Ambipolar organic transistors and near-infrared phototransistors based on a solution processable squarylium dye

Paul H. Wöbkenberg, John G. Labram, Jean-Marie, Swiecicki, Ksenia Parkhomenko, Dusan Sredojevic, Jean-Paul Gisselbrecht, Dago de Leeuw, Donal D. C. Bradley, Jean-Pierre Djukic*, Thomas D. Anthopoulos*

ESI

1) DFT computations

a) **SQ1**, vacuum**,** Becke-Perdew/TZ2P level.

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*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2008.01   September 22, 2008  *
*  ------------------------------------                                     *
*                                             Build 200901172115            *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
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*                                                                           *
************************  pentium64_linux / hpmpi  **************************

 ADF 2008.01  RunTime: Apr12-2009 17:33:44

 ============================
 A T T A C H E D   F I L E S
 ============================



 ==============================
 M O D E L   P A R A M E T E R S
 ==============================

 DENSITY FUNCTIONAL POTENTIAL (scf)
    LDA:                              VWN
    Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

 SPIN  (restricted / unrestr.)
    Molecule:                         Restricted
    Fragments:                        Restricted

 OTHER ASPECTS
    Relativistic Corrections:         ---
    Core Treatment:                   ---

    Electric Field:                   ---

    Hyperfine or Zeeman Interaction:  ---


 Fragment File(s)
 ----------------
 O:
         file : t21.O
         jobid: ADF 2008.01  RunTime: Apr12-2009 17:33:43
         title: Oxygen (TZ2P)
 C:
         file : t21.C
         jobid: ADF 2008.01  RunTime: Apr12-2009 17:33:42
         title: Carbon (TZ2P)
 H:
         file : t21.H
         jobid: ADF 2008.01  RunTime: Apr12-2009 17:33:41
         title: Hydrogen (TZ2P)



                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************


Geometry CYCLE 28
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ------------------------------------------
     1 O    -0.000007 -0.000002  0.000029
```

```
     2 C     0.000009 -0.000019 -0.000005
     3 C     0.000006 -0.000005  0.000003
     4 C    -0.000002  0.000000 -0.000007
     5 C     0.000003  0.000033  0.000012
     6 H    -0.000019  0.000019  0.000004
     7 C     0.000003 -0.000015  0.000046
     8 C     0.000012  0.000001  0.000009
     9 H     0.000010 -0.000008  0.000000
    10 H    -0.000006  0.000008 -0.000004
    11 H    -0.000001  0.000007  0.000019
    12 C     0.000004 -0.000030 -0.000002
    13 C    -0.000018  0.000024 -0.000011
    14 C     0.000008 -0.000003  0.000001
    15 C     0.000019 -0.000012 -0.000006
    16 C     0.000012 -0.000010 -0.000004
    17 H     0.000007  0.000000  0.000000
    18 C    -0.000028 -0.000015 -0.000007
    19 H     0.000007  0.000005 -0.000006
    20 C     0.000022  0.000017  0.000008
    21 C     0.000027  0.000005 -0.000004
    22 H     0.000007 -0.000004  0.000007
    23 C    -0.000004  0.000053 -0.000014
    24 H     0.000017  0.000012  0.000012
    25 C    -0.000075 -0.000036 -0.000033
    26 C    -0.000018 -0.000062  0.000034
    27 O     0.000007 -0.000001 -0.000002
    28 C     0.000005  0.000007  0.000004
    29 C     0.000004  0.000002 -0.000009
    30 C     0.000018 -0.000033  0.000002
    31 C    -0.000019  0.000002  0.000017
    32 H    -0.000021  0.000001 -0.000012
    33 C    -0.000005  0.000023  0.000012
    34 C     0.000004  0.000021 -0.000011
    35 H    -0.000005  0.000027 -0.000012
    36 H     0.000003 -0.000007 -0.000001
    37 H     0.000009 -0.000019  0.000007
    38 C    -0.000015  0.000037 -0.000009
    39 C     0.000020 -0.000013  0.000019
    40 C     0.000001 -0.000017 -0.000031
    41 C     0.000000  0.000016 -0.000016
    42 C    -0.000014  0.000017  0.000013
    43 H     0.000007  0.000036  0.000005
    44 C    -0.000010  0.000005  0.000015
    45 H    -0.000014  0.000006 -0.000002
    46 C     0.000013 -0.000016 -0.000004
    47 C    -0.000014  0.000009 -0.000004
    48 H    -0.000008 -0.000005 -0.000003
    49 C     0.000003  0.000038  0.000029
    50 H    -0.000016  0.000004 -0.000003
    51 C    -0.000005 -0.000030  0.000005
    52 C    -0.000021 -0.000066 -0.000020
    53 H     0.000020  0.000013 -0.000005
    54 H     0.000011  0.000003  0.000010
    55 H    -0.000032 -0.000030 -0.000072
    56 H     0.000005  0.000013  0.000006
    57 H     0.000004  0.000005  0.000016
    58 H     0.000011 -0.000003  0.000004
    59 H    -0.000002  0.000008 -0.000001
    60 H     0.000006 -0.000001  0.000001
    61 H    -0.000004  0.000002 -0.000002
    62 H    -0.000002  0.000005 -0.000003
    63 H     0.000003  0.000003 -0.000001
    64 H     0.000000 -0.000005 -0.000001
    65 H     0.000010  0.000002 -0.000001
    66 H    -0.000005  0.000003 -0.000004
    67 H     0.000003  0.000010 -0.000004
    68 H    -0.000007  0.000011  0.000009
    69 H     0.000047 -0.000028  0.000004
    70 H     0.000010 -0.000016 -0.000028
 ----------------------------------------

