0015   0.0032  -0.0019   0.0005   0.0036   0.0044
         Z    0.0122  -0.0045   0.0015  -0.0010   0.0083   0.0033
AT. 19 SI X    0.0130   0.0231   0.0000   0.0000   0.0000   0.0000
         Y    0.0000   0.0000   0.0059  -0.0088   0.0036  -0.0001
         Z    0.0000   0.0000   0.0045  -0.0041   0.0068  -0.0137
AT. 20 SI X    0.0130  -0.0231   0.0000   0.0000   0.0000   0.0000
         Y    0.0000   0.0000  -0.0059  -0.0088   0.0036   0.0001
         Z    0.0000   0.0000   0.0045   0.0041  -0.0068  -0.0137
AT. 21 O  X   -0.0013  -0.0083  -0.0010  -0.0093   0.0018   0.0122
         Y   -0.0008  -0.0100  -0.0089   0.0085   0.0134   0.0236
         Z    0.0013  -0.0004  -0.0037  -0.0033  -0.0045   0.0003
AT. 22 O  X   -0.0013  -0.0083   0.0010   0.0093  -0.0018  -0.0122
         Y    0.0008   0.0100  -0.0089   0.0085   0.0134   0.0236
         Z   -0.0013   0.0004  -0.0037  -0.0033  -0.0045   0.0003
AT. 23 O  X   -0.0013   0.0083  -0.0010   0.0093  -0.0018   0.0122
         Y    0.0008  -0.0100   0.0089   0.0085   0.0134  -0.0236
         Z    0.0013   0.0004  -0.0037   0.0033   0.0045   0.0003
AT. 24 O  X   -0.0013   0.0083   0.0010  -0.0093   0.0018  -0.0122
         Y   -0.0008   0.0100   0.0089   0.0085   0.0134  -0.0236
         Z   -0.0013  -0.0004  -0.0037   0.0033   0.0045   0.0003
AT. 25 O  X    0.0060   0.0000   0.0000   0.0016   0.0052   0.0000
         Y   -0.0172   0.0000   0.0000  -0.0265  -0.0177   0.0000
         Z    0.0000  -0.0030  -0.0102   0.0000   0.0000   0.0132
AT. 26 O  X    0.0060   0.0000   0.0000  -0.0016  -0.0052   0.0000
         Y    0.0172   0.0000   0.0000  -0.0265  -0.0177   0.0000
         Z    0.0000   0.0030  -0.0102   0.0000   0.0000   0.0132
AT. 27 O  X    0.0072   0.0000   0.0000   0.0191   0.0125   0.0000
         Y   -0.0031   0.0000   0.0000  -0.0017   0.0038   0.0000
         Z    0.0000   0.0057   0.0116   0.0000   0.0000  -0.0204
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AT. 28 O  X    0.0072   0.0000   0.0000  -0.0191  -0.0125   0.0000
        Y    0.0031   0.0000   0.0000  -0.0017   0.0038   0.0000
        Z    0.0000  -0.0057   0.0116   0.0000   0.0000  -0.0204
AT. 29 O  X    0.0029  -0.0019   0.0131  -0.0007  -0.0150   0.0170
        Y    0.0264   0.0301   0.0079  -0.0117  -0.0161   0.0186
        Z    0.0055   0.0176   0.0131  -0.0080  -0.0236   0.0245
AT. 30 O  X    0.0029  -0.0019  -0.0131   0.0007   0.0150  -0.0170
        Y   -0.0264  -0.0301   0.0079  -0.0117  -0.0161   0.0186
        Z   -0.0055  -0.0176   0.0131  -0.0080  -0.0236   0.0245
AT. 31 O  X    0.0029   0.0019   0.0131   0.0007   0.0150   0.0170
        Y   -0.0264   0.0301  -0.0079  -0.0117  -0.0161  -0.0186
        Z    0.0055  -0.0176   0.0131   0.0080   0.0236   0.0245
AT. 32 O  X    0.0029   0.0019  -0.0131  -0.0007  -0.0150  -0.0170
        Y    0.0264  -0.0301  -0.0079  -0.0117  -0.0161  -0.0186
        Z   -0.0055   0.0176   0.0131   0.0080   0.0236   0.0245
AT. 33 O  X   -0.0092   0.0140  -0.0027  -0.0055  -0.0040  -0.0081
        Y    0.0059  -0.0175  -0.0058   0.0008   0.0284   0.0275
        Z   -0.0220   0.0149  -0.0010  -0.0038   0.0134   0.0166
AT. 34 O  X   -0.0092   0.0140   0.0027   0.0055   0.0040   0.0081
        Y   -0.0059   0.0175  -0.0058   0.0008   0.0284   0.0275
        Z    0.0220  -0.0149  -0.0010  -0.0038   0.0134   0.0166
AT. 35 O  X   -0.0092  -0.0140  -0.0027   0.0055   0.0040  -0.0081
        Y   -0.0059  -0.0175   0.0058   0.0008   0.0284  -0.0275
        Z   -0.0220  -0.0149  -0.0010   0.0038  -0.0134   0.0166
AT. 36 O  X   -0.0092  -0.0140   0.0027  -0.0055  -0.0040   0.0081
        Y    0.0059   0.0175   0.0058   0.0008   0.0284  -0.0275
        Z    0.0220   0.0149  -0.0010   0.0038  -0.0134   0.0166
AT. 37 O  X    0.0101   0.0084   0.0072  -0.0001  -0.0203   0.0132
        Y   -0.0116  -0.0181  -0.0037   0.0036  -0.0047   0.0049
        Z   -0.0108  -0.0032  -0.0114   0.0093   0.0105  -0.0113
AT. 38 O  X    0.0101   0.0084  -0.0072   0.0001   0.0203  -0.0132
        Y    0.0116   0.0181  -0.0037   0.0036  -0.0047   0.0049
        Z    0.0108   0.0032  -0.0114   0.0093   0.0105  -0.0113
AT. 39 O  X    0.0101  -0.0084   0.0072   0.0001   0.0203   0.0132
        Y    0.0116  -0.0181   0.0037   0.0036  -0.0047  -0.0049
        Z   -0.0108   0.0032  -0.0114  -0.0093  -0.0105  -0.0113
AT. 40 O  X    0.0101  -0.0084  -0.0072  -0.0001  -0.0203  -0.0132
        Y   -0.0116   0.0181   0.0037   0.0036  -0.0047  -0.0049
        Z    0.0108  -0.0032  -0.0114  -0.0093  -0.0105  -0.0113
AT. 41 O  X   -0.0310  -0.0224  -0.0117   0.0027   0.0194  -0.0184
        Y    0.0032  -0.0041   0.0021  -0.0002   0.0067  -0.0058
        Z    0.0036  -0.0059   0.0014  -0.0049   0.0041  -0.0042
AT. 42 O  X   -0.0310  -0.0224   0.0117  -0.0027  -0.0194   0.0184
        Y   -0.0032   0.0041   0.0021  -0.0002   0.0067  -0.0058
        Z   -0.0036   0.0059   0.0014  -0.0049   0.0041  -0.0042
AT. 43 O  X   -0.0310   0.0224  -0.0117  -0.0027  -0.0194  -0.0184
        Y   -0.0032  -0.0041  -0.0021  -0.0002   0.0067   0.0058
        Z    0.0036   0.0059   0.0014   0.0049  -0.0041  -0.0042
AT. 44 O  X   -0.0310   0.0224   0.0117   0.0027   0.0194   0.0184
        Y    0.0032   0.0041  -0.0021  -0.0002   0.0067   0.0058
        Z   -0.0036  -0.0059   0.0014   0.0049  -0.0041  -0.0042
AT. 45 O  X    0.0177   0.0199   0.0423  -0.0362  -0.0022   0.0005
        Y    0.0106   0.0042   0.0277  -0.0235  -0.0029  -0.0039
        Z   -0.0081  -0.0078   0.0191  -0.0211   0.0120  -0.0068
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AT. 46 O  X   0.0177   0.0199  -0.0423   0.0362   0.0022  -0.0005
          Y  -0.0106  -0.0042   0.0277  -0.0235  -0.0029  -0.0039
          Z   0.0081   0.0078   0.0191  -0.0211   0.0120  -0.0068
AT. 47 O  X   0.0177  -0.0199   0.0423   0.0362   0.0022   0.0005
          Y  -0.0106   0.0042  -0.0277  -0.0235  -0.0029   0.0039
          Z  -0.0081   0.0078   0.0191   0.0211  -0.0120  -0.0068
AT. 48 O  X   0.0177  -0.0199  -0.0423  -0.0362  -0.0022  -0.0005
          Y   0.0106  -0.0042  -0.0277  -0.0235  -0.0029   0.0039
          Z   0.0081  -0.0078   0.0191   0.0211  -0.0120  -0.0068


FREQ(CM**-1)   399.43   412.91   412.92   420.72   424.87   430.88


AT.  1 CA X  -0.0066   0.0043   0.0000   0.0000   0.0078   0.0000
          Y   0.0000   0.0000   0.0013  -0.0009   0.0000  -0.0020
          Z   0.0000   0.0000  -0.0008  -0.0002   0.0000   0.0082
AT.  2 CA X  -0.0066  -0.0043   0.0000   0.0000  -0.0078   0.0000
          Y   0.0000   0.0000   0.0013   0.0009   0.0000   0.0020
          Z   0.0000   0.0000   0.0008  -0.0002   0.0000   0.0082
AT.  3 CA X   0.0007   0.0000  -0.0046   0.0000   0.0000   0.0000
          Y   0.0070   0.0000  -0.0018   0.0000   0.0000   0.0000
          Z   0.0000   0.0025   0.0000   0.0053  -0.0042   0.0008
AT.  4 CA X   0.0007   0.0000   0.0046   0.0000   0.0000   0.0000
          Y  -0.0070   0.0000  -0.0018   0.0000   0.0000   0.0000
          Z   0.0000  -0.0025   0.0000   0.0053   0.0042   0.0008
AT.  5 CA X   0.0031  -0.0034   0.0044  -0.0015   0.0034  -0.0003
          Y   0.0049  -0.0002  -0.0019  -0.0006   0.0055  -0.0033
          Z   0.0053   0.0023  -0.0002   0.0017   0.0054  -0.0054
AT.  6 CA X   0.0031  -0.0034  -0.0044   0.0015   0.0034   0.0003
          Y  -0.0049   0.0002  -0.0019  -0.0006  -0.0055  -0.0033
          Z  -0.0053  -0.0023  -0.0002   0.0017  -0.0054  -0.0054
AT.  7 CA X   0.0031   0.0034  -0.0044  -0.0015  -0.0034  -0.0003
          Y  -0.0049  -0.0002  -0.0019   0.0006   0.0055   0.0033
          Z   0.0053  -0.0023   0.0002   0.0017  -0.0054  -0.0054
AT.  8 CA X   0.0031   0.0034   0.0044   0.0015  -0.0034   0.0003
          Y   0.0049   0.0002  -0.0019   0.0006  -0.0055   0.0033
          Z  -0.0053   0.0023   0.0002   0.0017   0.0054  -0.0054
AT.  9 CA X   0.0014  -0.0003   0.0046  -0.0040   0.0041  -0.0025
          Y   0.0005  -0.0013   0.0049  -0.0061   0.0034   0.0020
          Z  -0.0019   0.0028  -0.0004   0.0000  -0.0014  -0.0060
AT. 10 CA X   0.0014  -0.0003  -0.0046   0.0040   0.0041   0.0025
          Y  -0.0005   0.0013   0.0049  -0.0061  -0.0034   0.0020
          Z   0.0019  -0.0028  -0.0004   0.0000   0.0014  -0.0060
AT. 11 CA X   0.0014   0.0003  -0.0046  -0.0040  -0.0041  -0.0025
          Y  -0.0005  -0.0013   0.0049   0.0061   0.0034  -0.0020
          Z  -0.0019  -0.0028   0.0004   0.0000   0.0014  -0.0060
AT. 12 CA X   0.0014   0.0003   0.0046   0.0040  -0.0041   0.0025
          Y   0.0005   0.0013   0.0049   0.0061  -0.0034  -0.0020
          Z   0.0019   0.0028   0.0004   0.0000  -0.0014  -0.0060
AT. 13 SI X   0.0022   0.0000  -0.0044   0.0000   0.0000   0.0000
          Y  -0.0002   0.0000   0.0003   0.0000   0.0000   0.0000
          Z   0.0000   0.0038   0.0000  -0.0016   0.0002   0.0093
AT. 14 SI X   0.0022   0.0000   0.0044   0.0000   0.0000   0.0000
          Y   0.0002   0.0000   0.0003   0.0000   0.0000   0.0000
          Z   0.0000  -0.0038   0.0000  -0.0016  -0.0002   0.0093
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AT. 15 SI X  -0.0065   0.0028   0.0054   0.0007   0.0078   0.0152
        Y   0.0047  -0.0041   0.0007   0.0008   0.0012  -0.0018
        Z   0.0002  -0.0003  -0.0027  -0.0008  -0.0002   0.0006
AT. 16 SI X  -0.0065   0.0028  -0.0054  -0.0007   0.0078  -0.0152
        Y  -0.0047   0.0041   0.0007   0.0008  -0.0012  -0.0018
        Z  -0.0002   0.0003  -0.0027  -0.0008   0.0002   0.0006
AT. 17 SI X  -0.0065  -0.0028  -0.0054   0.0007  -0.0078   0.0152
        Y  -0.0047  -0.0041   0.0007  -0.0008   0.0012   0.0018
        Z   0.0002   0.0003   0.0027  -0.0008   0.0002   0.0006
AT. 18 SI X  -0.0065  -0.0028   0.0054  -0.0007  -0.0078  -0.0152
        Y   0.0047   0.0041   0.0007  -0.0008  -0.0012   0.0018
        Z  -0.0002  -0.0003   0.0027  -0.0008  -0.0002   0.0006
AT. 19 SI X   0.0082  -0.0095   0.0000   0.0000  -0.0160   0.0000
        Y   0.0000   0.0000  -0.0035   0.0000   0.0000  -0.0104
        Z   0.0000   0.0000   0.0013   0.0149   0.0000   0.0211
AT. 20 SI X   0.0082   0.0095   0.0000   0.0000   0.0160   0.0000
        Y   0.0000   0.0000  -0.0035   0.0000   0.0000   0.0104
        Z   0.0000   0.0000  -0.0013   0.0149   0.0000   0.0211
AT. 21 O  X   0.0079   0.0093   0.0133   0.0130  -0.0119  -0.0044
        Y  -0.0259   0.0382  -0.0252   0.0441  -0.0307  -0.0066
        Z   0.0128  -0.0031   0.0168  -0.0073   0.0018   0.0084
AT. 22 O  X   0.0079   0.0093  -0.0133  -0.0130  -0.0119   0.0044
        Y   0.0259  -0.0382  -0.0252   0.0441   0.0307  -0.0066
        Z  -0.0128   0.0031   0.0168  -0.0073  -0.0018   0.0084
AT. 23 O  X   0.0079  -0.0093  -0.0133   0.0130   0.0119  -0.0044
        Y   0.0259   0.0382  -0.0252  -0.0441  -0.0307   0.0066
        Z   0.0128   0.0031  -0.0168  -0.0073  -0.0018   0.0084
AT. 24 O  X   0.0079  -0.0093   0.0133  -0.0130   0.0119   0.0044
        Y  -0.0259  -0.0382  -0.0252  -0.0441   0.0307   0.0066
        Z  -0.0128  -0.0031  -0.0168  -0.0073   0.0018   0.0084
AT. 25 O  X  -0.0132   0.0000  -0.0178   0.0000   0.0000   0.0000
        Y   0.0473   0.0000   0.0538   0.0000   0.0000   0.0000
        Z   0.0000   0.0203   0.0000   0.0222  -0.0157  -0.0108
AT. 26 O  X  -0.0132   0.0000   0.0178   0.0000   0.0000   0.0000
        Y  -0.0473   0.0000   0.0538   0.0000   0.0000   0.0000
        Z   0.0000  -0.0203   0.0000   0.0222   0.0157  -0.0108
AT. 27 O  X  -0.0307   0.0000  -0.0349   0.0000   0.0000   0.0000
        Y  -0.0015   0.0000   0.0007   0.0000   0.0000   0.0000
        Z   0.0000  -0.0358   0.0000  -0.0348   0.0267   0.0016
AT. 28 O  X  -0.0307   0.0000   0.0349   0.0000   0.0000   0.0000
        Y   0.0015   0.0000   0.0007   0.0000   0.0000   0.0000
        Z   0.0000   0.0358   0.0000  -0.0348  -0.0267   0.0016
AT. 29 O  X  -0.0014   0.0065  -0.0106  -0.0091   0.0121  -0.0160
        Y  -0.0123   0.0166  -0.0106  -0.0086   0.0062   0.0215
        Z  -0.0049   0.0089  -0.0143  -0.0130   0.0052  -0.0103
AT. 30 O  X  -0.0014   0.0065   0.0106   0.0091   0.0121   0.0160
        Y   0.0123  -0.0166  -0.0106  -0.0086  -0.0062   0.0215
        Z   0.0049  -0.0089  -0.0143  -0.0130  -0.0052  -0.0103
AT. 31 O  X  -0.0014  -0.0065   0.0106  -0.0091  -0.0121  -0.0160
        Y   0.0123   0.0166  -0.0106   0.0086   0.0062  -0.0215
        Z  -0.0049  -0.0089   0.0143  -0.0130  -0.0052  -0.0103
AT. 32 O  X  -0.0014  -0.0065  -0.0106   0.0091  -0.0121   0.0160
        Y  -0.0123  -0.0166  -0.0106   0.0086  -0.0062  -0.0215
        Z   0.0049   0.0089   0.0143  -0.0130   0.0052  -0.0103
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AT. 33 O  X   -0.0037  -0.0007  -0.0074   0.0070   0.0004   0.0132
        Y   -0.0164  -0.0167   0.0103  -0.0189  -0.0211   0.0089
        Z   -0.0179  -0.0074  -0.0014  -0.0013  -0.0201  -0.0037
AT. 34 O  X   -0.0037  -0.0007   0.0074  -0.0070   0.0004  -0.0132
        Y    0.0164   0.0167   0.0103  -0.0189   0.0211   0.0089
        Z    0.0179   0.0074  -0.0014  -0.0013   0.0201  -0.0037
AT. 35 O  X   -0.0037   0.0007   0.0074   0.0070  -0.0004   0.0132
        Y    0.0164  -0.0167   0.0103   0.0189  -0.0211  -0.0089
        Z   -0.0179   0.0074   0.0014  -0.0013   0.0201  -0.0037
AT. 36 O  X   -0.0037   0.0007  -0.0074  -0.0070  -0.0004  -0.0132
        Y   -0.0164   0.0167   0.0103   0.0189   0.0211  -0.0089
        Z    0.0179  -0.0074   0.0014  -0.0013  -0.0201  -0.0037
AT. 37 O  X   -0.0114   0.0147  -0.0048  -0.0016   0.0138   0.0150
        Y   -0.0036   0.0040  -0.0023  -0.0079   0.0138  -0.0168
        Z    0.0112  -0.0145   0.0074   0.0027  -0.0111   0.0023
AT. 38 O  X   -0.0114   0.0147   0.0048   0.0016   0.0138  -0.0150
        Y    0.0036  -0.0040  -0.0023  -0.0079  -0.0138  -0.0168
        Z   -0.0112   0.0145   0.0074   0.0027   0.0111   0.0023
AT. 39 O  X   -0.0114  -0.0147   0.0048  -0.0016  -0.0138   0.0150
        Y    0.0036   0.0040  -0.0023   0.0079   0.0138   0.0168
        Z    0.0112   0.0145  -0.0074   0.0027   0.0111   0.0023
AT. 40 O  X   -0.0114  -0.0147  -0.0048   0.0016  -0.0138  -0.0150
        Y   -0.0036  -0.0040  -0.0023   0.0079  -0.0138   0.0168
        Z   -0.0112  -0.0145  -0.0074   0.0027  -0.0111   0.0023
AT. 41 O  X    0.0085  -0.0162   0.0076   0.0029  -0.0168  -0.0220
        Y    0.0064  -0.0047   0.0008   0.0009   0.0006  -0.0042
        Z   -0.0067   0.0089   0.0026   0.0015  -0.0004   0.0115
AT. 42 O  X    0.0085  -0.0162  -0.0076  -0.0029  -0.0168   0.0220
        Y   -0.0064   0.0047   0.0008   0.0009  -0.0006  -0.0042
        Z    0.0067  -0.0089   0.0026   0.0015   0.0004   0.0115
AT. 43 O  X    0.0085   0.0162  -0.0076   0.0029   0.0168  -0.0220
        Y   -0.0064  -0.0047   0.0008  -0.0009   0.0006   0.0042
        Z   -0.0067  -0.0089  -0.0026   0.0015   0.0004   0.0115
AT. 44 O  X    0.0085   0.0162   0.0076  -0.0029   0.0168   0.0220
        Y    0.0064   0.0047   0.0008  -0.0009  -0.0006   0.0042
        Z    0.0067   0.0089  -0.0026   0.0015  -0.0004   0.0115
AT. 45 O  X    0.0205  -0.0185  -0.0121   0.0054  -0.0182  -0.0078
        Y    0.0067  -0.0013  -0.0056   0.0146  -0.0016   0.0201
        Z    0.0015  -0.0065  -0.0060   0.0030  -0.0006  -0.0138
AT. 46 O  X    0.0205  -0.0185   0.0121  -0.0054  -0.0182   0.0078
        Y   -0.0067   0.0013  -0.0056   0.0146   0.0016   0.0201
        Z   -0.0015   0.0065  -0.0060   0.0030   0.0006  -0.0138
AT. 47 O  X    0.0205   0.0185   0.0121   0.0054   0.0182  -0.0078
        Y   -0.0067  -0.0013  -0.0056  -0.0146  -0.0016  -0.0201
        Z    0.0015   0.0065   0.0060   0.0030   0.0006  -0.0138
AT. 48 O  X    0.0205   0.0185  -0.0121  -0.0054   0.0182   0.0078
        Y    0.0067   0.0013  -0.0056  -0.0146   0.0016  -0.0201
        Z   -0.0015  -0.0065   0.0060   0.0030  -0.0006  -0.0138


FREQ(CM**-1)    432.50   437.99   472.31   476.71   481.05   482.64


AT.  1 CA X    0.0047   0.0000   0.0000  -0.0062   0.0000   0.0009
        Y    0.0000  -0.0011  -0.0006   0.0000  -0.0027   0.0000
        Z    0.0000   0.0033   0.0022   0.0000   0.0026   0.0000
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AT.  2 CA X   0.0047   0.0000   0.0000   0.0062   0.0000   0.0009
        Y   0.0000  -0.0011   0.0006   0.0000  -0.0027   0.0000
        Z   0.0000  -0.0033   0.0022   0.0000  -0.0026   0.0000
AT.  3 CA X   0.0000  -0.0049   0.0000   0.0000   0.0028  -0.0008
        Y   0.0013   0.0016   0.0000   0.0000  -0.0003   0.0026
        Z   0.0000   0.0000   0.0020  -0.0008   0.0000   0.0000
AT.  4 CA X   0.0000   0.0049   0.0000   0.0000  -0.0028  -0.0008
        Y  -0.0013   0.0016   0.0000   0.0000  -0.0003  -0.0026
        Z   0.0000   0.0000   0.0020   0.0008   0.0000   0.0000
AT.  5 CA X   0.0020   0.0036   0.0015  -0.0006  -0.0014   0.0013
        Y  -0.0045  -0.0011   0.0007  -0.0005  -0.0017   0.0026
        Z  -0.0069   0.0000  -0.0007  -0.0021  -0.0035   0.0032
AT.  6 CA X   0.0020  -0.0036  -0.0015  -0.0006   0.0014   0.0013
        Y   0.0045  -0.0011   0.0007   0.0005  -0.0017  -0.0026
        Z   0.0069   0.0000  -0.0007   0.0021  -0.0035  -0.0032
AT.  7 CA X   0.0020  -0.0036   0.0015   0.0006   0.0014   0.0013
        Y   0.0045  -0.0011  -0.0007  -0.0005  -0.0017  -0.0026
        Z  -0.0069   0.0000  -0.0007   0.0021   0.0035   0.0032
AT.  8 CA X   0.0020   0.0036  -0.0015   0.0006  -0.0014   0.0013
        Y  -0.0045  -0.0011  -0.0007   0.0005  -0.0017   0.0026
        Z   0.0069   0.0000  -0.0007  -0.0021   0.0035  -0.0032
AT.  9 CA X  -0.0006  -0.0049  -0.0026  -0.0028  -0.0008   0.0008
        Y   0.0005   0.0012  -0.0006   0.0009   0.0018  -0.0042
        Z  -0.0017   0.0057   0.0003   0.0056  -0.0022   0.0013
AT. 10 CA X  -0.0006   0.0049   0.0026  -0.0028   0.0008   0.0008
        Y  -0.0005   0.0012  -0.0006  -0.0009   0.0018   0.0042
        Z   0.0017   0.0057   0.0003  -0.0056  -0.0022  -0.0013
AT. 11 CA X  -0.0006   0.0049  -0.0026   0.0028   0.0008   0.0008
        Y  -0.0005   0.0012   0.0006   0.0009   0.0018   0.0042
        Z  -0.0017  -0.0057   0.0003  -0.0056   0.0022   0.0013
AT. 12 CA X  -0.0006  -0.0049   0.0026   0.0028  -0.0008   0.0008
        Y   0.0005   0.0012   0.0006  -0.0009   0.0018  -0.0042
        Z   0.0017  -0.0057   0.0003   0.0056   0.0022  -0.0013
AT. 13 SI X   0.0033   0.0024   0.0000   0.0000  -0.0119  -0.0034
        Y  -0.0028   0.0033   0.0000   0.0000   0.0023   0.0001
        Z   0.0000   0.0000  -0.0174  -0.0104   0.0000   0.0000
AT. 14 SI X   0.0033  -0.0024   0.0000   0.0000   0.0119  -0.0034
        Y   0.0028   0.0033   0.0000   0.0000   0.0023  -0.0001
        Z   0.0000   0.0000  -0.0174   0.0104   0.0000   0.0000
AT. 15 SI X   0.0078  -0.0106  -0.0007  -0.0017  -0.0001  -0.0040
        Y   0.0008   0.0032  -0.0102   0.0098   0.0098   0.0130
        Z   0.0042   0.0057  -0.0201   0.0123   0.0183   0.0011
AT. 16 SI X   0.0078   0.0106   0.0007  -0.0017   0.0001  -0.0040
        Y  -0.0008   0.0032  -0.0102  -0.0098   0.0098  -0.0130
        Z  -0.0042   0.0057  -0.0201  -0.0123   0.0183  -0.0011
AT. 17 SI X   0.0078   0.0106  -0.0007   0.0017   0.0001  -0.0040
        Y  -0.0008   0.0032   0.0102   0.0098   0.0098  -0.0130
        Z   0.0042  -0.0057  -0.0201  -0.0123  -0.0183   0.0011
AT. 18 SI X   0.0078  -0.0106   0.0007   0.0017  -0.0001  -0.0040
        Y   0.0008   0.0032   0.0102  -0.0098   0.0098   0.0130
        Z  -0.0042  -0.0057  -0.0201   0.0123  -0.0183  -0.0011
AT. 19 SI X  -0.0024   0.0000   0.0000   0.0127   0.0000   0.0002
        Y   0.0000   0.0030   0.0162   0.0000  -0.0173   0.0000
        Z   0.0000  -0.0293  -0.0049   0.0000   0.0135   0.0000
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AT. 20 SI X  -0.0024   0.0000   0.0000  -0.0127   0.0000   0.0002
        Y   0.0000   0.0030  -0.0162   0.0000  -0.0173   0.0000
        Z   0.0000   0.0293  -0.0049   0.0000  -0.0135   0.0000
AT. 21 O  X   0.0085  -0.0028   0.0134   0.0097   0.0096   0.0013
        Y  -0.0166  -0.0042  -0.0041   0.0041   0.0018   0.0032
        Z   0.0049   0.0002  -0.0062  -0.0061   0.0096   0.0021
AT. 22 O  X   0.0085   0.0028  -0.0134   0.0097  -0.0096   0.0013
        Y   0.0166  -0.0042  -0.0041  -0.0041   0.0018  -0.0032
        Z  -0.0049   0.0002  -0.0062   0.0061   0.0096  -0.0021
AT. 23 O  X   0.0085   0.0028   0.0134  -0.0097  -0.0096   0.0013
        Y   0.0166  -0.0042   0.0041   0.0041   0.0018  -0.0032
        Z   0.0049  -0.0002  -0.0062   0.0061  -0.0096   0.0021
AT. 24 O  X   0.0085  -0.0028  -0.0134  -0.0097   0.0096   0.0013
        Y  -0.0166  -0.0042   0.0041  -0.0041   0.0018   0.0032
        Z  -0.0049  -0.0002  -0.0062  -0.0061  -0.0096  -0.0021
AT. 25 O  X  -0.0076   0.0057   0.0000   0.0000  -0.0112  -0.0007
        Y   0.0413   0.0072   0.0000   0.0000  -0.0032  -0.0121
        Z   0.0000   0.0000   0.0148   0.0116   0.0000   0.0000
AT. 26 O  X  -0.0076  -0.0057   0.0000   0.0000   0.0112  -0.0007
        Y  -0.0413   0.0072   0.0000   0.0000  -0.0032   0.0121
        Z   0.0000   0.0000   0.0148  -0.0116   0.0000   0.0000
AT. 27 O  X  -0.0229  -0.0044   0.0000   0.0000   0.0099   0.0043
        Y  -0.0029   0.0040   0.0000   0.0000   0.0035  -0.0013
        Z   0.0000   0.0000   0.0148   0.0079   0.0000   0.0000
AT. 28 O  X  -0.0229   0.0044   0.0000   0.0000  -0.0099   0.0043
        Y   0.0029   0.0040   0.0000   0.0000   0.0035   0.0013
        Z   0.0000   0.0000   0.0148  -0.0079   0.0000   0.0000
AT. 29 O  X   0.0068   0.0180   0.0052  -0.0063  -0.0073   0.0064
        Y   0.0203  -0.0240   0.0225  -0.0239  -0.0204  -0.0280
        Z   0.0096   0.0144  -0.0017  -0.0030  -0.0011  -0.0088
AT. 30 O  X   0.0068  -0.0180  -0.0052  -0.0063   0.0073   0.0064
        Y  -0.0203  -0.0240   0.0225   0.0239  -0.0204   0.0280
        Z  -0.0096   0.0144  -0.0017   0.0030  -0.0011   0.0088
AT. 31 O  X   0.0068  -0.0180   0.0052   0.0063   0.0073   0.0064
        Y  -0.0203  -0.0240  -0.0225  -0.0239  -0.0204   0.0280
        Z   0.0096  -0.0144  -0.0017   0.0030   0.0011  -0.0088
AT. 32 O  X   0.0068   0.0180  -0.0052   0.0063  -0.0073   0.0064
        Y   0.0203  -0.0240  -0.0225   0.0239  -0.0204  -0.0280
        Z  -0.0096  -0.0144  -0.0017  -0.0030   0.0011   0.0088
AT. 33 O  X  -0.0023   0.0089   0.0121   0.0123   0.0137  -0.0177
        Y   0.0293   0.0059  -0.0082  -0.0144  -0.0058   0.0215
        Z   0.0048  -0.0093   0.0153   0.0152   0.0216  -0.0007
AT. 34 O  X  -0.0023  -0.0089  -0.0121   0.0123  -0.0137  -0.0177
        Y  -0.0293   0.0059  -0.0082   0.0144  -0.0058  -0.0215
        Z  -0.0048  -0.0093   0.0153  -0.0152   0.0216   0.0007
AT. 35 O  X  -0.0023  -0.0089   0.0121  -0.0123  -0.0137  -0.0177
        Y  -0.0293   0.0059   0.0082  -0.0144  -0.0058  -0.0215
        Z   0.0048   0.0093   0.0153  -0.0152  -0.0216  -0.0007
AT. 36 O  X  -0.0023   0.0089  -0.0121  -0.0123   0.0137  -0.0177
        Y   0.0293   0.0059   0.0082   0.0144  -0.0058   0.0215
        Z  -0.0048   0.0093   0.0153   0.0152  -0.0216   0.0007
AT. 37 O  X   0.0140  -0.0104  -0.0158   0.0178   0.0190   0.0115
        Y   0.0079   0.0182  -0.0110   0.0238   0.0057   0.0307
        Z  -0.0074  -0.0012  -0.0019   0.0039  -0.0007  -0.0012
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AT. 38 O X   0.0140   0.0104   0.0158   0.0178 -0.0190   0.0115
         Y -0.0079   0.0182 -0.0110 -0.0238   0.0057 -0.0307
         Z   0.0074 -0.0012 -0.0019 -0.0039 -0.0007   0.0012
AT. 39 O X   0.0140   0.0104 -0.0158 -0.0178 -0.0190   0.0115
         Y -0.0079   0.0182   0.0110   0.0238   0.0057 -0.0307
         Z -0.0074   0.0012 -0.0019 -0.0039   0.0007 -0.0012
AT. 40 O X   0.0140 -0.0104   0.0158 -0.0178   0.0190   0.0115
         Y   0.0079   0.0182   0.0110 -0.0238   0.0057   0.0307
         Z   0.0074   0.0012 -0.0019   0.0039   0.0007   0.0012
AT. 41 O X -0.0193   0.0194   0.0017 -0.0070 -0.0010 -0.0059
         Y -0.0006   0.0041 -0.0081   0.0096   0.0080   0.0148
         Z   0.0010 -0.0155   0.0221 -0.0215 -0.0192 -0.0161
AT. 42 O X -0.0193 -0.0194 -0.0017 -0.0070   0.0010 -0.0059
         Y   0.0006   0.0041 -0.0081 -0.0096   0.0080 -0.0148
         Z -0.0010 -0.0155   0.0221   0.0215 -0.0192   0.0161
AT. 43 O X -0.0193 -0.0194   0.0017   0.0070   0.0010 -0.0059
         Y   0.0006   0.0041   0.0081   0.0096   0.0080 -0.0148
         Z   0.0010   0.0155   0.0221   0.0215   0.0192 -0.0161
AT. 44 O X -0.0193   0.0194 -0.0017   0.0070 -0.0010 -0.0059
         Y -0.0006   0.0041   0.0081 -0.0096   0.0080   0.0148
         Z -0.0010   0.0155   0.0221 -0.0215   0.0192   0.0161
AT. 45 O X -0.0164   0.0142 -0.0094 -0.0065   0.0058   0.0068
         Y -0.0077 -0.0176 -0.0048 -0.0096   0.0100   0.0001
         Z -0.0004   0.0065   0.0081 -0.0036 -0.0094   0.0063
AT. 46 O X -0.0164 -0.0142   0.0094 -0.0065 -0.0058   0.0068
         Y   0.0077 -0.0176 -0.0048   0.0096   0.0100 -0.0001
         Z   0.0004   0.0065   0.0081   0.0036 -0.0094 -0.0063
AT. 47 O X -0.0164 -0.0142 -0.0094   0.0065 -0.0058   0.0068
         Y   0.0077 -0.0176   0.0048 -0.0096   0.0100 -0.0001
         Z -0.0004 -0.0065   0.0081   0.0036   0.0094   0.0063
AT. 48 O X -0.0164   0.0142   0.0094   0.0065   0.0058   0.0068
         Y -0.0077 -0.0176   0.0048   0.0096   0.0100   0.0001
         Z   0.0004 -0.0065   0.0081 -0.0036   0.0094 -0.0063

FREQ(CM**-1)   498.39   509.86   511.46   513.52   522.35   531.30

AT. 1 CA X   0.0006 -0.0015   0.0000   0.0000   0.0051   0.0011
         Y   0.0000   0.0000   0.0004 -0.0017   0.0000   0.0000
         Z   0.0000   0.0000 -0.0005 -0.0008   0.0000   0.0000
AT. 2 CA X -0.0006 -0.0015   0.0000   0.0000 -0.0051   0.0011
         Y   0.0000   0.0000 -0.0004 -0.0017   0.0000   0.0000
         Z   0.0000   0.0000 -0.0005   0.0008   0.0000   0.0000
AT. 3 CA X   0.0000 -0.0022   0.0000 -0.0004   0.0000 -0.0046
         Y   0.0000   0.0003   0.0000   0.0021   0.0000 -0.0008
         Z   0.0032   0.0000   0.0040   0.0000 -0.0059   0.0000
AT. 4 CA X   0.0000 -0.0022   0.0000   0.0004   0.0000 -0.0046
         Y   0.0000 -0.0003   0.0000   0.0021   0.0000   0.0008
         Z -0.0032   0.0000   0.0040   0.0000   0.0059   0.0000
AT. 5 CA X -0.0016   0.0015   0.0020 -0.0027   0.0036   0.0020
         Y -0.0033 -0.0011   0.0015 -0.0014 -0.0005 -0.0001
         Z -0.0016   0.0014 -0.0011   0.0009 -0.0008   0.0015
AT. 6 CA X -0.0016   0.0015 -0.0020   0.0027   0.0036   0.0020
         Y   0.0033   0.0011   0.0015 -0.0014   0.0005   0.0001
         Z   0.0016 -0.0014 -0.0011   0.0009   0.0008 -0.0015