--------------------------------------
Geometry Convergence after Step  28
--------------------------------------
current energy                          -16.02975033 Hartree
abs of energy change               0.00000966     0.00100000    T
constrained gradient max           0.00007540     0.00100000    T
constrained gradient rms           0.00001752     0.00066667    T
gradient max                       0.00007505
gradient rms                       0.00001762
cart. step max                     0.00318895     0.01000000    T
cart. step rms                     0.00078158     0.00666667    T


 Number of elements of the density matrix on this node (used, total):    138300   1107816
```

```
 ====================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ====================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   46896
    Points in the Atomic Polyhedra                392391
    Points in the Outer Region                     53264
    ------------------------------------------------
    Total                                         492551

    Sum of Weights                                110615.974416

 Total nr. of points:     492551
 Nr. of blocks:             3849
 Block length:               128
 Nr. of dummy points:        121


 Test of Precision of the Numerical Integration Grid
 ====================================================

 Integral of the Total Core Density:                   0.00000000000000


 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.466016264767291	4475.3480	103203.99	431805.46
Delta V^Pauli Coulomb:	-77.584469746276753	-2111.1808	-48684.99	-203698.00
Delta V^Pauli LDA-XC:	-21.664263768317426	-589.5146	-13594.53	-56879.52
Delta V^Pauli GGA-Exchange:	1.144481007273473	31.1429	718.17	3004.83
Delta V^Pauli GGA-Correlation:	-0.280305871560481	-7.6275	-175.89	-735.94
Total Pauli Repulsion:	66.081457885886110	1798.1680	41466.75	173496.84
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	66.081457885886110	1798.1680	41466.75	173496.84
Electrostatic Interaction:	-13.047318523032144	-355.0356	-8187.32	-34255.73
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	53.034139362853963	1443.1324	33279.43	139241.11
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-69.037940043976889	-1878.6179	-43321.97	-181259.09
Total Orbital Interactions:	-69.063956987904135	-1879.3259	-43338.29	-181327.39

Alternative Decomposition Orb.Int.

Kinetic:	-149.323710169783681	-4063.3049	-93702.05	-392049.35
Coulomb:	74.172216532969159	2018.3287	46543.77	194739.13
XC:	6.087536648910349	165.6503	3819.99	15982.83
Total Orbital Interactions:	-69.063956987904177	-1879.3259	-43338.29	-181327.39
Residu (E=Steric+OrbInt+Res):	0.000067243489818	0.0018	0.04	0.18
Total Bonding Energy:	-16.029750381560355	-436.1917	-10058.82	-42086.10

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.047318523032144	-355.0356	-8187.32	-34255.73
Kinetic Energy:	15.142306094983610	412.0431	9501.94	39756.12
Coulomb (Steric+OrbInt) Energy:	-3.412185969817770	-92.8503	-2141.18	-8958.69
XC Energy:	-14.712551983694086	-400.3489	-9232.27	-38627.80
Total Bonding Energy:	-16.029750381560390	-436.1917	-10058.82	-42086.10