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AT.  7 CA X    0.0016   0.0015   0.0020   0.0027  -0.0036   0.0020
        Y   -0.0033   0.0011  -0.0015  -0.0014  -0.0005   0.0001
        Z    0.0016   0.0014  -0.0011  -0.0009   0.0008   0.0015
AT.  8 CA X    0.0016   0.0015  -0.0020  -0.0027  -0.0036   0.0020
        Y    0.0033  -0.0011  -0.0015  -0.0014   0.0005  -0.0001
        Z   -0.0016  -0.0014  -0.0011  -0.0009  -0.0008  -0.0015
AT.  9 CA X   -0.0032  -0.0022  -0.0013  -0.0004   0.0006   0.0001
        Y   -0.0002   0.0002  -0.0029  -0.0005   0.0025  -0.0003
        Z   -0.0048   0.0031   0.0007  -0.0011   0.0007   0.0042
AT. 10 CA X   -0.0032  -0.0022   0.0013   0.0004   0.0006   0.0001
        Y    0.0002  -0.0002  -0.0029  -0.0005  -0.0025   0.0003
        Z    0.0048  -0.0031   0.0007  -0.0011  -0.0007  -0.0042
AT. 11 CA X    0.0032  -0.0022  -0.0013   0.0004  -0.0006   0.0001
        Y   -0.0002  -0.0002   0.0029  -0.0005   0.0025   0.0003
        Z    0.0048   0.0031   0.0007   0.0011  -0.0007   0.0042
AT. 12 CA X    0.0032  -0.0022   0.0013  -0.0004  -0.0006   0.0001
        Y    0.0002   0.0002   0.0029  -0.0005  -0.0025  -0.0003
        Z   -0.0048  -0.0031   0.0007   0.0011   0.0007  -0.0042
AT. 13 SI X    0.0000   0.0117   0.0000   0.0019   0.0000   0.0252
        Y    0.0000   0.0020   0.0000   0.0057   0.0000   0.0030
        Z    0.0217   0.0000  -0.0109   0.0000   0.0040   0.0000
AT. 14 SI X    0.0000   0.0117   0.0000  -0.0019   0.0000   0.0252
        Y    0.0000  -0.0020   0.0000   0.0057   0.0000  -0.0030
        Z   -0.0217   0.0000  -0.0109   0.0000  -0.0040   0.0000
AT. 15 SI X   -0.0124   0.0190   0.0075   0.0081  -0.0092  -0.0049
        Y    0.0086   0.0007   0.0153   0.0141  -0.0039  -0.0024
        Z   -0.0086   0.0023  -0.0067  -0.0065   0.0084   0.0013
AT. 16 SI X   -0.0124   0.0190  -0.0075  -0.0081  -0.0092  -0.0049
        Y   -0.0086  -0.0007   0.0153   0.0141   0.0039   0.0024
        Z    0.0086  -0.0023  -0.0067  -0.0065  -0.0084  -0.0013
AT. 17 SI X    0.0124   0.0190   0.0075  -0.0081   0.0092  -0.0049
        Y    0.0086  -0.0007  -0.0153   0.0141  -0.0039   0.0024
        Z    0.0086   0.0023  -0.0067   0.0065  -0.0084   0.0013
AT. 18 SI X    0.0124   0.0190  -0.0075   0.0081   0.0092  -0.0049
        Y   -0.0086   0.0007  -0.0153   0.0141   0.0039  -0.0024
        Z   -0.0086  -0.0023  -0.0067   0.0065   0.0084  -0.0013
AT. 19 SI X    0.0006   0.0084   0.0000   0.0000   0.0036  -0.0048
        Y    0.0000   0.0000  -0.0100  -0.0050   0.0000   0.0000
        Z    0.0000   0.0000   0.0023   0.0005   0.0000   0.0000
AT. 20 SI X   -0.0006   0.0084   0.0000   0.0000  -0.0036  -0.0048
        Y    0.0000   0.0000   0.0100  -0.0050   0.0000   0.0000
        Z    0.0000   0.0000   0.0023  -0.0005   0.0000   0.0000
AT. 21 O  X   -0.0180  -0.0101   0.0105  -0.0026   0.0001  -0.0262
        Y    0.0093  -0.0011  -0.0035  -0.0033  -0.0059  -0.0060
        Z    0.0084  -0.0073  -0.0037   0.0031   0.0001  -0.0259
AT. 22 O  X   -0.0180  -0.0101  -0.0105   0.0026   0.0001  -0.0262
        Y   -0.0093   0.0011  -0.0035  -0.0033   0.0059   0.0060
        Z   -0.0084   0.0073  -0.0037   0.0031  -0.0001   0.0259
AT. 23 O  X    0.0180  -0.0101   0.0105   0.0026  -0.0001  -0.0262
        Y    0.0093   0.0011   0.0035  -0.0033  -0.0059   0.0060
        Z   -0.0084  -0.0073  -0.0037  -0.0031  -0.0001  -0.0259
AT. 24 O  X    0.0180  -0.0101  -0.0105  -0.0026  -0.0001  -0.0262
        Y   -0.0093  -0.0011   0.0035  -0.0033   0.0059  -0.0060
        Z    0.0084   0.0073  -0.0037  -0.0031   0.0001   0.0259
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AT. 25 O  X    0.0000   0.0130   0.0000   0.0041   0.0000   0.0281
         Y    0.0000  -0.0037   0.0000  -0.0050   0.0000   0.0053
         Z   -0.0279   0.0000   0.0151   0.0000  -0.0018   0.0000
AT. 26 O  X    0.0000   0.0130   0.0000  -0.0041   0.0000   0.0281
         Y    0.0000   0.0037   0.0000  -0.0050   0.0000  -0.0053
         Z    0.0279   0.0000   0.0151   0.0000   0.0018   0.0000
AT. 27 O  X    0.0000  -0.0058   0.0000   0.0005   0.0000  -0.0254
         Y    0.0000   0.0023   0.0000   0.0075   0.0000   0.0023
         Z   -0.0195   0.0000   0.0087   0.0000   0.0031   0.0000
AT. 28 O  X    0.0000  -0.0058   0.0000  -0.0005   0.0000  -0.0254
         Y    0.0000  -0.0023   0.0000   0.0075   0.0000  -0.0023
         Z    0.0195   0.0000   0.0087   0.0000  -0.0031   0.0000
AT. 29 O  X    0.0180  -0.0209   0.0060   0.0043   0.0058   0.0018
         Y   -0.0142  -0.0010  -0.0124  -0.0096  -0.0002  -0.0043
         Z   -0.0021  -0.0184  -0.0232  -0.0232   0.0211   0.0118
AT. 30 O  X    0.0180  -0.0209  -0.0060  -0.0043   0.0058   0.0018
         Y    0.0142   0.0010  -0.0124  -0.0096   0.0002   0.0043
         Z    0.0021   0.0184  -0.0232  -0.0232  -0.0211  -0.0118
AT. 31 O  X   -0.0180  -0.0209   0.0060  -0.0043  -0.0058   0.0018
         Y   -0.0142   0.0010   0.0124  -0.0096  -0.0002   0.0043
         Z    0.0021  -0.0184  -0.0232   0.0232  -0.0211   0.0118
AT. 32 O  X   -0.0180  -0.0209  -0.0060   0.0043  -0.0058   0.0018
         Y    0.0142  -0.0010   0.0124  -0.0096   0.0002  -0.0043
         Z   -0.0021   0.0184  -0.0232   0.0232   0.0211  -0.0118
AT. 33 O  X    0.0199   0.0152  -0.0064   0.0033   0.0083  -0.0025
         Y   -0.0096   0.0080   0.0268  -0.0285   0.0214  -0.0074
         Z   -0.0064  -0.0068   0.0140  -0.0153   0.0099  -0.0071
AT. 34 O  X    0.0199   0.0152   0.0064  -0.0033   0.0083  -0.0025
         Y    0.0096  -0.0080   0.0268  -0.0285  -0.0214   0.0074
         Z    0.0064   0.0068   0.0140  -0.0153  -0.0099   0.0071
AT. 35 O  X   -0.0199   0.0152  -0.0064  -0.0033  -0.0083  -0.0025
         Y   -0.0096  -0.0080  -0.0268  -0.0285   0.0214   0.0074
         Z    0.0064  -0.0068   0.0140   0.0153  -0.0099  -0.0071
AT. 36 O  X   -0.0199   0.0152   0.0064   0.0033  -0.0083  -0.0025
         Y    0.0096   0.0080  -0.0268  -0.0285  -0.0214  -0.0074
         Z   -0.0064   0.0068   0.0140   0.0153   0.0099   0.0071
AT. 37 O  X    0.0032  -0.0133  -0.0111  -0.0162   0.0186   0.0116
         Y    0.0087   0.0051   0.0043   0.0066  -0.0122   0.0063
         Z   -0.0104   0.0264   0.0128   0.0149  -0.0204  -0.0101
AT. 38 O  X    0.0032  -0.0133   0.0111   0.0162   0.0186   0.0116
         Y   -0.0087  -0.0051   0.0043   0.0066   0.0122  -0.0063
         Z    0.0104  -0.0264   0.0128   0.0149   0.0204   0.0101
AT. 39 O  X   -0.0032  -0.0133  -0.0111   0.0162  -0.0186   0.0116
         Y    0.0087  -0.0051  -0.0043   0.0066  -0.0122  -0.0063
         Z    0.0104   0.0264   0.0128  -0.0149   0.0204  -0.0101
AT. 40 O  X   -0.0032  -0.0133   0.0111  -0.0162  -0.0186   0.0116
         Y   -0.0087   0.0051  -0.0043   0.0066   0.0122   0.0063
         Z   -0.0104  -0.0264   0.0128  -0.0149  -0.0204   0.0101
AT. 41 O  X    0.0094  -0.0209  -0.0148  -0.0182   0.0231   0.0079
         Y    0.0110  -0.0010   0.0161   0.0143  -0.0036  -0.0021
         Z   -0.0005  -0.0056   0.0024   0.0028  -0.0027  -0.0072
AT. 42 O  X    0.0094  -0.0209   0.0148   0.0182   0.0231   0.0079
         Y   -0.0110   0.0010   0.0161   0.0143   0.0036   0.0021
         Z    0.0005   0.0056   0.0024   0.0028   0.0027   0.0072
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AT. 43 O  X  -0.0094  -0.0209  -0.0148   0.0182  -0.0231   0.0079
       Y   0.0110   0.0010  -0.0161   0.0143  -0.0036   0.0021
       Z   0.0005  -0.0056   0.0024  -0.0028   0.0027  -0.0072
AT. 44 O  X  -0.0094  -0.0209   0.0148  -0.0182  -0.0231   0.0079
       Y  -0.0110  -0.0010  -0.0161   0.0143   0.0036  -0.0021
       Z  -0.0005   0.0056   0.0024  -0.0028  -0.0027   0.0072
AT. 45 O  X   0.0119   0.0018   0.0087   0.0125  -0.0197  -0.0040
       Y   0.0051  -0.0058  -0.0006  -0.0017  -0.0065   0.0016
       Z   0.0024   0.0024   0.0014   0.0038  -0.0104  -0.0007
AT. 46 O  X   0.0119   0.0018  -0.0087  -0.0125  -0.0197  -0.0040
       Y  -0.0051   0.0058  -0.0006  -0.0017   0.0065  -0.0016
       Z  -0.0024  -0.0024   0.0014   0.0038   0.0104   0.0007
AT. 47 O  X  -0.0119   0.0018   0.0087  -0.0125   0.0197  -0.0040
       Y   0.0051   0.0058   0.0006  -0.0017  -0.0065  -0.0016
       Z  -0.0024   0.0024   0.0014  -0.0038   0.0104  -0.0007
AT. 48 O  X  -0.0119   0.0018  -0.0087   0.0125   0.0197  -0.0040
       Y  -0.0051  -0.0058   0.0006  -0.0017   0.0065   0.0016
       Z   0.0024  -0.0024   0.0014  -0.0038  -0.0104   0.0007


FREQ(CM**-1)    533.88    539.94    548.56    556.18    565.71    567.77


AT.  1 CA X   0.0000   0.0000  -0.0001   0.0002   0.0003   0.0000
       Y  -0.0002   0.0003   0.0000   0.0000   0.0000   0.0001
       Z  -0.0002   0.0032   0.0000   0.0000   0.0000   0.0010
AT.  2 CA X   0.0000   0.0000  -0.0001  -0.0002   0.0003   0.0000
       Y  -0.0002  -0.0003   0.0000   0.0000   0.0000   0.0001
       Z   0.0002   0.0032   0.0000   0.0000   0.0000  -0.0010
AT.  3 CA X   0.0042   0.0000  -0.0026   0.0000  -0.0005   0.0003
       Y   0.0014   0.0000   0.0015   0.0000  -0.0034  -0.0004
       Z   0.0000  -0.0064   0.0000  -0.0015   0.0000   0.0000
AT.  4 CA X  -0.0042   0.0000  -0.0026   0.0000  -0.0005  -0.0003
       Y   0.0014   0.0000  -0.0015   0.0000   0.0034  -0.0004
       Z   0.0000  -0.0064   0.0000   0.0015   0.0000   0.0000
AT.  5 CA X   0.0039  -0.0001   0.0011   0.0001  -0.0006  -0.0005
       Y  -0.0017   0.0008   0.0008   0.0011  -0.0028  -0.0028
       Z  -0.0016  -0.0018  -0.0036   0.0019  -0.0024  -0.0002
AT.  6 CA X  -0.0039   0.0001   0.0011   0.0001  -0.0006   0.0005
       Y  -0.0017   0.0008  -0.0008  -0.0011   0.0028  -0.0028
       Z  -0.0016  -0.0018   0.0036  -0.0019   0.0024  -0.0002
AT.  7 CA X  -0.0039  -0.0001   0.0011  -0.0001  -0.0006   0.0005
       Y  -0.0017  -0.0008  -0.0008   0.0011   0.0028  -0.0028
       Z   0.0016  -0.0018  -0.0036  -0.0019  -0.0024   0.0002
AT.  8 CA X   0.0039   0.0001   0.0011  -0.0001  -0.0006  -0.0005
       Y  -0.0017  -0.0008   0.0008  -0.0011  -0.0028  -0.0028
       Z   0.0016  -0.0018   0.0036   0.0019   0.0024   0.0002
AT.  9 CA X   0.0006   0.0008  -0.0015   0.0056   0.0008  -0.0005
       Y   0.0002   0.0002  -0.0036   0.0014   0.0018   0.0017
       Z   0.0018   0.0028  -0.0033  -0.0012  -0.0041  -0.0033
AT. 10 CA X  -0.0006  -0.0008  -0.0015   0.0056   0.0008   0.0005
       Y   0.0002   0.0002   0.0036  -0.0014  -0.0018   0.0017
       Z   0.0018   0.0028   0.0033   0.0012   0.0041  -0.0033
AT. 11 CA X  -0.0006   0.0008  -0.0015  -0.0056   0.0008   0.0005
       Y   0.0002  -0.0002   0.0036   0.0014  -0.0018   0.0017
       Z  -0.0018   0.0028  -0.0033   0.0012  -0.0041   0.0033
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AT. 12 CA X   0.0006  -0.0008  -0.0015  -0.0056   0.0008  -0.0005
        Y    0.0002  -0.0002  -0.0036  -0.0014   0.0018   0.0017
        Z   -0.0018   0.0028   0.0033  -0.0012   0.0041   0.0033
AT. 13 SI X   0.0178   0.0000   0.0079   0.0000  -0.0022  -0.0048
        Y    0.0028   0.0000  -0.0049   0.0000   0.0284   0.0246
        Z    0.0000  -0.0137   0.0000   0.0159   0.0000   0.0000
AT. 14 SI X  -0.0178   0.0000   0.0079   0.0000  -0.0022   0.0048
        Y    0.0028   0.0000   0.0049   0.0000  -0.0284   0.0246
        Z    0.0000  -0.0137   0.0000  -0.0159   0.0000   0.0000
AT. 15 SI X  -0.0038  -0.0088  -0.0008   0.0062  -0.0001  -0.0052
        Y    0.0059   0.0025   0.0065  -0.0065   0.0016   0.0014
        Z   -0.0037   0.0027  -0.0114   0.0088  -0.0006  -0.0039
AT. 16 SI X   0.0038   0.0088  -0.0008   0.0062  -0.0001   0.0052
        Y    0.0059   0.0025  -0.0065   0.0065  -0.0016   0.0014
        Z   -0.0037   0.0027   0.0114  -0.0088   0.0006  -0.0039
AT. 17 SI X   0.0038  -0.0088  -0.0008  -0.0062  -0.0001   0.0052
        Y    0.0059  -0.0025  -0.0065  -0.0065  -0.0016   0.0014
        Z    0.0037   0.0027  -0.0114  -0.0088  -0.0006   0.0039
AT. 18 SI X  -0.0038   0.0088  -0.0008  -0.0062  -0.0001  -0.0052
        Y    0.0059  -0.0025   0.0065   0.0065   0.0016   0.0014
        Z    0.0037   0.0027   0.0114   0.0088   0.0006   0.0039
AT. 19 SI X   0.0000   0.0000  -0.0064   0.0014  -0.0024   0.0000
        Y   -0.0067  -0.0076   0.0000   0.0000   0.0000   0.0023
        Z    0.0144   0.0142   0.0000   0.0000   0.0000   0.0045
AT. 20 SI X   0.0000   0.0000  -0.0064  -0.0014  -0.0024   0.0000
        Y   -0.0067   0.0076   0.0000   0.0000   0.0000   0.0023
        Z   -0.0144   0.0142   0.0000   0.0000   0.0000  -0.0045
AT. 21 O  X  -0.0256   0.0213  -0.0065  -0.0227  -0.0074  -0.0002
        Y   -0.0077  -0.0096   0.0029   0.0040  -0.0303  -0.0244
        Z   -0.0254  -0.0086  -0.0140   0.0074   0.0180   0.0229
AT. 22 O  X   0.0256  -0.0213  -0.0065  -0.0227  -0.0074   0.0002
        Y   -0.0077  -0.0096  -0.0029  -0.0040   0.0303  -0.0244
        Z   -0.0254  -0.0086   0.0140  -0.0074  -0.0180   0.0229
AT. 23 O  X   0.0256   0.0213  -0.0065   0.0227  -0.0074   0.0002
        Y   -0.0077   0.0096  -0.0029   0.0040   0.0303  -0.0244
        Z    0.0254  -0.0086  -0.0140  -0.0074   0.0180  -0.0229
AT. 24 O  X  -0.0256  -0.0213  -0.0065   0.0227  -0.0074  -0.0002
        Y   -0.0077   0.0096   0.0029  -0.0040  -0.0303  -0.0244
        Z    0.0254  -0.0086   0.0140   0.0074  -0.0180  -0.0229
AT. 25 O  X   0.0279   0.0000   0.0059   0.0000   0.0185   0.0092
        Y    0.0109   0.0000   0.0085   0.0000  -0.0264  -0.0278
        Z    0.0000   0.0346   0.0000  -0.0344   0.0000   0.0000
AT. 26 O  X  -0.0279   0.0000   0.0059   0.0000   0.0185  -0.0092
        Y    0.0109   0.0000  -0.0085   0.0000   0.0264  -0.0278
        Z    0.0000   0.0346   0.0000   0.0344   0.0000   0.0000
AT. 27 O  X  -0.0264   0.0000  -0.0104   0.0000  -0.0022   0.0061
        Y    0.0028   0.0000  -0.0061   0.0000   0.0335   0.0286
        Z    0.0000   0.0258   0.0000  -0.0231   0.0000   0.0000
AT. 28 O  X   0.0264   0.0000  -0.0104   0.0000  -0.0022  -0.0061
        Y    0.0028   0.0000   0.0061   0.0000  -0.0335   0.0286
        Z    0.0000   0.0258   0.0000   0.0231   0.0000   0.0000
AT. 29 O  X   0.0035   0.0019   0.0172  -0.0188   0.0036   0.0105
        Y   -0.0094  -0.0046   0.0014   0.0042   0.0012   0.0033
        Z   -0.0026   0.0058  -0.0115  -0.0006  -0.0012   0.0036
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AT. 30 O  X   -0.0035  -0.0019   0.0172  -0.0188   0.0036  -0.0105
        Y   -0.0094  -0.0046  -0.0014  -0.0042  -0.0012   0.0033
        Z   -0.0026   0.0058   0.0115   0.0006   0.0012   0.0036
AT. 31 O  X   -0.0035   0.0019   0.0172   0.0188   0.0036  -0.0105
        Y   -0.0094   0.0046  -0.0014   0.0042  -0.0012   0.0033
        Z    0.0026   0.0058  -0.0115   0.0006  -0.0012  -0.0036
AT. 32 O  X    0.0035  -0.0019   0.0172   0.0188   0.0036   0.0105
        Y   -0.0094   0.0046   0.0014  -0.0042   0.0012   0.0033
        Z    0.0026   0.0058   0.0115  -0.0006   0.0012  -0.0036
AT. 33 O  X    0.0112  -0.0110  -0.0024  -0.0110  -0.0015   0.0064
        Y   -0.0011  -0.0027   0.0108   0.0064   0.0049   0.0025
        Z    0.0026  -0.0108   0.0267   0.0155   0.0054  -0.0058
AT. 34 O  X   -0.0112   0.0110  -0.0024  -0.0110  -0.0015  -0.0064
        Y   -0.0011  -0.0027  -0.0108  -0.0064  -0.0049   0.0025
        Z    0.0026  -0.0108  -0.0267  -0.0155  -0.0054  -0.0058
AT. 35 O  X   -0.0112  -0.0110  -0.0024   0.0110  -0.0015  -0.0064
        Y   -0.0011   0.0027  -0.0108   0.0064  -0.0049   0.0025
        Z   -0.0026  -0.0108   0.0267  -0.0155   0.0054   0.0058
AT. 36 O  X    0.0112   0.0110  -0.0024   0.0110  -0.0015   0.0064
        Y   -0.0011   0.0027   0.0108  -0.0064   0.0049   0.0025
        Z   -0.0026  -0.0108  -0.0267   0.0155  -0.0054   0.0058
AT. 37 O  X    0.0121   0.0208  -0.0174   0.0040  -0.0023   0.0037
        Y   -0.0066  -0.0081  -0.0096   0.0088  -0.0028  -0.0114
        Z   -0.0031  -0.0062  -0.0001   0.0110  -0.0019  -0.0083
AT. 38 O  X   -0.0121  -0.0208  -0.0174   0.0040  -0.0023  -0.0037
        Y   -0.0066  -0.0081   0.0096  -0.0088   0.0028  -0.0114
        Z   -0.0031  -0.0062   0.0001  -0.0110   0.0019  -0.0083
AT. 39 O  X   -0.0121   0.0208  -0.0174  -0.0040  -0.0023  -0.0037
        Y   -0.0066   0.0081   0.0096   0.0088   0.0028  -0.0114
        Z    0.0031  -0.0062  -0.0001  -0.0110  -0.0019   0.0083
AT. 40 O  X    0.0121  -0.0208  -0.0174  -0.0040  -0.0023   0.0037
        Y   -0.0066   0.0081  -0.0096  -0.0088  -0.0028  -0.0114
        Z    0.0031  -0.0062   0.0001   0.0110   0.0019   0.0083
AT. 41 O  X    0.0055   0.0083  -0.0025  -0.0090   0.0009   0.0076
        Y    0.0069   0.0030   0.0082  -0.0080   0.0008   0.0038
        Z   -0.0013  -0.0049   0.0168  -0.0100   0.0048   0.0064
AT. 42 O  X   -0.0055  -0.0083  -0.0025  -0.0090   0.0009  -0.0076
        Y    0.0069   0.0030  -0.0082   0.0080  -0.0008   0.0038
        Z   -0.0013  -0.0049  -0.0168   0.0100  -0.0048   0.0064
AT. 43 O  X   -0.0055   0.0083  -0.0025   0.0090   0.0009  -0.0076
        Y    0.0069  -0.0030  -0.0082  -0.0080  -0.0008   0.0038
        Z    0.0013  -0.0049   0.0168   0.0100   0.0048  -0.0064
AT. 44 O  X    0.0055  -0.0083  -0.0025   0.0090   0.0009   0.0076
        Y    0.0069  -0.0030   0.0082   0.0080   0.0008   0.0038
        Z    0.0013  -0.0049  -0.0168  -0.0100  -0.0048  -0.0064
AT. 45 O  X   -0.0086  -0.0127   0.0182  -0.0075   0.0023  -0.0090
        Y    0.0068   0.0100   0.0092  -0.0071   0.0017   0.0029
        Z   -0.0050  -0.0091   0.0097  -0.0011   0.0024  -0.0005
AT. 46 O  X    0.0086   0.0127   0.0182  -0.0075   0.0023   0.0090
        Y    0.0068   0.0100  -0.0092   0.0071  -0.0017   0.0029
        Z   -0.0050  -0.0091  -0.0097   0.0011  -0.0024  -0.0005
AT. 47 O  X    0.0086  -0.0127   0.0182   0.0075   0.0023   0.0090
        Y    0.0068  -0.0100  -0.0092  -0.0071  -0.0017   0.0029
        Z    0.0050  -0.0091   0.0097   0.0011   0.0024   0.0005
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AT. 48 O X   -0.0086   0.0127   0.0182   0.0075   0.0023 -0.0090
         Y   0.0068 -0.0100   0.0092   0.0071   0.0017   0.0029
         Z   0.0050 -0.0091 -0.0097 -0.0011 -0.0024   0.0005

FREQ(CM**-1)   568.30   577.01   578.69   587.70   668.57   679.24

AT. 1 CA X   0.0000   0.0000   0.0021 -0.0010   0.0037 -0.0013
         Y   0.0013 -0.0002   0.0000   0.0000   0.0000   0.0000
         Z   0.0002   0.0021   0.0000   0.0000   0.0000   0.0000
AT. 2 CA X   0.0000   0.0000   0.0021   0.0010   0.0037   0.0013
         Y   -0.0013 -0.0002   0.0000   0.0000   0.0000   0.0000
         Z   0.0002 -0.0021   0.0000   0.0000   0.0000   0.0000
AT. 3 CA X   0.0000 -0.0068   0.0008   0.0000   0.0005   0.0000
         Y   0.0000   0.0008 -0.0009   0.0000   0.0001   0.0000
         Z   0.0031   0.0000   0.0000   0.0004   0.0000 -0.0007
AT. 4 CA X   0.0000   0.0068   0.0008   0.0000   0.0005   0.0000
         Y   0.0000   0.0008   0.0009   0.0000 -0.0001   0.0000
         Z   0.0031   0.0000   0.0000 -0.0004   0.0000   0.0007
AT. 5 CA X   -0.0002   0.0004   0.0000   0.0006 -0.0003   0.0000
         Y   0.0016 -0.0001 -0.0017 -0.0006   0.0002 -0.0001
         Z   0.0003   0.0022 -0.0007   0.0025   0.0002   0.0000
AT. 6 CA X   0.0002 -0.0004   0.0000   0.0006 -0.0003   0.0000
         Y   0.0016 -0.0001   0.0017   0.0006 -0.0002   0.0001
         Z   0.0003   0.0022   0.0007 -0.0025 -0.0002   0.0000
AT. 7 CA X   -0.0002 -0.0004   0.0000 -0.0006 -0.0003   0.0000
         Y   -0.0016 -0.0001   0.0017 -0.0006 -0.0002 -0.0001
         Z   0.0003 -0.0022 -0.0007 -0.0025   0.0002   0.0000
AT. 8 CA X   0.0002   0.0004   0.0000 -0.0006 -0.0003   0.0000
         Y   -0.0016 -0.0001 -0.0017   0.0006   0.0002   0.0001
         Z   0.0003 -0.0022   0.0007   0.0025 -0.0002   0.0000
AT. 9 CA X   0.0022 -0.0036 -0.0028   0.0038 -0.0017 -0.0013
         Y   -0.0012 -0.0012 -0.0016   0.0021 -0.0020 -0.0022
         Z   -0.0031   0.0002 -0.0040   0.0025   0.0002 -0.0006
AT. 10 CA X   -0.0022   0.0036 -0.0028   0.0038 -0.0017 -0.0013
         Y   -0.0012 -0.0012   0.0016 -0.0021   0.0020   0.0022
         Z   -0.0031   0.0002   0.0040 -0.0025 -0.0002   0.0006
AT. 11 CA X   0.0022   0.0036 -0.0028 -0.0038 -0.0017   0.0013
         Y   0.0012 -0.0012   0.0016   0.0021   0.0020 -0.0022
         Z   -0.0031 -0.0002 -0.0040 -0.0025   0.0002   0.0006
AT. 12 CA X   -0.0022 -0.0036 -0.0028 -0.0038 -0.0017   0.0013
         Y   0.0012 -0.0012 -0.0016 -0.0021 -0.0020   0.0022
         Z   -0.0031 -0.0002   0.0040   0.0025 -0.0002 -0.0006
AT. 13 SI X   0.0000 -0.0060 -0.0023   0.0000   0.0010   0.0000
         Y   0.0000 -0.0143 -0.0003   0.0000 -0.0008   0.0000
         Z   0.0097   0.0000   0.0000   0.0022   0.0000 -0.0011
AT. 14 SI X   0.0000   0.0060 -0.0023   0.0000   0.0010   0.0000
         Y   0.0000 -0.0143   0.0003   0.0000   0.0008   0.0000
         Z   0.0097   0.0000   0.0000 -0.0022   0.0000   0.0011
AT. 15 SI X   -0.0107 -0.0078 -0.0009   0.0040   0.0097   0.0089
         Y   0.0076   0.0071 -0.0118   0.0118   0.0092   0.0086
         Z   -0.0100 -0.0083 -0.0006   0.0032   0.0154   0.0144
AT. 16 SI X   0.0107   0.0078 -0.0009   0.0040   0.0097   0.0089
         Y   0.0076   0.0071   0.0118 -0.0118 -0.0092 -0.0086
         Z   -0.0100 -0.0083   0.0006 -0.0032 -0.0154 -0.0144

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AT.  17 SI X   -0.0107   0.0078  -0.0009  -0.0040   0.0097  -0.0089
        Y   -0.0076   0.0071   0.0118   0.0118  -0.0092   0.0086
        Z   -0.0100   0.0083  -0.0006  -0.0032   0.0154  -0.0144
AT.  18 SI X    0.0107  -0.0078  -0.0009  -0.0040   0.0097  -0.0089
        Y   -0.0076   0.0071  -0.0118  -0.0118   0.0092  -0.0086
        Z   -0.0100   0.0083   0.0006   0.0032  -0.0154   0.0144
AT.  19 SI X    0.0000   0.0000  -0.0210   0.0136  -0.0196  -0.0193
        Y    0.0007  -0.0002   0.0000   0.0000   0.0000   0.0000
        Z    0.0134   0.0095   0.0000   0.0000   0.0000   0.0000
AT.  20 SI X    0.0000   0.0000  -0.0210  -0.0136  -0.0196   0.0193
        Y   -0.0007  -0.0002   0.0000   0.0000   0.0000   0.0000
        Z    0.0134  -0.0095   0.0000   0.0000   0.0000   0.0000
AT.  21 O  X   -0.0128   0.0125   0.0031  -0.0050   0.0003  -0.0025
        Y    0.0029   0.0167   0.0000   0.0018   0.0024   0.0024
        Z    0.0049   0.0019   0.0030   0.0005   0.0019   0.0011
AT.  22 O  X    0.0128  -0.0125   0.0031  -0.0050   0.0003  -0.0025
        Y    0.0029   0.0167   0.0000  -0.0018  -0.0024  -0.0024
        Z    0.0049   0.0019  -0.0030  -0.0005  -0.0019  -0.0011
AT.  23 O  X   -0.0128  -0.0125   0.0031   0.0050   0.0003   0.0025
        Y   -0.0029   0.0167   0.0000   0.0018  -0.0024   0.0024
        Z    0.0049  -0.0019   0.0030  -0.0005   0.0019  -0.0011
AT.  24 O  X    0.0128   0.0125   0.0031   0.0050   0.0003   0.0025
        Y   -0.0029   0.0167   0.0000  -0.0018   0.0024  -0.0024
        Z    0.0049  -0.0019  -0.0030   0.0005  -0.0019   0.0011
AT.  25 O  X    0.0000  -0.0171  -0.0030   0.0000  -0.0017   0.0000
        Y    0.0000   0.0124   0.0013   0.0000  -0.0011   0.0000
        Z   -0.0200   0.0000   0.0000  -0.0073   0.0000  -0.0030
AT.  26 O  X    0.0000   0.0171  -0.0030   0.0000  -0.0017   0.0000
        Y    0.0000   0.0124  -0.0013   0.0000   0.0011   0.0000
        Z   -0.0200   0.0000   0.0000   0.0073   0.0000   0.0030
AT.  27 O  X    0.0000   0.0098   0.0029   0.0000   0.0014   0.0000
        Y    0.0000  -0.0155   0.0008   0.0000  -0.0016   0.0000
        Z   -0.0138   0.0000   0.0000  -0.0034   0.0000  -0.0018
AT.  28 O  X    0.0000  -0.0098   0.0029   0.0000   0.0014   0.0000
        Y    0.0000  -0.0155  -0.0008   0.0000   0.0016   0.0000
        Z   -0.0138   0.0000   0.0000   0.0034   0.0000   0.0018
AT.  29 O  X    0.0191   0.0195  -0.0060   0.0025  -0.0081  -0.0073
        Y   -0.0049  -0.0072   0.0098  -0.0054  -0.0079  -0.0071
        Z   -0.0025  -0.0018   0.0060  -0.0127   0.0039   0.0045
AT.  30 O  X   -0.0191  -0.0195  -0.0060   0.0025  -0.0081  -0.0073
        Y   -0.0049  -0.0072  -0.0098   0.0054   0.0079   0.0071
        Z   -0.0025  -0.0018  -0.0060   0.0127  -0.0039  -0.0045
AT.  31 O  X    0.0191  -0.0195  -0.0060  -0.0025  -0.0081   0.0073
        Y    0.0049  -0.0072  -0.0098  -0.0054   0.0079  -0.0071
        Z   -0.0025   0.0018   0.0060   0.0127   0.0039  -0.0045
AT.  32 O  X   -0.0191   0.0195  -0.0060  -0.0025  -0.0081   0.0073
        Y    0.0049  -0.0072   0.0098   0.0054  -0.0079   0.0071
        Z   -0.0025   0.0018  -0.0060  -0.0127  -0.0039   0.0045
AT.  33 O  X   -0.0158   0.0147   0.0130   0.0037   0.0046  -0.0033
        Y    0.0045  -0.0057  -0.0080  -0.0102   0.0045  -0.0066
        Z    0.0138  -0.0136   0.0009  -0.0067  -0.0072   0.0078
AT.  34 O  X    0.0158  -0.0147   0.0130   0.0037   0.0046  -0.0033
        Y    0.0045  -0.0057   0.0080   0.0102  -0.0045   0.0066
        Z    0.0138  -0.0136  -0.0009   0.0067   0.0072  -0.0078
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AT. 35 O  X  -0.0158  -0.0147   0.0130  -0.0037   0.0046   0.0033
         Y  -0.0045  -0.0057   0.0080  -0.0102  -0.0045  -0.0066
         Z   0.0138   0.0136   0.0009   0.0067  -0.0072  -0.0078
AT. 36 O  X   0.0158   0.0147   0.0130  -0.0037   0.0046   0.0033
         Y  -0.0045  -0.0057  -0.0080   0.0102   0.0045   0.0066
         Z   0.0138   0.0136  -0.0009  -0.0067   0.0072   0.0078
AT. 37 O  X   0.0052   0.0031   0.0014  -0.0073   0.0043   0.0035
         Y  -0.0182  -0.0146   0.0277  -0.0319  -0.0257  -0.0221
         Z  -0.0114  -0.0103  -0.0037   0.0111  -0.0119  -0.0139
AT. 38 O  X  -0.0052  -0.0031   0.0014  -0.0073   0.0043   0.0035
         Y  -0.0182  -0.0146  -0.0277   0.0319   0.0257   0.0221
         Z  -0.0114  -0.0103   0.0037  -0.0111   0.0119   0.0139
AT. 39 O  X   0.0052  -0.0031   0.0014   0.0073   0.0043  -0.0035
         Y   0.0182  -0.0146  -0.0277  -0.0319   0.0257  -0.0221
         Z  -0.0114   0.0103  -0.0037  -0.0111  -0.0119   0.0139
AT. 40 O  X  -0.0052   0.0031   0.0014   0.0073   0.0043  -0.0035
         Y   0.0182  -0.0146   0.0277   0.0319  -0.0257   0.0221
         Z  -0.0114   0.0103   0.0037   0.0111   0.0119  -0.0139
AT. 41 O  X   0.0132   0.0121  -0.0072  -0.0021  -0.0030  -0.0029
         Y   0.0109   0.0092  -0.0128   0.0127   0.0102   0.0092
         Z   0.0130   0.0118  -0.0030   0.0070  -0.0063  -0.0064
AT. 42 O  X  -0.0132  -0.0121  -0.0072  -0.0021  -0.0030  -0.0029
         Y   0.0109   0.0092   0.0128  -0.0127  -0.0102  -0.0092
         Z   0.0130   0.0118   0.0030  -0.0070   0.0063   0.0064
AT. 43 O  X   0.0132  -0.0121  -0.0072   0.0021  -0.0030   0.0029
         Y  -0.0109   0.0092   0.0128   0.0127  -0.0102   0.0092
         Z   0.0130  -0.0118  -0.0030  -0.0070  -0.0063   0.0064
AT. 44 O  X  -0.0132   0.0121  -0.0072   0.0021  -0.0030   0.0029
         Y  -0.0109   0.0092  -0.0128  -0.0127   0.0102  -0.0092
         Z   0.0130  -0.0118   0.0030   0.0070   0.0063  -0.0064
AT. 45 O  X  -0.0142  -0.0108   0.0211  -0.0186   0.0008   0.0058
         Y   0.0063   0.0057   0.0163  -0.0138   0.0182   0.0205
         Z  -0.0008  -0.0008   0.0197  -0.0173   0.0126   0.0157
AT. 46 O  X   0.0142   0.0108   0.0211  -0.0186   0.0008   0.0058
         Y   0.0063   0.0057  -0.0163   0.0138  -0.0182  -0.0205
         Z  -0.0008  -0.0008  -0.0197   0.0173  -0.0126  -0.0157
AT. 47 O  X  -0.0142   0.0108   0.0211   0.0186   0.0008  -0.0058
         Y  -0.0063   0.0057  -0.0163  -0.0138  -0.0182   0.0205
         Z  -0.0008   0.0008   0.0197   0.0173   0.0126  -0.0157
AT. 48 O  X   0.0142  -0.0108   0.0211   0.0186   0.0008  -0.0058
         Y  -0.0063   0.0057   0.0163   0.0138   0.0182  -0.0205
         Z  -0.0008   0.0008  -0.0197  -0.0173  -0.0126   0.0157