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): 0.0072354438
2. Electrostatic (Fit correction): 0.0000000000

```
********** NBO 5.0 **********
          N A T U R A L   A T O M I C   O R B I T A L   A N D
        N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
*******************************************************************************
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     on behalf of the Theoretical Chemistry Institute.  All Rights Reserved.

         Cite this program as:

         NBO 5.0.  E. D. Glendening, J. K. Badenhoop, A. E. Reed,
         J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold
         (Theoretical Chemistry Institute, University of Wisconsin,
         Madison, WI, 2001); http://www.chem.wisc.edu/~nbo5

       /NLMO   / : Form Natural Localized Molecular Orbitals
       /DIST   / : Print atom distance table
       /AONBO  / : Write the AO to NBO transformation to LFN 37
       /AONLMO / : Write the AO to NLMO transformation to LFN 39
       /NBONLMO/ : Write the NBO to NLMO transformation to LFN 49
       /NLMOMO / : Write the NLMO to MO transformation to LFN 49
       /STERIC / : Print NBO/NLMO steric analysis
       /BNDIDX / : Print bond indices based on the NAO density matrix
       /FILE   / : Set to adfnbo

 Job title: ***squarain-iso1true_PW91_TZP

 Storage needed:     8585860 in NPA,     6873256 in NBO,
                     6875850 in NLMO (    10000000 available)


 Atom distance matrix: (Angstroms)
```

Atom		1	2	3	4	5	6	7	8
1.	O	0.0000	4.5582	1.2357	2.5302	3.5105	4.8181	5.7571	7.2003
2.	O	4.5582	0.0000	3.3228	2.4928	3.1816	3.0304	4.3815	5.2334
3.	C	1.2357	3.3228	0.0000	1.4846	2.7437	3.8991	5.0109	6.3985
4.	C	2.5302	2.4928	1.4846	0.0000	1.4083	2.4431	3.6197	4.9817
5.	C	3.5105	3.1816	2.7437	1.4083	0.0000	1.4392	2.3249	3.7771
6.	C	4.8181	3.0304	3.8991	2.4431	1.4392	0.0000	1.3787	2.5683
7.	C	5.7571	4.3815	5.0109	3.6197	2.3249	1.3787	0.0000	1.5000
8.	C	7.2003	5.2334	6.3985	4.9817	3.7771	2.5683	1.5000	0.0000
9.	C	5.3797	5.1960	4.9126	3.7283	2.3381	2.2727	1.4328	2.6121
10.	C	3.9884	4.6250	3.6257	2.6380	1.4496	2.3170	2.3570	3.8143
11.	C	3.8262	5.6126	3.8657	3.3364	2.5671	3.6765	3.6979	5.0979
12.	C	2.9608	5.5444	3.2378	3.1991	3.0483	4.4027	4.8033	6.2728
13.	C	4.9712	6.9914	5.1914	4.7353	3.8713	4.7878	4.4606	5.6705
14.	C	6.1855	7.7920	6.3242	5.6976	4.6181	5.2119	4.5196	5.4444
15.	C	6.8368	7.6793	6.7600	5.8834	4.6135	4.8125	3.8165	4.4302
16.	C	6.4800	6.5756	6.1645	5.0760	3.7082	3.5983	2.4708	3.0469
17.	C	8.3127	9.0592	8.2589	7.3682	6.0714	6.1026	4.9456	5.1849
18.	C	9.1970	9.9684	9.1717	8.2828	6.9874	7.0612	5.9259	6.1375
19.	C	8.6744	9.9041	8.7777	8.0633	6.8750	7.0248	5.9485	6.2333
20.	C	3.3229	1.2356	2.0878	1.4842	2.5904	2.9976	4.3618	5.4850
21.	C	2.4928	2.5303	1.4842	2.1107	3.5076	4.2744	5.5752	6.8015
22.	C	3.1813	3.5109	2.5901	3.5073	4.9108	5.6569	6.9723	8.1638
23.	C	3.0295	4.8184	2.9969	4.2735	5.6558	6.6344	7.8776	9.1791
24.	C	4.3805	5.7574	4.3609	5.5741	6.9709	7.8777	9.1597	10.4187
25.	C	5.2319	7.2005	5.4838	6.7998	8.1615	9.1783	10.4176	11.7335
26.	C	5.1953	5.3800	4.8572	5.8200	7.2205	7.8993	9.2443	10.3725
27.	C	4.6248	3.9889	3.9928	4.7094	6.0720	6.6001	7.9576	9.0128
28.	C	5.6128	3.8266	4.7949	5.1821	6.4213	6.6534	8.0040	8.8688
29.	C	5.5449	2.9603	4.5626	4.5956	5.6482	5.6364	6.9311	7.6594
30.	C	6.9915	4.9716	6.1996	6.5585	7.7646	7.8942	9.2358	9.9976
31.	C	7.7917	6.1853	7.1250	7.6385	8.9060	9.1349	10.4947	11.3063
32.	C	7.6786	6.8359	7.1969	7.9322	9.2778	9.7040	11.0775	12.0232
33.	C	6.5749	6.4797	6.2458	7.1616	8.5516	9.1596	10.5208	11.5937
34.	C	9.0583	8.3112	8.6447	9.4173	10.7674	11.2038	12.5799	13.5181
35.	C	9.9660	9.1982	9.5705	10.3526	11.6962	12.0733	13.4340	14.3131
36.	C	9.9051	8.6717	9.3852	10.0063	11.2998	11.6424	13.0170	13.8873
37.	H	5.1950	2.3032	4.1150	2.7055	2.2164	1.0858	2.2062	2.9335
38.	H	7.4717	4.8200	6.5379	5.1013	4.0987	2.7004	2.1453	1.0962
39.	H	7.8887	5.9549	7.1171	5.6793	4.4065	3.3033	2.1660	1.1002
40.	H	7.6084	5.9492	6.8935	5.5653	4.3716	3.2804	2.1661	1.1006
41.	H	5.1029	7.6763	5.5348	5.3280	4.6711	5.7259	5.5097	6.7490
42.	H	6.9321	8.8497	7.2026	6.6918	5.6739	6.3050	5.5911	6.4419
43.	H	7.3885	6.9652	6.9714	5.7808	4.3920	3.9352	2.6063	2.5878
44.	H	8.7665	8.9987	8.5769	7.5559	6.2027	5.9770	4.6965	4.6238
45.	H	2.3015	5.1950	2.6730	4.0992	5.3885	6.5362	7.6794	9.0623
46.	H	4.8184	7.4719	5.3004	6.6976	7.9939	9.1306	10.2953	11.6743
47.	H	5.9549	7.8895	6.2316	7.5683	8.9412	9.9204	11.1616	12.4486
48.	H	5.9465	7.6079	6.1258	7.3559	8.7054	9.7002	10.9587	12.2666
49.	H	7.6766	5.1038	6.7918	6.9592	8.0526	7.9902	9.2862	9.8971
50.	H	8.8494	6.9321	8.1413	8.5689	9.7903	9.9126	11.2565	11.9743
51.	H	6.9643	7.3879	6.8030	7.8425	9.2442	9.9611	11.3075	12.4443
52.	H	8.9974	8.7633	8.7190	9.6185	10.9975	11.5611	12.9331	13.9588
53.	H	8.4720	10.1867	8.7210	8.1596	7.0656	7.4255	6.4757	6.9617
54.	H	8.2997	9.5017	8.3868	7.7039	6.5714	6.6866	5.6618	5.9437