FREQ(CM**-1)   708.05   709.90   820.75   821.40   824.47   830.58

AT.  1 CA X   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
         Y   0.0019   0.0008   0.0002   0.0000   0.0002  -0.0001
         Z   0.0000   0.0004   0.0002   0.0000   0.0005  -0.0003
AT.  2 CA X   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
         Y  -0.0019   0.0008   0.0002   0.0000  -0.0002  -0.0001
         Z   0.0000  -0.0004  -0.0002   0.0000   0.0005   0.0003
AT.  3 CA X   0.0000  -0.0014  -0.0015   0.0005   0.0000  -0.0017
         Y   0.0000   0.0001   0.0002  -0.0008   0.0000  -0.0001
         Z  -0.0010   0.0000   0.0000   0.0000   0.0000   0.0000
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AT.  4 CA X   0.0000   0.0014   0.0015   0.0005   0.0000   0.0017
        Y   0.0000   0.0001   0.0002   0.0008   0.0000  -0.0001
        Z  -0.0010   0.0000   0.0000   0.0000   0.0000   0.0000
AT.  5 CA X  -0.0005  -0.0004   0.0004  -0.0009  -0.0003   0.0010
        Y   0.0002   0.0001  -0.0002  -0.0001  -0.0005   0.0005
        Z  -0.0007  -0.0005   0.0004  -0.0006  -0.0002   0.0010
AT.  6 CA X   0.0005   0.0004  -0.0004  -0.0009   0.0003  -0.0010
        Y   0.0002   0.0001  -0.0002   0.0001  -0.0005   0.0005
        Z  -0.0007  -0.0005   0.0004   0.0006  -0.0002   0.0010
AT.  7 CA X  -0.0005   0.0004  -0.0004  -0.0009  -0.0003  -0.0010
        Y  -0.0002   0.0001  -0.0002   0.0001   0.0005   0.0005
        Z  -0.0007   0.0005  -0.0004  -0.0006  -0.0002  -0.0010
AT.  8 CA X   0.0005  -0.0004   0.0004  -0.0009   0.0003   0.0010
        Y  -0.0002   0.0001  -0.0002  -0.0001   0.0005   0.0005
        Z  -0.0007   0.0005  -0.0004   0.0006  -0.0002  -0.0010
AT.  9 CA X  -0.0006  -0.0011  -0.0003   0.0005   0.0002  -0.0003
        Y  -0.0015   0.0015  -0.0003   0.0005  -0.0001  -0.0006
        Z   0.0009  -0.0007   0.0005  -0.0013   0.0005   0.0015
AT. 10 CA X   0.0006   0.0011   0.0003   0.0005  -0.0002   0.0003
        Y  -0.0015   0.0015  -0.0003  -0.0005  -0.0001  -0.0006
        Z   0.0009  -0.0007   0.0005   0.0013   0.0005   0.0015
AT. 11 CA X  -0.0006   0.0011   0.0003   0.0005   0.0002   0.0003
        Y   0.0015   0.0015  -0.0003  -0.0005   0.0001  -0.0006
        Z   0.0009   0.0007  -0.0005  -0.0013   0.0005  -0.0015
AT. 12 CA X   0.0006  -0.0011  -0.0003   0.0005  -0.0002  -0.0003
        Y   0.0015   0.0015  -0.0003   0.0005   0.0001  -0.0006
        Z   0.0009   0.0007  -0.0005   0.0013   0.0005  -0.0015
AT. 13 SI X   0.0000   0.0003   0.0111  -0.0139   0.0000   0.0004
        Y   0.0000   0.0003  -0.0009   0.0005   0.0000  -0.0026
        Z  -0.0003   0.0000   0.0000   0.0000   0.0074   0.0000
AT. 14 SI X   0.0000  -0.0003  -0.0111  -0.0139   0.0000  -0.0004
        Y   0.0000   0.0003  -0.0009  -0.0005   0.0000  -0.0026
        Z  -0.0003   0.0000   0.0000   0.0000   0.0074   0.0000
AT. 15 SI X   0.0101  -0.0083  -0.0040   0.0004   0.0049   0.0041
        Y   0.0076  -0.0080  -0.0021  -0.0002   0.0024   0.0017
        Z   0.0139  -0.0140  -0.0130   0.0004   0.0144   0.0058
AT. 16 SI X  -0.0101   0.0083   0.0040   0.0004  -0.0049  -0.0041
        Y   0.0076  -0.0080  -0.0021   0.0002   0.0024   0.0017
        Z   0.0139  -0.0140  -0.0130  -0.0004   0.0144   0.0058
AT. 17 SI X   0.0101   0.0083   0.0040   0.0004   0.0049  -0.0041
        Y  -0.0076  -0.0080  -0.0021   0.0002  -0.0024   0.0017
        Z   0.0139   0.0140   0.0130   0.0004   0.0144  -0.0058
AT. 18 SI X  -0.0101  -0.0083  -0.0040   0.0004  -0.0049   0.0041
        Y  -0.0076  -0.0080  -0.0021  -0.0002  -0.0024   0.0017
        Z   0.0139   0.0140   0.0130  -0.0004   0.0144  -0.0058
AT. 19 SI X   0.0000   0.0000   0.0000   0.0002   0.0000   0.0000
        Y   0.0215  -0.0226   0.0029   0.0000  -0.0053  -0.0023
        Z  -0.0161   0.0155  -0.0048   0.0000   0.0049   0.0039
AT. 20 SI X   0.0000   0.0000   0.0000   0.0002   0.0000   0.0000
        Y  -0.0215  -0.0226   0.0029   0.0000   0.0053  -0.0023
        Z  -0.0161  -0.0155   0.0048   0.0000   0.0049  -0.0039
AT. 21 O  X   0.0023   0.0013   0.0042  -0.0103   0.0043   0.0118
        Y  -0.0003  -0.0003  -0.0021   0.0069  -0.0032  -0.0086
        Z  -0.0015   0.0033  -0.0071   0.0198  -0.0068  -0.0255
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AT. 22 O  X   -0.0023  -0.0013  -0.0042  -0.0103  -0.0043  -0.0118
        Y   -0.0003  -0.0003  -0.0021  -0.0069  -0.0032  -0.0086
        Z   -0.0015   0.0033  -0.0071  -0.0198  -0.0068  -0.0255
AT. 23 O  X    0.0023  -0.0013  -0.0042  -0.0103   0.0043  -0.0118
        Y    0.0003  -0.0003  -0.0021  -0.0069   0.0032  -0.0086
        Z   -0.0015  -0.0033   0.0071   0.0198  -0.0068   0.0255
AT. 24 O  X   -0.0023   0.0013   0.0042  -0.0103  -0.0043   0.0118
        Y    0.0003  -0.0003  -0.0021   0.0069   0.0032  -0.0086
        Z   -0.0015  -0.0033   0.0071  -0.0198  -0.0068   0.0255
AT. 25 O  X    0.0000  -0.0021  -0.0278   0.0446   0.0000  -0.0262
        Y    0.0000  -0.0014  -0.0090   0.0145   0.0000  -0.0082
        Z    0.0034   0.0000   0.0000   0.0000   0.0014   0.0000
AT. 26 O  X    0.0000   0.0021   0.0278   0.0446   0.0000   0.0262
        Y    0.0000  -0.0014  -0.0090  -0.0145   0.0000  -0.0082
        Z    0.0034   0.0000   0.0000   0.0000   0.0014   0.0000
AT. 27 O  X    0.0000   0.0015  -0.0001   0.0018   0.0000  -0.0021
        Y    0.0000  -0.0002   0.0153  -0.0304   0.0000   0.0304
        Z    0.0016   0.0000   0.0000   0.0000   0.0014   0.0000
AT. 28 O  X    0.0000  -0.0015   0.0001   0.0018   0.0000   0.0021
        Y    0.0000  -0.0002   0.0153   0.0304   0.0000   0.0304
        Z    0.0016   0.0000   0.0000   0.0000   0.0014   0.0000
AT. 29 O  X   -0.0060   0.0073  -0.0091   0.0003   0.0115   0.0045
        Y   -0.0059   0.0059  -0.0088   0.0000   0.0103   0.0039
        Z    0.0032  -0.0026   0.0165  -0.0007  -0.0190  -0.0073
AT. 30 O  X    0.0060  -0.0073   0.0091   0.0003  -0.0115  -0.0045
        Y   -0.0059   0.0059  -0.0088   0.0000   0.0103   0.0039
        Z    0.0032  -0.0026   0.0165   0.0007  -0.0190  -0.0073
AT. 31 O  X   -0.0060  -0.0073   0.0091   0.0003   0.0115  -0.0045
        Y    0.0059   0.0059  -0.0088   0.0000  -0.0103   0.0039
        Z    0.0032   0.0026  -0.0165  -0.0007  -0.0190   0.0073
AT. 32 O  X    0.0060   0.0073  -0.0091   0.0003  -0.0115   0.0045
        Y    0.0059   0.0059  -0.0088   0.0000  -0.0103   0.0039
        Z    0.0032   0.0026  -0.0165   0.0007  -0.0190   0.0073
AT. 33 O  X    0.0045   0.0069  -0.0109  -0.0012  -0.0147   0.0078
        Y    0.0052   0.0067  -0.0052  -0.0008  -0.0067   0.0038
        Z   -0.0047  -0.0050   0.0013   0.0006   0.0021  -0.0019
AT. 34 O  X   -0.0045  -0.0069   0.0109  -0.0012   0.0147  -0.0078
        Y    0.0052   0.0067  -0.0052   0.0008  -0.0067   0.0038
        Z   -0.0047  -0.0050   0.0013  -0.0006   0.0021  -0.0019
AT. 35 O  X    0.0045  -0.0069   0.0109  -0.0012  -0.0147  -0.0078
        Y   -0.0052   0.0067  -0.0052   0.0008   0.0067   0.0038
        Z   -0.0047   0.0050  -0.0013   0.0006   0.0021   0.0019
AT. 36 O  X   -0.0045   0.0069  -0.0109  -0.0012   0.0147   0.0078
        Y   -0.0052   0.0067  -0.0052  -0.0008   0.0067   0.0038
        Z   -0.0047   0.0050  -0.0013  -0.0006   0.0021   0.0019
AT. 37 O  X   -0.0056   0.0046   0.0129  -0.0004  -0.0138  -0.0088
        Y   -0.0276   0.0276  -0.0024   0.0003   0.0031   0.0019
        Z   -0.0139   0.0121   0.0144  -0.0006  -0.0161  -0.0098
AT. 38 O  X    0.0056  -0.0046  -0.0129  -0.0004   0.0138   0.0088
        Y   -0.0276   0.0276  -0.0024  -0.0003   0.0031   0.0019
        Z   -0.0139   0.0121   0.0144   0.0006  -0.0161  -0.0098
AT. 39 O  X   -0.0056  -0.0046  -0.0129  -0.0004  -0.0138   0.0088
        Y    0.0276   0.0276  -0.0024  -0.0003  -0.0031   0.0019
        Z   -0.0139  -0.0121  -0.0144  -0.0006  -0.0161   0.0098
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AT. 40 O  X    0.0056   0.0046   0.0129  -0.0004   0.0138  -0.0088
          Y    0.0276   0.0276  -0.0024   0.0003  -0.0031   0.0019
          Z   -0.0139  -0.0121  -0.0144   0.0006  -0.0161   0.0098
AT. 41 O  X   -0.0014   0.0021   0.0000   0.0002   0.0006   0.0001
          Y    0.0132  -0.0136   0.0154  -0.0006  -0.0191  -0.0090
          Z   -0.0005   0.0010   0.0001  -0.0003  -0.0002   0.0001
AT. 42 O  X    0.0014  -0.0021   0.0000   0.0002  -0.0006  -0.0001
          Y    0.0132  -0.0136   0.0154   0.0006  -0.0191  -0.0090
          Z   -0.0005   0.0010   0.0001   0.0003  -0.0002   0.0001
AT. 43 O  X   -0.0014  -0.0021   0.0000   0.0002   0.0006  -0.0001
          Y   -0.0132  -0.0136   0.0154   0.0006   0.0191  -0.0090
          Z   -0.0005  -0.0010  -0.0001  -0.0003  -0.0002  -0.0001
AT. 44 O  X    0.0014   0.0021   0.0000   0.0002  -0.0006   0.0001
          Y   -0.0132  -0.0136   0.0154  -0.0006   0.0191  -0.0090
          Z   -0.0005  -0.0010  -0.0001   0.0003  -0.0002  -0.0001
AT. 45 O  X   -0.0053   0.0046   0.0006   0.0001  -0.0017  -0.0003
          Y   -0.0026   0.0029   0.0021   0.0000  -0.0005  -0.0015
          Z    0.0057  -0.0052  -0.0014   0.0000   0.0013   0.0008
AT. 46 O  X    0.0053  -0.0046  -0.0006   0.0001   0.0017   0.0003
          Y   -0.0026   0.0029   0.0021   0.0000  -0.0005  -0.0015
          Z    0.0057  -0.0052  -0.0014   0.0000   0.0013   0.0008
AT. 47 O  X   -0.0053  -0.0046  -0.0006   0.0001  -0.0017   0.0003
          Y    0.0026   0.0029   0.0021   0.0000   0.0005  -0.0015
          Z    0.0057   0.0052   0.0014   0.0000   0.0013  -0.0008
AT. 48 O  X    0.0053   0.0046   0.0006   0.0001   0.0017  -0.0003
          Y    0.0026   0.0029   0.0021   0.0000   0.0005  -0.0015
          Z    0.0057   0.0052   0.0014   0.0000   0.0013  -0.0008


FREQ(CM**-1)   848.30   850.95   864.05   882.44   884.51   888.48


AT.  1 CA X    0.0015  -0.0003  -0.0003   0.0000  -0.0001   0.0000
          Y    0.0000   0.0000   0.0000   0.0000   0.0000  -0.0006
          Z    0.0000   0.0000   0.0000   0.0008   0.0000   0.0007
AT.  2 CA X   -0.0015  -0.0003  -0.0003   0.0000   0.0001   0.0000
          Y    0.0000   0.0000   0.0000   0.0000   0.0000   0.0006
          Z    0.0000   0.0000   0.0000  -0.0008   0.0000   0.0007
AT.  3 CA X    0.0000   0.0008  -0.0009  -0.0007   0.0000   0.0000
          Y    0.0000  -0.0003  -0.0003  -0.0005   0.0000   0.0000
          Z   -0.0005   0.0000   0.0000   0.0000   0.0012   0.0006
AT.  4 CA X    0.0000   0.0008  -0.0009   0.0007   0.0000   0.0000
          Y    0.0000   0.0003   0.0003  -0.0005   0.0000   0.0000
          Z    0.0005   0.0000   0.0000   0.0000  -0.0012   0.0006
AT.  5 CA X    0.0001  -0.0005   0.0002  -0.0009  -0.0008  -0.0006
          Y    0.0000   0.0003  -0.0007   0.0004  -0.0005  -0.0006
          Z    0.0005  -0.0005  -0.0017   0.0008  -0.0004  -0.0006
AT.  6 CA X    0.0001  -0.0005   0.0002   0.0009  -0.0008   0.0006
          Y    0.0000  -0.0003   0.0007   0.0004   0.0005  -0.0006
          Z   -0.0005   0.0005   0.0017   0.0008   0.0004  -0.0006
AT.  7 CA X   -0.0001  -0.0005   0.0002   0.0009   0.0008  -0.0006
          Y    0.0000  -0.0003   0.0007   0.0004  -0.0005   0.0006
          Z   -0.0005  -0.0005  -0.0017  -0.0008   0.0004  -0.0006
AT.  8 CA X   -0.0001  -0.0005   0.0002  -0.0009   0.0008   0.0006
          Y    0.0000   0.0003  -0.0007   0.0004   0.0005   0.0006
          Z    0.0005   0.0005   0.0017  -0.0008  -0.0004  -0.0006
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AT.  9 CA X   0.0010   0.0000   0.0002  -0.0005   0.0001   0.0001
        Y   0.0001   0.0004   0.0006   0.0001   0.0000   0.0005
        Z  -0.0006  -0.0007  -0.0008  -0.0002  -0.0001  -0.0006
AT. 10 CA X   0.0010   0.0000   0.0002   0.0005   0.0001  -0.0001
        Y  -0.0001  -0.0004  -0.0006   0.0001   0.0000   0.0005
        Z   0.0006   0.0007   0.0008  -0.0002   0.0001  -0.0006
AT. 11 CA X  -0.0010   0.0000   0.0002   0.0005  -0.0001   0.0001
        Y   0.0001  -0.0004  -0.0006   0.0001   0.0000  -0.0005
        Z   0.0006  -0.0007  -0.0008   0.0002   0.0001  -0.0006
AT. 12 CA X  -0.0010   0.0000   0.0002  -0.0005  -0.0001  -0.0001
        Y  -0.0001   0.0004   0.0006   0.0001   0.0000  -0.0005
        Z  -0.0006   0.0007   0.0008   0.0002  -0.0001  -0.0006
AT. 13 SI X   0.0000  -0.0143   0.0259  -0.0273   0.0000   0.0000
        Y   0.0000  -0.0007   0.0065  -0.0051   0.0000   0.0000
        Z   0.0032   0.0000   0.0000   0.0000   0.0303   0.0212
AT. 14 SI X   0.0000  -0.0143   0.0259   0.0273   0.0000   0.0000
        Y   0.0000   0.0007  -0.0065  -0.0051   0.0000   0.0000
        Z  -0.0032   0.0000   0.0000   0.0000  -0.0303   0.0212
AT. 15 SI X  -0.0011  -0.0050  -0.0040  -0.0104  -0.0068   0.0003
        Y  -0.0039  -0.0040  -0.0029  -0.0036   0.0000  -0.0027
        Z  -0.0130  -0.0094  -0.0030   0.0003   0.0050  -0.0040
AT. 16 SI X  -0.0011  -0.0050  -0.0040   0.0104  -0.0068  -0.0003
        Y   0.0039   0.0040   0.0029  -0.0036   0.0000  -0.0027
        Z   0.0130   0.0094   0.0030   0.0003  -0.0050  -0.0040
AT. 17 SI X   0.0011  -0.0050  -0.0040   0.0104   0.0068   0.0003
        Y  -0.0039   0.0040   0.0029  -0.0036   0.0000   0.0027
        Z   0.0130  -0.0094  -0.0030  -0.0003  -0.0050  -0.0040
AT. 18 SI X   0.0011  -0.0050  -0.0040  -0.0104   0.0068  -0.0003
        Y   0.0039  -0.0040  -0.0029  -0.0036   0.0000   0.0027
        Z  -0.0130   0.0094   0.0030  -0.0003   0.0050  -0.0040
AT. 19 SI X  -0.0041  -0.0045   0.0001   0.0000  -0.0014   0.0000
        Y   0.0000   0.0000   0.0000  -0.0009   0.0000  -0.0091
        Z   0.0000   0.0000   0.0000   0.0000   0.0000   0.0120
AT. 20 SI X   0.0041  -0.0045   0.0001   0.0000   0.0014   0.0000
        Y   0.0000   0.0000   0.0000  -0.0009   0.0000   0.0091
        Z   0.0000   0.0000   0.0000   0.0000   0.0000   0.0120
AT. 21 O  X   0.0017   0.0069  -0.0118   0.0121   0.0143   0.0100
        Y  -0.0007  -0.0041   0.0072  -0.0059  -0.0099  -0.0068
        Z  -0.0023  -0.0104   0.0216  -0.0145  -0.0266  -0.0184
AT. 22 O  X   0.0017   0.0069  -0.0118  -0.0121   0.0143  -0.0100
        Y   0.0007   0.0041  -0.0072  -0.0059   0.0099  -0.0068
        Z   0.0023   0.0104  -0.0216  -0.0145   0.0266  -0.0184
AT. 23 O  X  -0.0017   0.0069  -0.0118  -0.0121  -0.0143   0.0100
        Y  -0.0007   0.0041  -0.0072  -0.0059  -0.0099   0.0068
        Z   0.0023  -0.0104   0.0216   0.0145   0.0266  -0.0184
AT. 24 O  X  -0.0017   0.0069  -0.0118   0.0121  -0.0143  -0.0100
        Y   0.0007  -0.0041   0.0072  -0.0059   0.0099   0.0068
        Z  -0.0023   0.0104  -0.0216   0.0145  -0.0266  -0.0184
AT. 25 O  X   0.0000   0.0111  -0.0213   0.0274   0.0000   0.0000
        Y   0.0000   0.0038  -0.0072   0.0089   0.0000   0.0000
        Z   0.0002   0.0000   0.0000   0.0000  -0.0015  -0.0016
AT. 26 O  X   0.0000   0.0111  -0.0213  -0.0274   0.0000   0.0000
        Y   0.0000  -0.0038   0.0072   0.0089   0.0000   0.0000
        Z  -0.0002   0.0000   0.0000   0.0000   0.0015  -0.0016
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AT. 27 O  X    0.0000   0.0016  -0.0021   0.0043   0.0000   0.0000
         Y    0.0000   0.0053  -0.0176   0.0110   0.0000   0.0000
         Z   -0.0004   0.0000   0.0000   0.0000  -0.0030  -0.0027
AT. 28 O  X    0.0000   0.0016  -0.0021  -0.0043   0.0000   0.0000
         Y    0.0000  -0.0053   0.0176   0.0110   0.0000   0.0000
         Z    0.0004   0.0000   0.0000   0.0000   0.0030  -0.0027
AT. 29 O  X   -0.0129  -0.0101  -0.0019   0.0023   0.0023  -0.0060
         Y   -0.0109  -0.0081  -0.0021   0.0022   0.0034  -0.0045
         Z    0.0245   0.0179   0.0079  -0.0013  -0.0074   0.0128
AT. 30 O  X   -0.0129  -0.0101  -0.0019  -0.0023   0.0023   0.0060
         Y    0.0109   0.0081   0.0021   0.0022  -0.0034  -0.0045
         Z   -0.0245  -0.0179  -0.0079  -0.0013   0.0074   0.0128
AT. 31 O  X    0.0129  -0.0101  -0.0019  -0.0023  -0.0023  -0.0060
         Y   -0.0109   0.0081   0.0021   0.0022   0.0034   0.0045
         Z   -0.0245   0.0179   0.0079   0.0013   0.0074   0.0128
AT. 32 O  X    0.0129  -0.0101  -0.0019   0.0023  -0.0023   0.0060
         Y    0.0109  -0.0081  -0.0021   0.0022  -0.0034   0.0045
         Z    0.0245  -0.0179  -0.0079   0.0013  -0.0074   0.0128
AT. 33 O  X   -0.0161   0.0191   0.0110  -0.0142  -0.0086   0.0107
         Y   -0.0060   0.0076   0.0048  -0.0064  -0.0042   0.0027
         Z    0.0010  -0.0006   0.0004   0.0009   0.0025   0.0015
AT. 34 O  X   -0.0161   0.0191   0.0110   0.0142  -0.0086  -0.0107
         Y    0.0060  -0.0076  -0.0048  -0.0064   0.0042   0.0027
         Z   -0.0010   0.0006  -0.0004   0.0009  -0.0025   0.0015
AT. 35 O  X    0.0161   0.0191   0.0110   0.0142   0.0086   0.0107
         Y   -0.0060  -0.0076  -0.0048  -0.0064  -0.0042  -0.0027
         Z   -0.0010  -0.0006   0.0004  -0.0009  -0.0025   0.0015
AT. 36 O  X    0.0161   0.0191   0.0110  -0.0142   0.0086  -0.0107
         Y    0.0060   0.0076   0.0048  -0.0064   0.0042  -0.0027
         Z    0.0010   0.0006  -0.0004  -0.0009   0.0025   0.0015
AT. 37 O  X   -0.0006   0.0005  -0.0033   0.0029   0.0011  -0.0142
         Y   -0.0006  -0.0014   0.0015   0.0007  -0.0011   0.0067
         Z    0.0010   0.0029  -0.0030   0.0037   0.0011  -0.0154
AT. 38 O  X   -0.0006   0.0005  -0.0033  -0.0029   0.0011   0.0142
         Y    0.0006   0.0014  -0.0015   0.0007   0.0011   0.0067
         Z   -0.0010  -0.0029   0.0030   0.0037  -0.0011  -0.0154
AT. 39 O  X    0.0006   0.0005  -0.0033  -0.0029  -0.0011  -0.0142
         Y   -0.0006   0.0014  -0.0015   0.0007  -0.0011  -0.0067
         Z   -0.0010   0.0029  -0.0030  -0.0037  -0.0011  -0.0154
AT. 40 O  X    0.0006   0.0005  -0.0033   0.0029  -0.0011   0.0142
         Y    0.0006  -0.0014   0.0015   0.0007   0.0011  -0.0067
         Z    0.0010  -0.0029   0.0030  -0.0037   0.0011  -0.0154
AT. 41 O  X    0.0002  -0.0007   0.0002   0.0002  -0.0009  -0.0003
         Y    0.0236   0.0227   0.0117   0.0089   0.0006   0.0126
         Z    0.0014   0.0015   0.0014   0.0012  -0.0005   0.0012
AT. 42 O  X    0.0002  -0.0007   0.0002  -0.0002  -0.0009   0.0003
         Y   -0.0236  -0.0227  -0.0117   0.0089  -0.0006   0.0126
         Z   -0.0014  -0.0015  -0.0014   0.0012   0.0005   0.0012
AT. 43 O  X   -0.0002  -0.0007   0.0002  -0.0002   0.0009  -0.0003
         Y    0.0236  -0.0227  -0.0117   0.0089   0.0006  -0.0126
         Z   -0.0014   0.0015   0.0014  -0.0012   0.0005   0.0012
AT. 44 O  X   -0.0002  -0.0007   0.0002   0.0002   0.0009   0.0003
         Y   -0.0236   0.0227   0.0117   0.0089  -0.0006  -0.0126
         Z    0.0014  -0.0015  -0.0014  -0.0012  -0.0005   0.0012
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AT. 45 O  X   0.0036   0.0038   0.0022   0.0006   0.0006   0.0005
        Y  -0.0072  -0.0066  -0.0043   0.0012   0.0010  -0.0006
        Z  -0.0070  -0.0054  -0.0042  -0.0005   0.0014  -0.0006
AT. 46 O  X   0.0036   0.0038   0.0022  -0.0006   0.0006  -0.0005
        Y   0.0072   0.0066   0.0043   0.0012  -0.0010  -0.0006
        Z   0.0070   0.0054   0.0042  -0.0005  -0.0014  -0.0006
AT. 47 O  X  -0.0036   0.0038   0.0022  -0.0006  -0.0006   0.0005
        Y  -0.0072   0.0066   0.0043   0.0012   0.0010   0.0006
        Z   0.0070  -0.0054  -0.0042   0.0005  -0.0014  -0.0006
AT. 48 O  X  -0.0036   0.0038   0.0022   0.0006  -0.0006  -0.0005
        Y   0.0072  -0.0066  -0.0043   0.0012  -0.0010   0.0006
        Z  -0.0070   0.0054   0.0042   0.0005   0.0014  -0.0006