55.	H	9.7700	10.8726	9.8589	9.1103	7.8919	7.9433	6.7915	6.8938
56.	H	9.0257	10.2487	9.1311	8.3828	7.1767	7.4585	6.4513	6.8700
57.	H	10.2373	10.9326	10.2121	9.3062	7.9912	7.9771	6.7736	6.8097
58.	H	9.2164	9.6172	9.0832	8.0951	6.7731	6.7527	5.6214	5.7697
59.	H	3.6568	6.5897	4.1538	4.2729	4.1214	5.4398	5.7238	7.1543
60.	H	3.1176	4.9847	3.0953	2.9210	2.9132	4.1931	4.7674	6.2153
61.	H	1.9495	5.3106	2.4947	2.8819	3.1138	4.5478	5.1274	6.6231
62.	H	4.9846	3.1151	4.0954	4.2276	5.2687	5.3498	6.5904	7.3778
63.	H	6.5902	3.6565	5.5980	5.5127	6.4427	6.2340	7.4602	8.0087
64.	H	5.3119	1.9498	4.1929	3.9433	4.8988	4.7924	6.1086	6.8292
65.	H	10.9311	10.2376	10.5737	11.3816	12.7328	13.1280	14.4934	15.3788
66.	H	10.2444	9.0267	9.7392	10.3941	11.6898	11.9387	13.2856	14.0669
67.	H	9.6148	9.2205	9.3115	10.1866	11.5447	11.9825	13.3251	14.2422
68.	H	9.5037	8.2939	8.9788	9.5706	10.8422	11.2224	12.5903	13.4944
69.	H	10.1894	8.4724	9.5562	10.0412	11.2829	11.4906	12.8523	13.6213
70.	H	10.8729	9.7670	10.4042	11.0660	12.3684	12.7322	14.1071	14.9833

Atom		9	10	11	12	13	14	15	16
1.	O	5.3797	3.9884	3.8262	2.9608	4.9712	6.1855	6.8368	6.4800
2.	O	5.1960	4.6250	5.6126	5.5444	6.9914	7.7920	7.6793	6.5756
3.	C	4.9126	3.6257	3.8657	3.2378	5.1914	6.3242	6.7600	6.1645
4.	C	3.7283	2.6380	3.3364	3.1991	4.7353	5.6976	5.8834	5.0760
5.	C	2.3381	1.4496	2.5671	3.0483	3.8713	4.6181	4.6135	3.7082
6.	C	2.2727	2.3170	3.6765	4.4027	4.7878	5.2119	4.8125	3.5983
7.	C	1.4328	2.3570	3.6979	4.8033	4.4606	4.5196	3.8165	2.4708
8.	C	2.6121	3.8143	5.0979	6.2728	5.6705	5.4444	4.4302	3.0469
9.	C	0.0000	1.4788	2.5586	3.8962	3.0838	3.0953	2.5408	1.3955
10.	C	1.4788	0.0000	1.4040	2.5108	2.5036	3.1693	3.2658	2.6069
11.	C	2.5586	1.4040	0.0000	1.5000	1.4179	2.5719	3.2680	3.2002
12.	C	3.8962	2.5108	1.5000	0.0000	2.4655	3.8286	4.7190	4.6821
13.	C	3.0838	2.5036	1.4179	2.4655	0.0000	1.3899	2.5396	3.0866
14.	C	3.0953	3.1693	2.5719	3.8286	1.3899	0.0000	1.4053	2.4708
15.	C	2.5408	3.2658	3.2680	4.7190	2.5396	1.4053	0.0000	1.3972
16.	C	1.3955	2.6069	3.2002	4.6821	3.0866	2.4708	1.3972	0.0000
17.	C	3.8653	4.7702	4.7704	6.1902	3.8696	2.5201	1.5282	2.5074
18.	C	4.8448	5.6489	5.4473	6.7369	4.3987	3.1073	2.5458	3.5622
19.	C	4.8363	5.5692	5.4416	6.7911	4.4233	3.1051	2.5430	3.5911
20.	C	4.8578	3.9930	4.7948	4.5623	6.1996	7.1255	7.1979	6.2467
21.	C	5.8208	4.7095	5.1816	4.5943	6.5581	7.6390	7.9336	7.1629
22.	C	7.2212	6.0716	6.4198	5.6453	7.7632	8.9059	9.2790	8.5529
23.	C	7.8984	6.5982	6.6502	5.6319	7.8908	9.1328	9.7033	9.1591
24.	C	9.2431	7.9552	7.9998	6.9250	9.2314	10.4917	11.0763	10.5200
25.	C	10.3700	9.0092	8.8630	7.6518	9.9912	11.3014	12.0202	11.5913
26.	C	9.5445	8.3821	8.6445	7.7100	9.9605	11.1594	11.5935	10.8831
27.	C	8.3836	7.3362	7.7898	7.0498	9.1562	10.2690	10.5631	9.7452
28.	C	8.6479	7.7914	8.4564	7.9124	9.8466	10.8513	10.9744	10.0196
29.	C	7.7156	7.0534	7.9147	7.6314	9.2885	10.1536	10.1111	9.0605
30.	C	9.9640	9.1576	9.8462	9.2854	11.2434	12.2427	12.3338	11.3386
31.	C	11.1612	10.2688	10.8489	10.1485	12.2406	13.3104	13.4890	12.5437
32.	C	11.5933	10.5611	10.9700	10.1040	12.3295	13.4867	13.8068	12.9692
33.	C	10.8825	9.7430	10.0151	9.0535	11.3341	12.5411	12.9687	12.2338
34.	C	13.0902	12.0366	12.3971	11.4656	13.7445	14.9311	15.2878	14.4671
35.	C	13.9885	12.9827	13.4005	12.5365	14.7424	15.8889	16.1996	15.3546
36.	C	13.6027	12.6005	13.0005	12.0773	14.3701	15.5502	15.8657	14.9937