FREQ(CM**-1)   896.00   897.65   903.84   915.95   922.86   932.31


AT.  1 CA X   0.0000  -0.0008  -0.0016   0.0000   0.0000  -0.0001
        Y  -0.0007   0.0000   0.0000   0.0006   0.0000   0.0000
        Z   0.0013   0.0000   0.0000  -0.0018  -0.0003   0.0000
AT.  2 CA X   0.0000  -0.0008   0.0016   0.0000   0.0000  -0.0001
        Y  -0.0007   0.0000   0.0000  -0.0006   0.0000   0.0000
        Z  -0.0013   0.0000   0.0000  -0.0018  -0.0003   0.0000
AT.  3 CA X  -0.0006   0.0002   0.0000   0.0000   0.0000   0.0001
        Y   0.0004   0.0000   0.0000   0.0000   0.0000   0.0007
        Z   0.0000   0.0000  -0.0011   0.0021  -0.0013   0.0000
AT.  4 CA X   0.0006   0.0002   0.0000   0.0000   0.0000   0.0001
        Y   0.0004   0.0000   0.0000   0.0000   0.0000  -0.0007
        Z   0.0000   0.0000   0.0011   0.0021  -0.0013   0.0000
AT.  5 CA X  -0.0002  -0.0001   0.0007  -0.0002  -0.0004  -0.0002
        Y  -0.0002  -0.0001   0.0004   0.0000  -0.0001   0.0007
        Z  -0.0007   0.0000   0.0005   0.0008   0.0001   0.0001
AT.  6 CA X   0.0002  -0.0001   0.0007   0.0002   0.0004  -0.0002
        Y  -0.0002   0.0001  -0.0004   0.0000  -0.0001  -0.0007
        Z  -0.0007   0.0000  -0.0005   0.0008   0.0001  -0.0001
AT.  7 CA X   0.0002  -0.0001  -0.0007  -0.0002  -0.0004  -0.0002
        Y  -0.0002   0.0001   0.0004   0.0000   0.0001  -0.0007
        Z   0.0007   0.0000  -0.0005   0.0008   0.0001   0.0001
AT.  8 CA X  -0.0002  -0.0001  -0.0007   0.0002   0.0004  -0.0002
        Y  -0.0002  -0.0001  -0.0004   0.0000   0.0001   0.0007
        Z   0.0007   0.0000   0.0005   0.0008   0.0001  -0.0001
AT.  9 CA X  -0.0014  -0.0001   0.0011   0.0001   0.0005   0.0003
        Y  -0.0002   0.0005   0.0006  -0.0004   0.0005   0.0001
        Z   0.0004   0.0012   0.0015   0.0000   0.0004   0.0001
AT. 10 CA X   0.0014  -0.0001   0.0011  -0.0001  -0.0005   0.0003
        Y  -0.0002  -0.0005  -0.0006  -0.0004   0.0005  -0.0001
        Z   0.0004  -0.0012  -0.0015   0.0000   0.0004  -0.0001
AT. 11 CA X   0.0014  -0.0001  -0.0011   0.0001   0.0005   0.0003
        Y  -0.0002  -0.0005   0.0006   0.0004  -0.0005  -0.0001
        Z  -0.0004   0.0012  -0.0015   0.0000   0.0004   0.0001
AT. 12 CA X  -0.0014  -0.0001  -0.0011  -0.0001  -0.0005   0.0003
        Y  -0.0002   0.0005  -0.0006   0.0004  -0.0005   0.0001
        Z  -0.0004  -0.0012   0.0015   0.0000   0.0004  -0.0001
AT. 13 SI X   0.0007  -0.0023   0.0000   0.0000   0.0000   0.0033
        Y  -0.0030  -0.0028   0.0000   0.0000   0.0000  -0.0308
        Z   0.0000   0.0000  -0.0029   0.0213  -0.0074   0.0000
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AT. 14 SI X  -0.0007  -0.0023   0.0000   0.0000   0.0000   0.0033
        Y  -0.0030   0.0028   0.0000   0.0000   0.0000   0.0308
        Z   0.0000   0.0000   0.0029   0.0213  -0.0074   0.0000
AT. 15 SI X  -0.0045   0.0106  -0.0018  -0.0077  -0.0172  -0.0060
        Y   0.0033   0.0016  -0.0004  -0.0007  -0.0053  -0.0023
        Z   0.0036   0.0038   0.0113   0.0018   0.0114   0.0045
AT. 16 SI X   0.0045   0.0106  -0.0018   0.0077   0.0172  -0.0060
        Y   0.0033  -0.0016   0.0004  -0.0007  -0.0053   0.0023
        Z   0.0036  -0.0038  -0.0113   0.0018   0.0114  -0.0045
AT. 17 SI X   0.0045   0.0106   0.0018  -0.0077  -0.0172  -0.0060
        Y   0.0033  -0.0016  -0.0004   0.0007   0.0053   0.0023
        Z  -0.0036   0.0038  -0.0113   0.0018   0.0114   0.0045
AT. 18 SI X  -0.0045   0.0106   0.0018   0.0077   0.0172  -0.0060
        Y   0.0033   0.0016   0.0004   0.0007   0.0053  -0.0023
        Z  -0.0036  -0.0038   0.0113   0.0018   0.0114  -0.0045
AT. 19 SI X   0.0000   0.0104   0.0076   0.0000   0.0000   0.0004
        Y   0.0131   0.0000   0.0000   0.0155  -0.0037   0.0000
        Z  -0.0149   0.0000   0.0000  -0.0048   0.0033   0.0000
AT. 20 SI X   0.0000   0.0104  -0.0076   0.0000   0.0000   0.0004
        Y   0.0131   0.0000   0.0000  -0.0155   0.0037   0.0000
        Z   0.0149   0.0000   0.0000  -0.0048   0.0033   0.0000
AT. 21 O  X   0.0002   0.0013  -0.0021   0.0089  -0.0037  -0.0080
        Y   0.0001  -0.0005   0.0008  -0.0062   0.0023   0.0052
        Z   0.0000  -0.0014   0.0025  -0.0188   0.0064   0.0127
AT. 22 O  X  -0.0002   0.0013  -0.0021  -0.0089   0.0037  -0.0080
        Y   0.0001   0.0005  -0.0008  -0.0062   0.0023  -0.0052
        Z   0.0000   0.0014  -0.0025  -0.0188   0.0064  -0.0127
AT. 23 O  X  -0.0002   0.0013   0.0021   0.0089  -0.0037  -0.0080
        Y   0.0001   0.0005   0.0008   0.0062  -0.0023  -0.0052
        Z   0.0000  -0.0014  -0.0025  -0.0188   0.0064   0.0127
AT. 24 O  X   0.0002   0.0013   0.0021  -0.0089   0.0037  -0.0080
        Y   0.0001  -0.0005  -0.0008   0.0062  -0.0023   0.0052
        Z   0.0000   0.0014   0.0025  -0.0188   0.0064  -0.0127
AT. 25 O  X  -0.0013   0.0020   0.0000   0.0000   0.0000   0.0093
        Y  -0.0002   0.0008   0.0000   0.0000   0.0000   0.0032
        Z   0.0000   0.0000  -0.0011  -0.0034   0.0014   0.0000
AT. 26 O  X   0.0013   0.0020   0.0000   0.0000   0.0000   0.0093
        Y  -0.0002  -0.0008   0.0000   0.0000   0.0000  -0.0032
        Z   0.0000   0.0000   0.0011  -0.0034   0.0014   0.0000
AT. 27 O  X  -0.0003   0.0004   0.0000   0.0000   0.0000  -0.0007
        Y   0.0050   0.0047   0.0000   0.0000   0.0000   0.0356
        Z   0.0000   0.0000   0.0002  -0.0040   0.0015   0.0000
AT. 28 O  X   0.0003   0.0004   0.0000   0.0000   0.0000  -0.0007
        Y   0.0050  -0.0047   0.0000   0.0000   0.0000  -0.0356
        Z   0.0000   0.0000  -0.0002  -0.0040   0.0015   0.0000
AT. 29 O  X   0.0078  -0.0042   0.0025   0.0050   0.0084   0.0038
        Y   0.0056  -0.0024   0.0029   0.0037   0.0069   0.0025
        Z  -0.0166   0.0078  -0.0034  -0.0117  -0.0135  -0.0060
AT. 30 O  X  -0.0078  -0.0042   0.0025  -0.0050  -0.0084   0.0038
        Y   0.0056   0.0024  -0.0029   0.0037   0.0069  -0.0025
        Z  -0.0166  -0.0078   0.0034  -0.0117  -0.0135   0.0060
AT. 31 O  X  -0.0078  -0.0042  -0.0025   0.0050   0.0084   0.0038
        Y   0.0056   0.0024   0.0029  -0.0037  -0.0069  -0.0025
        Z   0.0166   0.0078   0.0034  -0.0117  -0.0135  -0.0060
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AT. 32 O  X    0.0078  -0.0042  -0.0025  -0.0050  -0.0084   0.0038
        Y    0.0056  -0.0024  -0.0029  -0.0037  -0.0069   0.0025
        Z    0.0166  -0.0078  -0.0034  -0.0117  -0.0135   0.0060
AT. 33 O  X    0.0081  -0.0029  -0.0116   0.0027   0.0232   0.0068
        Y    0.0015  -0.0025  -0.0032   0.0017   0.0089   0.0030
        Z    0.0011   0.0007  -0.0001  -0.0006  -0.0031  -0.0010
AT. 34 O  X   -0.0081  -0.0029  -0.0116  -0.0027  -0.0232   0.0068
        Y    0.0015   0.0025   0.0032   0.0017   0.0089  -0.0030
        Z    0.0011  -0.0007   0.0001  -0.0006  -0.0031   0.0010
AT. 35 O  X   -0.0081  -0.0029   0.0116   0.0027   0.0232   0.0068
        Y    0.0015   0.0025  -0.0032  -0.0017  -0.0089  -0.0030
        Z   -0.0011   0.0007   0.0001  -0.0006  -0.0031  -0.0010
AT. 36 O  X    0.0081  -0.0029   0.0116  -0.0027  -0.0232   0.0068
        Y    0.0015  -0.0025   0.0032  -0.0017  -0.0089   0.0030
        Z   -0.0011  -0.0007  -0.0001  -0.0006  -0.0031   0.0010
AT. 37 O  X    0.0201  -0.0246  -0.0233   0.0142  -0.0042  -0.0003
        Y   -0.0086   0.0091   0.0085  -0.0060   0.0022   0.0003
        Z    0.0228  -0.0287  -0.0271   0.0176  -0.0056  -0.0010
AT. 38 O  X   -0.0201  -0.0246  -0.0233  -0.0142   0.0042  -0.0003
        Y   -0.0086  -0.0091  -0.0085  -0.0060   0.0022  -0.0003
        Z    0.0228   0.0287   0.0271   0.0176  -0.0056   0.0010
AT. 39 O  X   -0.0201  -0.0246   0.0233   0.0142  -0.0042  -0.0003
        Y   -0.0086  -0.0091   0.0085   0.0060  -0.0022  -0.0003
        Z   -0.0228  -0.0287   0.0271   0.0176  -0.0056  -0.0010
AT. 40 O  X    0.0201  -0.0246   0.0233  -0.0142   0.0042  -0.0003
        Y   -0.0086   0.0091  -0.0085   0.0060  -0.0022   0.0003
        Z   -0.0228   0.0287  -0.0271   0.0176  -0.0056   0.0010
AT. 41 O  X    0.0006  -0.0013  -0.0009   0.0002   0.0009   0.0007
        Y   -0.0144   0.0005   0.0042  -0.0021   0.0111   0.0044
        Z   -0.0004  -0.0015  -0.0017   0.0007  -0.0014  -0.0007
AT. 42 O  X   -0.0006  -0.0013  -0.0009  -0.0002  -0.0009   0.0007
        Y   -0.0144  -0.0005  -0.0042  -0.0021   0.0111  -0.0044
        Z   -0.0004   0.0015   0.0017   0.0007  -0.0014   0.0007
AT. 43 O  X   -0.0006  -0.0013   0.0009   0.0002   0.0009   0.0007
        Y   -0.0144  -0.0005   0.0042   0.0021  -0.0111  -0.0044
        Z    0.0004  -0.0015   0.0017   0.0007  -0.0014  -0.0007
AT. 44 O  X    0.0006  -0.0013   0.0009  -0.0002  -0.0009   0.0007
        Y   -0.0144   0.0005  -0.0042   0.0021  -0.0111   0.0044
        Z    0.0004   0.0015  -0.0017   0.0007  -0.0014   0.0007
AT. 45 O  X    0.0011   0.0061   0.0070   0.0062  -0.0011  -0.0003
        Y    0.0001  -0.0059  -0.0087  -0.0055   0.0000  -0.0006
        Z    0.0002  -0.0073  -0.0101  -0.0035   0.0003  -0.0008
AT. 46 O  X   -0.0011   0.0061   0.0070  -0.0062   0.0011  -0.0003
        Y    0.0001   0.0059   0.0087  -0.0055   0.0000   0.0006
        Z    0.0002   0.0073   0.0101  -0.0035   0.0003   0.0008
AT. 47 O  X   -0.0011   0.0061  -0.0070   0.0062  -0.0011  -0.0003
        Y    0.0001   0.0059  -0.0087   0.0055   0.0000   0.0006
        Z   -0.0002  -0.0073   0.0101  -0.0035   0.0003  -0.0008
AT. 48 O  X    0.0011   0.0061  -0.0070  -0.0062   0.0011  -0.0003
        Y    0.0001  -0.0059   0.0087   0.0055   0.0000  -0.0006
        Z   -0.0002   0.0073  -0.0101  -0.0035   0.0003   0.0008


FREQ(CM**-1)   934.85   947.57   948.72   959.90   975.30   977.69
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AT.  1 CA X    0.0000   0.0004   0.0012   0.0000   0.0004   0.0000
        Y    0.0001   0.0000   0.0000   0.0000   0.0000  -0.0007
        Z   -0.0003   0.0000   0.0000  -0.0003   0.0000   0.0000
AT.  2 CA X    0.0000   0.0004  -0.0012   0.0000   0.0004   0.0000
        Y    0.0001   0.0000   0.0000   0.0000   0.0000   0.0007
        Z    0.0003   0.0000   0.0000   0.0003   0.0000   0.0000
AT.  3 CA X    0.0009  -0.0003   0.0000   0.0000  -0.0001   0.0000
        Y    0.0006   0.0004   0.0000   0.0002   0.0003   0.0000
        Z    0.0000   0.0000  -0.0010   0.0000   0.0000   0.0000
AT.  4 CA X   -0.0009  -0.0003   0.0000   0.0000  -0.0001   0.0000
        Y    0.0006  -0.0004   0.0000   0.0002  -0.0003   0.0000
        Z    0.0000   0.0000   0.0010   0.0000   0.0000   0.0000
AT.  5 CA X    0.0000   0.0004   0.0010  -0.0018   0.0002   0.0001
        Y    0.0008   0.0001   0.0004  -0.0001   0.0007  -0.0006
        Z   -0.0002  -0.0014  -0.0002   0.0004  -0.0003  -0.0003
AT.  6 CA X    0.0000   0.0004   0.0010   0.0018   0.0002  -0.0001
        Y    0.0008  -0.0001  -0.0004  -0.0001  -0.0007  -0.0006
        Z   -0.0002   0.0014   0.0002   0.0004   0.0003  -0.0003
AT.  7 CA X    0.0000   0.0004  -0.0010   0.0018   0.0002   0.0001
        Y    0.0008  -0.0001   0.0004  -0.0001  -0.0007   0.0006
        Z    0.0002  -0.0014   0.0002  -0.0004  -0.0003  -0.0003
AT.  8 CA X    0.0000   0.0004  -0.0010  -0.0018   0.0002  -0.0001
        Y    0.0008   0.0001  -0.0004  -0.0001   0.0007   0.0006
        Z    0.0002   0.0014  -0.0002  -0.0004   0.0003  -0.0003
AT.  9 CA X    0.0004  -0.0005  -0.0001  -0.0004   0.0000  -0.0002
        Y    0.0000  -0.0004   0.0001  -0.0004  -0.0002   0.0005
        Z   -0.0004  -0.0018  -0.0005  -0.0008  -0.0001   0.0002
AT. 10 CA X   -0.0004  -0.0005  -0.0001   0.0004   0.0000   0.0002
        Y    0.0000   0.0004  -0.0001  -0.0004   0.0002   0.0005
        Z   -0.0004   0.0018   0.0005  -0.0008   0.0001   0.0002
AT. 11 CA X   -0.0004  -0.0005   0.0001   0.0004   0.0000  -0.0002
        Y    0.0000   0.0004   0.0001  -0.0004   0.0002  -0.0005
        Z    0.0004  -0.0018   0.0005   0.0008  -0.0001   0.0002
AT. 12 CA X    0.0004  -0.0005   0.0001  -0.0004   0.0000   0.0002
        Y    0.0000  -0.0004  -0.0001  -0.0004  -0.0002  -0.0005
        Z    0.0004   0.0018  -0.0005   0.0008   0.0001   0.0002
AT. 13 SI X    0.0043   0.0039   0.0000  -0.0126   0.0012   0.0000
        Y   -0.0323  -0.0097   0.0000  -0.0021  -0.0035   0.0000
        Z    0.0000   0.0000  -0.0077   0.0000   0.0000  -0.0012
AT. 14 SI X   -0.0043   0.0039   0.0000   0.0126   0.0012   0.0000
        Y   -0.0323   0.0097   0.0000  -0.0021   0.0035   0.0000
        Z    0.0000   0.0000   0.0077   0.0000   0.0000  -0.0012
AT. 15 SI X    0.0013   0.0146  -0.0122   0.0129  -0.0019   0.0076
        Y   -0.0015  -0.0014  -0.0148   0.0087   0.0188  -0.0214
        Z    0.0005  -0.0141   0.0057  -0.0114  -0.0042   0.0031
AT. 16 SI X   -0.0013   0.0146  -0.0122  -0.0129  -0.0019  -0.0076
        Y   -0.0015   0.0014   0.0148   0.0087  -0.0188  -0.0214
        Z    0.0005   0.0141  -0.0057  -0.0114   0.0042   0.0031
AT. 17 SI X   -0.0013   0.0146   0.0122  -0.0129  -0.0019   0.0076
        Y   -0.0015   0.0014  -0.0148   0.0087  -0.0188   0.0214
        Z   -0.0005  -0.0141  -0.0057   0.0114  -0.0042   0.0031
AT. 18 SI X    0.0013   0.0146   0.0122   0.0129  -0.0019  -0.0076
        Y   -0.0015  -0.0014   0.0148   0.0087   0.0188   0.0214
        Z   -0.0005   0.0141   0.0057   0.0114   0.0042   0.0031
```

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AT.  19 SI X    0.0000  -0.0002   0.0064   0.0000  -0.0145   0.0000
         Y   -0.0017   0.0000   0.0000   0.0090   0.0000   0.0025
         Z    0.0005   0.0000   0.0000   0.0033   0.0000   0.0022
AT.  20 SI X    0.0000  -0.0002  -0.0064   0.0000  -0.0145   0.0000
         Y   -0.0017   0.0000   0.0000   0.0090   0.0000  -0.0025
         Z   -0.0005   0.0000   0.0000  -0.0033   0.0000   0.0022
AT.  21 O  X   -0.0087  -0.0029  -0.0034   0.0055  -0.0011  -0.0003
         Y    0.0056   0.0019   0.0019  -0.0017   0.0009   0.0000
         Z    0.0149   0.0079   0.0070  -0.0039   0.0028   0.0010
AT.  22 O  X    0.0087  -0.0029  -0.0034  -0.0055  -0.0011   0.0003
         Y    0.0056  -0.0019  -0.0019  -0.0017  -0.0009   0.0000
         Z    0.0149  -0.0079  -0.0070  -0.0039  -0.0028   0.0010
AT.  23 O  X    0.0087  -0.0029   0.0034  -0.0055  -0.0011  -0.0003
         Y    0.0056  -0.0019   0.0019  -0.0017  -0.0009   0.0000
         Z   -0.0149   0.0079  -0.0070   0.0039   0.0028   0.0010
AT.  24 O  X   -0.0087  -0.0029   0.0034   0.0055  -0.0011   0.0003
         Y    0.0056   0.0019  -0.0019  -0.0017   0.0009   0.0000
         Z   -0.0149  -0.0079   0.0070   0.0039  -0.0028   0.0010
AT.  25 O  X    0.0096  -0.0007   0.0000   0.0149   0.0001   0.0000
         Y    0.0031   0.0010   0.0000   0.0033   0.0006   0.0000
         Z    0.0000   0.0000   0.0007   0.0000   0.0000   0.0001
AT.  26 O  X   -0.0096  -0.0007   0.0000  -0.0149   0.0001   0.0000
         Y    0.0031  -0.0010   0.0000   0.0033  -0.0006   0.0000
         Z    0.0000   0.0000  -0.0007   0.0000   0.0000   0.0001
AT.  27 O  X   -0.0007  -0.0001   0.0000   0.0044   0.0001   0.0000
         Y    0.0367   0.0101   0.0000   0.0027   0.0029   0.0000
         Z    0.0000   0.0000   0.0020   0.0000   0.0000   0.0007
AT.  28 O  X    0.0007  -0.0001   0.0000  -0.0044   0.0001   0.0000
         Y    0.0367  -0.0101   0.0000   0.0027  -0.0029   0.0000
         Z    0.0000   0.0000  -0.0020   0.0000   0.0000   0.0007
AT.  29 O  X   -0.0011  -0.0084   0.0084  -0.0098  -0.0041   0.0035
         Y   -0.0001  -0.0069   0.0059  -0.0068  -0.0037   0.0034
         Z    0.0006   0.0171  -0.0117   0.0161   0.0076  -0.0065
AT.  30 O  X    0.0011  -0.0084   0.0084   0.0098  -0.0041  -0.0035
         Y   -0.0001   0.0069  -0.0059  -0.0068   0.0037   0.0034
         Z    0.0006  -0.0171   0.0117   0.0161  -0.0076  -0.0065
AT.  31 O  X    0.0011  -0.0084  -0.0084   0.0098  -0.0041   0.0035
         Y   -0.0001   0.0069   0.0059  -0.0068   0.0037  -0.0034
         Z   -0.0006   0.0171   0.0117  -0.0161   0.0076  -0.0065
AT.  32 O  X   -0.0011  -0.0084  -0.0084  -0.0098  -0.0041  -0.0035
         Y   -0.0001  -0.0069  -0.0059  -0.0068  -0.0037  -0.0034
         Z   -0.0006  -0.0171  -0.0117  -0.0161  -0.0076  -0.0065
AT.  33 O  X    0.0009  -0.0196  -0.0106   0.0149   0.0065  -0.0161
         Y    0.0009  -0.0073  -0.0039   0.0050   0.0035  -0.0066
         Z    0.0003   0.0047   0.0012  -0.0018  -0.0004   0.0017
AT.  34 O  X   -0.0009  -0.0196  -0.0106  -0.0149   0.0065   0.0161
         Y    0.0009   0.0073   0.0039   0.0050  -0.0035  -0.0066
         Z    0.0003  -0.0047  -0.0012  -0.0018   0.0004   0.0017
AT.  35 O  X   -0.0009  -0.0196   0.0106  -0.0149   0.0065  -0.0161
         Y    0.0009   0.0073  -0.0039   0.0050  -0.0035   0.0066
         Z   -0.0003   0.0047  -0.0012   0.0018  -0.0004   0.0017
AT.  36 O  X    0.0009  -0.0196   0.0106   0.0149   0.0065   0.0161
         Y    0.0009  -0.0073   0.0039   0.0050   0.0035   0.0066
         Z   -0.0003  -0.0047   0.0012   0.0018   0.0004   0.0017
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AT. 37 O  X   -0.0017  0.0054  0.0064  0.0021  0.0021  0.0013
          Y    0.0007 -0.0013 -0.0008 -0.0020 -0.0021  0.0006
          Z   -0.0022  0.0080  0.0060  0.0038  0.0020  0.0019
AT. 38 O  X    0.0017  0.0054  0.0064 -0.0021  0.0021 -0.0013
          Y    0.0007  0.0013  0.0008 -0.0020  0.0021  0.0006
          Z   -0.0022 -0.0080 -0.0060  0.0038 -0.0020  0.0019
AT. 39 O  X    0.0017  0.0054 -0.0064 -0.0021  0.0021  0.0013
          Y    0.0007  0.0013 -0.0008 -0.0020  0.0021 -0.0006
          Z    0.0022  0.0080 -0.0060 -0.0038  0.0020  0.0019
AT. 40 O  X   -0.0017  0.0054 -0.0064  0.0021  0.0021 -0.0013
          Y    0.0007 -0.0013  0.0008 -0.0020 -0.0021 -0.0006
          Z    0.0022 -0.0080  0.0060 -0.0038 -0.0020  0.0019
AT. 41 O  X   -0.0002 -0.0006  0.0018 -0.0012  0.0003 -0.0011
          Y    0.0017  0.0011  0.0208 -0.0119 -0.0229  0.0242
          Z   -0.0006  0.0029 -0.0003  0.0020  0.0010 -0.0010
AT. 42 O  X    0.0002 -0.0006  0.0018  0.0012  0.0003  0.0011
          Y    0.0017 -0.0011 -0.0208 -0.0119  0.0229  0.0242
          Z   -0.0006 -0.0029  0.0003  0.0020 -0.0010 -0.0010
AT. 43 O  X    0.0002 -0.0006 -0.0018  0.0012  0.0003 -0.0011
          Y    0.0017 -0.0011  0.0208 -0.0119  0.0229 -0.0242
          Z    0.0006  0.0029  0.0003 -0.0020  0.0010 -0.0010
AT. 44 O  X   -0.0002 -0.0006 -0.0018 -0.0012  0.0003  0.0011
          Y    0.0017  0.0011 -0.0208 -0.0119 -0.0229 -0.0242
          Z    0.0006 -0.0029 -0.0003 -0.0020 -0.0010 -0.0010
AT. 45 O  X   -0.0008 -0.0022 -0.0078  0.0053  0.0102  0.0031
          Y    0.0004  0.0043  0.0095 -0.0058 -0.0119 -0.0024
          Z    0.0004  0.0050  0.0093 -0.0041 -0.0116 -0.0033
AT. 46 O  X    0.0008 -0.0022 -0.0078 -0.0053  0.0102 -0.0031
          Y    0.0004 -0.0043 -0.0095 -0.0058  0.0119 -0.0024
          Z    0.0004 -0.0050 -0.0093 -0.0041  0.0116 -0.0033
AT. 47 O  X    0.0008 -0.0022  0.0078 -0.0053  0.0102  0.0031
          Y    0.0004 -0.0043  0.0095 -0.0058  0.0119  0.0024
          Z   -0.0004  0.0050 -0.0093  0.0041 -0.0116 -0.0033
AT. 48 O  X   -0.0008 -0.0022  0.0078  0.0053  0.0102 -0.0031
          Y    0.0004  0.0043 -0.0095 -0.0058 -0.0119  0.0024
          Z   -0.0004 -0.0050  0.0093  0.0041  0.0116 -0.0033


FREQ(CM**-1)   982.23   994.82   999.45  1016.14  1039.67  1043.90


AT.  1 CA X    0.0000 -0.0015 -0.0020  0.0004  0.0000  0.0000
          Y   -0.0007  0.0000  0.0000  0.0000  0.0002  0.0006
          Z   -0.0004  0.0000  0.0000  0.0000  0.0006  0.0016
AT.  2 CA X    0.0000 -0.0015  0.0020 -0.0004  0.0000  0.0000
          Y   -0.0007  0.0000  0.0000  0.0000  0.0002 -0.0006
          Z    0.0004  0.0000  0.0000  0.0000 -0.0006  0.0016
AT.  3 CA X    0.0001  0.0002  0.0000  0.0000 -0.0002  0.0000
          Y    0.0001  0.0000  0.0000  0.0000  0.0000  0.0000
          Z    0.0000  0.0000  0.0010 -0.0001  0.0000 -0.0010
AT.  4 CA X   -0.0001  0.0002  0.0000  0.0000  0.0002  0.0000
          Y    0.0001  0.0000  0.0000  0.0000  0.0000  0.0000
          Z    0.0000  0.0000 -0.0010  0.0001  0.0000 -0.0010
AT.  5 CA X    0.0002 -0.0003 -0.0008  0.0003  0.0010  0.0001
          Y   -0.0006  0.0003  0.0004  0.0000 -0.0001  0.0002
          Z   -0.0001 -0.0001  0.0003 -0.0009 -0.0003 -0.0007
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AT.  6 CA X   -0.0002 -0.0003 -0.0008  0.0003 -0.0010 -0.0001
       Y   -0.0006 -0.0003 -0.0004  0.0000 -0.0001  0.0002
       Z   -0.0001  0.0001 -0.0003  0.0009 -0.0003 -0.0007
AT.  7 CA X   -0.0002 -0.0003  0.0008 -0.0003 -0.0010  0.0001
       Y   -0.0006 -0.0003  0.0004  0.0000 -0.0001 -0.0002
       Z    0.0001 -0.0001 -0.0003  0.0009  0.0003 -0.0007
AT.  8 CA X    0.0002 -0.0003  0.0008 -0.0003  0.0010 -0.0001
       Y   -0.0006  0.0003 -0.0004  0.0000 -0.0001 -0.0002
       Z    0.0001  0.0001  0.0003 -0.0009  0.0003 -0.0007
AT.  9 CA X    0.0004  0.0004 -0.0003 -0.0013  0.0001  0.0001
       Y   -0.0002 -0.0004  0.0001  0.0003  0.0001  0.0000
       Z   -0.0001 -0.0008  0.0006  0.0002  0.0003  0.0001
AT. 10 CA X   -0.0004  0.0004 -0.0003 -0.0013 -0.0001 -0.0001
       Y   -0.0002  0.0004 -0.0001 -0.0003  0.0001  0.0000
       Z   -0.0001  0.0008 -0.0006 -0.0002  0.0003  0.0001
AT. 11 CA X   -0.0004  0.0004  0.0003  0.0013 -0.0001  0.0001
       Y   -0.0002  0.0004  0.0001  0.0003  0.0001  0.0000
       Z    0.0001 -0.0008 -0.0006 -0.0002 -0.0003  0.0001
AT. 12 CA X    0.0004  0.0004  0.0003  0.0013  0.0001 -0.0001
       Y   -0.0002 -0.0004 -0.0001 -0.0003  0.0001  0.0000
       Z    0.0001  0.0008  0.0006  0.0002 -0.0003  0.0001
AT. 13 SI X    0.0017 -0.0003  0.0000  0.0000  0.0040  0.0000
       Y   -0.0009 -0.0008  0.0000  0.0000 -0.0007  0.0000
       Z    0.0000  0.0000  0.0059 -0.0042  0.0000 -0.0055
AT. 14 SI X   -0.0017 -0.0003  0.0000  0.0000 -0.0040  0.0000
       Y   -0.0009  0.0008  0.0000  0.0000 -0.0007  0.0000
       Z    0.0000  0.0000 -0.0059  0.0042  0.0000 -0.0055
AT. 15 SI X   -0.0082 -0.0061  0.0146 -0.0051 -0.0073  0.0003
       Y    0.0195  0.0107 -0.0161 -0.0019  0.0042  0.0036
       Z   -0.0019 -0.0055  0.0022  0.0052  0.0018 -0.0003
AT. 16 SI X    0.0082 -0.0061  0.0146 -0.0051  0.0073 -0.0003
       Y    0.0195 -0.0107  0.0161  0.0019  0.0042  0.0036
       Z   -0.0019  0.0055 -0.0022 -0.0052  0.0018 -0.0003
AT. 17 SI X    0.0082 -0.0061 -0.0146  0.0051  0.0073  0.0003
       Y    0.0195 -0.0107 -0.0161 -0.0019  0.0042 -0.0036
       Z    0.0019 -0.0055 -0.0022 -0.0052 -0.0018 -0.0003
AT. 18 SI X   -0.0082 -0.0061 -0.0146  0.0051 -0.0073 -0.0003
       Y    0.0195  0.0107  0.0161  0.0019  0.0042 -0.0036
       Z    0.0019  0.0055  0.0022  0.0052 -0.0018 -0.0003
AT. 19 SI X    0.0000  0.0225 -0.0020 -0.0271  0.0000  0.0000
       Y   -0.0088  0.0000  0.0000  0.0000  0.0178  0.0182
       Z   -0.0042  0.0000  0.0000  0.0000  0.0211  0.0230
AT. 20 SI X    0.0000  0.0225  0.0020  0.0271  0.0000  0.0000
       Y   -0.0088  0.0000  0.0000  0.0000  0.0178 -0.0182
       Z    0.0042  0.0000  0.0000  0.0000 -0.0211  0.0230
AT. 21 O  X   -0.0013 -0.0001  0.0028 -0.0011 -0.0021 -0.0020
       Y    0.0002  0.0002 -0.0012  0.0010  0.0006  0.0014
       Z    0.0015  0.0004 -0.0058  0.0040  0.0026  0.0055
AT. 22 O  X    0.0013 -0.0001  0.0028 -0.0011  0.0021  0.0020
       Y    0.0002 -0.0002  0.0012 -0.0010  0.0006  0.0014
       Z    0.0015 -0.0004  0.0058 -0.0040  0.0026  0.0055
AT. 23 O  X    0.0013 -0.0001 -0.0028  0.0011  0.0021 -0.0020
       Y    0.0002 -0.0002 -0.0012  0.0010  0.0006 -0.0014
       Z   -0.0015  0.0004  0.0058 -0.0040 -0.0026  0.0055
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AT. 24 O  X  -0.0013  -0.0001  -0.0028   0.0011  -0.0021   0.0020
        Y   0.0002   0.0002   0.0012  -0.0010   0.0006  -0.0014
        Z  -0.0015  -0.0004  -0.0058   0.0040  -0.0026   0.0055
AT. 25 O  X  -0.0014   0.0005   0.0000   0.0000  -0.0044   0.0000
        Y  -0.0005   0.0003   0.0000   0.0000  -0.0007   0.0000
        Z   0.0000   0.0000  -0.0003   0.0013   0.0000   0.0018
AT. 26 O  X   0.0014   0.0005   0.0000   0.0000   0.0044   0.0000
        Y  -0.0005  -0.0003   0.0000   0.0000  -0.0007   0.0000
        Z   0.0000   0.0000   0.0003  -0.0013   0.0000   0.0018
AT. 27 O  X  -0.0003   0.0002   0.0000   0.0000  -0.0013   0.0000
        Y   0.0014   0.0004   0.0000   0.0000   0.0007   0.0000
        Z   0.0000   0.0000  -0.0014   0.0016   0.0000   0.0018
AT. 28 O  X   0.0003   0.0002   0.0000   0.0000   0.0013   0.0000
        Y   0.0014  -0.0004   0.0000   0.0000   0.0007   0.0000
        Z   0.0000   0.0000   0.0014  -0.0016   0.0000   0.0018
AT. 29 O  X  -0.0025  -0.0035  -0.0006   0.0052   0.0027  -0.0006
        Y  -0.0027  -0.0032   0.0012   0.0033   0.0008  -0.0007
        Z   0.0058   0.0082  -0.0033  -0.0083  -0.0019   0.0027
AT. 30 O  X   0.0025  -0.0035  -0.0006   0.0052  -0.0027   0.0006
        Y  -0.0027   0.0032  -0.0012  -0.0033   0.0008  -0.0007
        Z   0.0058  -0.0082   0.0033   0.0083  -0.0019   0.0027
AT. 31 O  X   0.0025  -0.0035   0.0006  -0.0052  -0.0027  -0.0006
        Y  -0.0027   0.0032   0.0012   0.0033   0.0008   0.0007
        Z  -0.0058   0.0082   0.0033   0.0083   0.0019   0.0027
AT. 32 O  X  -0.0025  -0.0035   0.0006  -0.0052   0.0027   0.0006
        Y  -0.0027  -0.0032  -0.0012  -0.0033   0.0008   0.0007
        Z  -0.0058  -0.0082  -0.0033  -0.0083   0.0019   0.0027
AT. 33 O  X  -0.0175   0.0129   0.0231  -0.0019  -0.0102   0.0004
        Y  -0.0067   0.0045   0.0084  -0.0010  -0.0033   0.0008
        Z   0.0017  -0.0003  -0.0023   0.0025   0.0010  -0.0003
AT. 34 O  X   0.0175   0.0129   0.0231  -0.0019   0.0102  -0.0004
        Y  -0.0067  -0.0045  -0.0084   0.0010  -0.0033   0.0008
        Z   0.0017   0.0003   0.0023  -0.0025   0.0010  -0.0003
AT. 35 O  X   0.0175   0.0129  -0.0231   0.0019   0.0102   0.0004
        Y  -0.0067  -0.0045   0.0084  -0.0010  -0.0033  -0.0008
        Z  -0.0017  -0.0003   0.0023  -0.0025  -0.0010  -0.0003
AT. 36 O  X  -0.0175   0.0129  -0.0231   0.0019  -0.0102  -0.0004
        Y  -0.0067   0.0045  -0.0084   0.0010  -0.0033  -0.0008
        Z  -0.0017   0.0003  -0.0023   0.0025  -0.0010  -0.0003
AT. 37 O  X  -0.0026  -0.0039  -0.0036   0.0099  -0.0003  -0.0026
        Y   0.0007   0.0026   0.0007  -0.0043  -0.0003  -0.0003
        Z  -0.0041  -0.0022  -0.0030   0.0067  -0.0028  -0.0051
AT. 38 O  X   0.0026  -0.0039  -0.0036   0.0099   0.0003   0.0026
        Y   0.0007  -0.0026  -0.0007   0.0043  -0.0003  -0.0003
        Z  -0.0041   0.0022   0.0030  -0.0067  -0.0028  -0.0051
AT. 39 O  X   0.0026  -0.0039   0.0036  -0.0099   0.0003  -0.0026
        Y   0.0007  -0.0026   0.0007  -0.0043  -0.0003   0.0003
        Z   0.0041  -0.0022   0.0030  -0.0067   0.0028  -0.0051
AT. 40 O  X  -0.0026  -0.0039   0.0036  -0.0099  -0.0003   0.0026
        Y   0.0007   0.0026  -0.0007   0.0043  -0.0003   0.0003
        Z   0.0041   0.0022  -0.0030   0.0067   0.0028  -0.0051
AT. 41 O  X   0.0011   0.0014  -0.0033   0.0019   0.0028   0.0002
        Y  -0.0217  -0.0096   0.0167   0.0004  -0.0036  -0.0030
        Z   0.0007   0.0020  -0.0013  -0.0019   0.0001   0.0003
```

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AT. 42 O  X  -0.0011   0.0014  -0.0033   0.0019  -0.0028  -0.0002
         Y  -0.0217   0.0096  -0.0167  -0.0004  -0.0036  -0.0030
         Z   0.0007  -0.0020   0.0013   0.0019   0.0001   0.0003
AT. 43 O  X  -0.0011   0.0014   0.0033  -0.0019  -0.0028   0.0002
         Y  -0.0217   0.0096   0.0167   0.0004  -0.0036   0.0030
         Z  -0.0007   0.0020   0.0013   0.0019  -0.0001   0.0003
AT. 44 O  X   0.0011   0.0014   0.0033  -0.0019   0.0028  -0.0002
         Y  -0.0217  -0.0096  -0.0167  -0.0004  -0.0036   0.0030
         Z  -0.0007  -0.0020  -0.0013  -0.0019  -0.0001   0.0003
AT. 45 O  X  -0.0070  -0.0147   0.0038   0.0169   0.0142   0.0149
         Y   0.0069   0.0160  -0.0027  -0.0160  -0.0169  -0.0179
         Z   0.0058   0.0157  -0.0026  -0.0155  -0.0181  -0.0190
AT. 46 O  X   0.0070  -0.0147   0.0038   0.0169  -0.0142  -0.0149
         Y   0.0069  -0.0160   0.0027   0.0160  -0.0169  -0.0179
         Z   0.0058  -0.0157   0.0026   0.0155  -0.0181  -0.0190
AT. 47 O  X   0.0070  -0.0147  -0.0038  -0.0169  -0.0142   0.0149
         Y   0.0069  -0.0160  -0.0027  -0.0160  -0.0169   0.0179
         Z  -0.0058   0.0157   0.0026   0.0155   0.0181  -0.0190
AT. 48 O  X  -0.0070  -0.0147  -0.0038  -0.0169   0.0142  -0.0149
         Y   0.0069   0.0160   0.0027   0.0160  -0.0169   0.0179
         Z  -0.0058  -0.0157  -0.0026  -0.0155   0.0181  -0.0190
```

****

VIBRATIONAL TEMPERATURES (K) [MODE NUMBER;IRREP]

TO MODES

```
 131.0 [   4;B1 ]  135.7 [   5;B2 ]  143.5 [   6;A2 ]  159.3 [   7;A2 ]
 163.2 [   8;B2 ]  166.0 [   9;B1 ]  168.0 [  10;A1 ]  181.1 [  11;B1 ]
 183.3 [  12;A1 ]  185.4 [  13;A2 ]  187.0 [  14;B2 ]  205.7 [  15;B1 ]
 209.2 [  16;B2 ]  211.6 [  17;A2 ]  216.2 [  18;A1 ]  219.9 [  19;B2 ]
 226.3 [  20;A1 ]  234.0 [  21;B1 ]  237.1 [  22;A2 ]  244.9 [  23;B2 ]
 251.6 [  24;B1 ]  258.9 [  25;B2 ]  261.8 [  26;B1 ]  262.2 [  27;A2 ]
 266.3 [  28;A1 ]  276.2 [  29;B2 ]  279.4 [  30;B1 ]  287.5 [  31;A2 ]
 288.4 [  32;A1 ]  292.3 [  33;B1 ]  298.7 [  34;B2 ]  299.1 [  35;A1 ]
 300.1 [  36;B1 ]  317.8 [  37;A2 ]  319.1 [  38;A1 ]  322.5 [  39;B2 ]
 333.7 [  40;A1 ]  337.2 [  41;B1 ]  347.6 [  42;A2 ]  351.3 [  43;B2 ]
 354.0 [  44;A1 ]  354.2 [  45;B2 ]  356.2 [  46;A2 ]  363.3 [  47;A1 ]
 365.0 [  48;A2 ]  365.1 [  49;B2 ]  366.8 [  50;B1 ]  370.8 [  51;A1 ]
 372.3 [  52;A2 ]  379.3 [  53;A2 ]  389.0 [  54;B1 ]  389.7 [  55;A1 ]
 392.6 [  56;B2 ]  401.0 [  57;B1 ]  404.0 [  58;A1 ]  409.5 [  59;B1 ]
 409.8 [  60;A2 ]  410.3 [  61;B2 ]  426.8 [  62;B2 ]  430.4 [  63;A2 ]
 430.6 [  64;A1 ]  438.0 [  65;B2 ]  444.2 [  66;B1 ]  460.4 [  67;B2 ]
 460.8 [  68;A1 ]  462.3 [  69;A2 ]  472.8 [  70;A2 ]  474.9 [  71;B1 ]
 484.4 [  72;B1 ]  490.3 [  73;A1 ]  494.9 [  74;B2 ]  501.8 [  75;A1 ]
 506.6 [  76;B1 ]  513.2 [  77;A2 ]  519.5 [  78;B2 ]  522.0 [  79;A1 ]
 538.2 [  80;A2 ]  556.9 [  81;B1 ]  557.0 [  82;B2 ]  571.2 [  83;B2 ]
 572.7 [  84;B1 ]  574.7 [  85;A1 ]  594.1 [  86;A2 ]  594.1 [  87;B2 ]
 605.3 [  88;B1 ]  611.3 [  89;A2 ]  619.9 [  90;B1 ]  622.3 [  91;A1 ]
 630.2 [  92;B2 ]  679.5 [  93;B1 ]  685.9 [  94;A2 ]  692.1 [  95;B2 ]
 694.4 [  96;A1 ]  717.1 [  97;A2 ]  733.6 [  98;A1 ]  735.9 [  99;B1 ]
 738.8 [ 100;B2 ]  751.5 [ 101;A2 ]  764.4 [ 102;A1 ]  768.1 [ 103;B2 ]
 776.9 [ 104;B1 ]  789.2 [ 105;A1 ]  800.2 [ 106;A2 ]  813.9 [ 107;A1 ]
 816.9 [ 108;B2 ]  817.7 [ 109;B1 ]  830.2 [ 110;B2 ]  832.6 [ 111;A1 ]
```

845.6 [112;A2]   961.9 [113;A1]   977.3 [114;A2]   1018.7 [115;B1]
1021.4 [116;B2] 1180.9 [117;B2] 1181.8 [118;A1] 1186.2 [119;B1]
1195.0 [120;B2] 1220.5 [121;A2] 1224.3 [122;A1] 1243.2 [123;A1]
1269.6 [124;B2] 1272.6 [125;A2] 1278.3 [126;B1] 1289.1 [127;B2]
1291.5 [128;A1] 1300.4 [129;A2] 1317.8 [130;B1] 1327.8 [131;B1]
1341.4 [132;A1] 1345.0 [133;B2] 1363.3 [134;A1] 1365.0 [135;A2]
1381.1 [136;B2] 1403.2 [137;A1] 1406.7 [138;B1] 1413.2 [139;B2]
1431.3 [140;A1] 1438.0 [141;A2] 1462.0 [142;A2] 1495.9 [143;B2]
1501.9 [144;B1]

****

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	:	-12552.663455967000	-341575.337991487060	-32957013.25915588
E0	:	0.141217051241	3.842711323946	370.76531578

****

THERMODYNAMIC FUNCTIONS WITH VIBRATIONAL CONTRIBUTIONS

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

		AU/CELL	EV/CELL	KJ/MOL
ET	:	0.049741151466	1.353525543306	130.59537477
PV	:	0.000015160639	0.000412541947	0.03980425
TS	:	0.086321595997	2.348930044387	226.63731835
ET+PV-TS	:	-0.036565283893	-0.994991959134	-96.00213933
EL+E0+ET+PV-TS:		-12552.558804199651	-341572.490272122202	-32956738.49597942

OTHER THERMODINAMIC FUNCTIONS:

		mHARTREE/(CELL*K)	mEV/(CELL*K)	J/(MOL*K)
ENTROPY	:	0.289524051643	7.878349972790	760.14529047
HEAT CAPACITY	:	0.310037302589	8.436543909057	814.00282323

****
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT END   TELAPSE   29311.22 TCPU   28863.17
 EEEEEEEEEE TERMINATION DATE 15 05 2011 TIME 23:21:28.0
 NODE   0 CPU TIME =   28863.166
 NODE   1 CPU TIME =   28854.258
 NODE   2 CPU TIME =   28849.949
 NODE   3 CPU TIME =   28862.611
 NODE   4 CPU TIME =   28867.518
 NODE   5 CPU TIME =   28868.051

```
NODE    6 CPU TIME =    28868.711
NODE    7 CPU TIME =    28860.894
NODE    8 CPU TIME =    28995.620
NODE    9 CPU TIME =    28978.039
NODE   10 CPU TIME =    28976.067
NODE   11 CPU TIME =    28974.701
NODE   12 CPU TIME =    28971.848
NODE   13 CPU TIME =    28994.685
NODE   14 CPU TIME =    28969.453
NODE   15 CPU TIME =    28984.998
   TOTAL CPU TIME =   462740.571
Sun May 15 23:21:28 CEST 2011
Contents of temporary directory in master node n025.leo1:
total 3005417
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 dffit3.dat
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe8
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 ERROR.pe9
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe0
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe1
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe10
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe11
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:48 fort.10.pe12
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:48 fort.10.pe13
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:48 fort.10.pe14
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:48 fort.10.pe15
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe2
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:48 fort.10.pe3
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe4
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:48 fort.10.pe5
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:48 fort.10.pe6
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe7
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:48 fort.10.pe8
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:48 fort.10.pe9
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe0
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe1
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe10
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe11
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe12
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe13
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe14
```

```
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe15
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe2
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe3
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe4
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe5
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe6
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe7
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe8
-rw-r--r--+ 1 c71460 c714 17751376 May 15 22:48 fort.11.pe9
-rw-r--r--+ 1 c71460 c714    77748 May 15 21:18 fort.12
-rw-r--r--+ 1 c71460 c714 17655624 May 11 09:34 fort.13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe8
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.17.pe9
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe0
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe8
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.18.pe9
-rw-r--r--+ 1 c71460 c714     6720 May 15 23:21 fort.19.pe0
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe1
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe10
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe11
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe12
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe13
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe14
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe15
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe2
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe3
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe4
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe5
```

```
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe6
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe7
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe8
-rw-r--r--+ 1 c71460 c714   437212 May 15 23:21 fort.19.pe9
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe0
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe8
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.1.pe9
-rw-r--r--+ 1 c71460 c714  6077012 May 11 09:35 fort.20
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.28
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.29
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe0
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe8
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.38.pe9
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe0
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe1
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe10
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe11
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe12
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe13
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe14
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe15
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe2
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe3
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe4
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe5
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe6
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe7
-rw-r--r--+ 1 c71460 c714        0 May 11 08:31 fort.3.pe8
```

```
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.3.pe9
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe0
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe1
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe10
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe11
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe12
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe13
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe14
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe15
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe2
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe3
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe4
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe5
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe6
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe7
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe8
-rw-r--r--+ 1 c71460 c714         0 May 11 08:31 fort.40.pe9
-rw-r--r--+ 1 c71460 c714    159795 May 15 23:21 fort.65
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe0
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe1
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe10
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe11
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe12
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe13
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe14
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe15
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe2
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe3
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe4
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe5
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe6
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe7
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe8
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.71.pe9
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe0
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-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe10
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe11
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe12
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe13
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe14
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe15
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe2
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe3
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe4
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe5
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe6
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe7
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe8
-rw-r--r--+ 1 c71460 c714  44378040 May 15 22:47 fort.72.pe9
-rw-r--r--+ 1 c71460 c714     41664 May 15 23:21 fort.8.pe0
-rw-r--r--+ 1 c71460 c714  32256528 May 15 22:43 fort.8.pe1
-rw-r--r--+ 1 c71460 c714  32256528 May 15 22:42 fort.8.pe10
-rw-r--r--+ 1 c71460 c714  32256528 May 15 22:42 fort.8.pe11
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-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:42 fort.8.pe12
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:42 fort.8.pe13
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:42 fort.8.pe14
-rw-r--r--+ 1 c71460 c714 40320664 May 15 22:43 fort.8.pe15
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:42 fort.8.pe2
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:43 fort.8.pe3
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:42 fort.8.pe4
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:43 fort.8.pe5
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:42 fort.8.pe6
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:43 fort.8.pe7
-rw-r--r--+ 1 c71460 c714 24192400 May 15 22:43 fort.8.pe8
-rw-r--r--+ 1 c71460 c714 32256528 May 15 22:42 fort.8.pe9
-rw-r--r--+ 1 c71460 c714  6077012 May 11 09:35 fort.9
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe0
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe1
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe10
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe11
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe12
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe13
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe14
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe15
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe2
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe3
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe4
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe5
-rw-r--r--+ 1 c71460 c714  8939624 May 15 22:43 fort.95.pe6
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-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe10
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe11
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe12
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe13
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe14
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe15
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe2
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe3
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe4
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe5
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe6
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe7
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe8
-rw-r--r--+ 1 c71460 c714  8875608 May 15 21:17 fort.96.pe9
-rw-r--r--+ 1 c71460 c714 10938630 May 15 23:21 FREQINFO.DAT
-rw-r--r--+ 1 c71460 c714   440640 May 15 23:21 HESSFREQ.DAT
-rw-r--r--+ 1 c71460 c714     3777 May 15 15:12 INPUT
-rw-r--r--+ 1 c71460 c714     3777 May 15 15:12 Kilchoanite-FREQ.d12
-rw-r--r--+ 1 c71460 c714        0 May 11 10:18 OPTalist
-rw-r--r--+ 1 c71460 c714        0 May 11 10:18 OPTclist
-rw-r--r--+ 1 c71460 c714        0 May 11 10:18 scanlist
-rw-r--r--+ 1 c71460 c714    21024 May 11 08:31 SCFOUT.LOG
wave function binary file /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.f9
```

file HESSFREQ.DAT saved as /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.hessfreq
file SCFOUT.LOG saved as /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.SCFLOG
file FREQINFO.DAT saved as /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.freqinfo
file fort.13 saved as /mnt/x4540/hpc-scratch/c71460/leo1/Kilchoanite/Kilchoanite-FREQ.f13