37.	H	3.3282	3.3529	4.6698	5.2183	5.8433	6.2977	5.8652	4.6040
38.	H	3.4934	4.4812	5.8345	6.8642	6.5654	6.4600	5.5042	4.1120
39.	H	2.9567	4.2492	5.3911	6.6009	5.8060	5.4530	4.3652	3.0815
40.	H	2.9676	4.2632	5.4961	6.7727	5.9144	5.5108	4.3704	3.0791
41.	H	4.1584	3.4191	2.1053	2.5188	1.0918	2.0868	3.4353	4.1493
42.	H	4.1751	4.2276	3.4607	4.5174	2.0883	1.0933	2.1185	3.4116
43.	H	2.0958	3.5138	4.2646	5.7300	4.1641	3.4087	2.1061	1.0937
44.	H	3.8867	5.0511	5.3343	6.8101	4.6530	3.3986	2.1230	2.5038
45.	H	7.5071	6.1279	5.9855	4.8754	7.1368	8.4141	9.0992	8.6903
46.	H	10.0983	8.6866	8.3861	7.1143	9.4181	10.7450	11.5600	11.2495
47.	H	11.1408	9.8056	9.6936	8.5326	10.8058	12.0886	12.7894	12.3553
48.	H	10.9341	9.5680	9.3986	8.1261	10.5352	11.8734	12.6094	12.1718
49.	H	10.1436	9.4779	10.2916	9.8661	11.6883	12.6040	12.5767	11.5010
50.	H	12.0052	11.1812	11.8209	11.1640	13.2212	14.2609	14.3821	13.3872
51.	H	11.5690	10.3554	10.4982	9.4293	11.7687	13.0236	13.5483	12.8967
52.	H	13.3340	12.1957	12.4338	11.4022	13.7420	14.9780	15.4320	14.6942
53.	H	5.2232	5.6921	5.2951	6.5055	4.1084	2.8794	2.8468	4.1022
54.	H	4.6479	5.3758	5.3991	6.7579	4.5689	3.4077	2.7823	3.5430
55.	H	5.7721	6.6075	6.5153	7.8688	5.4748	4.1264	3.4937	4.4599
56.	H	5.2286	5.7703	5.2981	6.4433	4.0778	2.8791	2.8470	4.0733
57.	H	5.7807	6.6756	6.5202	7.8219	5.4545	4.1276	3.4964	4.4382
58.	H	4.6640	5.5179	5.4108	6.6662	4.5301	3.4128	2.7876	3.4930
59.	H	4.6828	3.4204	2.1536	1.0952	2.5217	3.8900	5.0105	5.2465
60.	H	4.1012	2.7510	2.1470	1.0985	3.2526	4.5424	5.2806	5.0466
61.	H	4.3466	2.8914	2.1655	1.1036	3.1702	4.4889	5.3377	5.2324
62.	H	7.2762	6.5985	7.4390	7.2172	8.7653	9.6009	9.5746	8.5789
63.	H	8.3720	7.8523	8.8066	8.6218	10.1637	10.9514	10.8033	9.6851
64.	H	6.9507	6.3398	7.2598	7.0374	8.6489	9.4921	9.4077	8.3144
65.	H	15.0363	14.0092	14.3907	13.4806	15.7257	16.8949	17.2349	16.4046
66.	H	13.9408	13.0268	13.5539	12.7895	14.9195	16.0110	16.2275	15.3099
67.	H	13.8186	12.7884	13.1712	12.3125	14.4803	15.6204	15.9592	15.1598
68.	H	13.1370	12.1110	12.4611	11.4953	13.8202	15.0208	15.3691	14.5225
69.	H	13.5438	12.6363	13.1482	12.3267	14.5426	15.6673	15.8868	14.9392

70.	H	14.6769	13.6540	14.0166	13.0518	15.3747	16.5744	16.9198	16.0660

	Atom	17	18	19	20	21	22	23	24
1.	O	8.3127	9.1970	8.6744	3.3229	2.4928	3.1813	3.0295	4.3805
2.	O	9.0592	9.9684	9.9041	1.2356	2.5303	3.5109	4.8184	5.7574
3.	C	8.2589	9.1717	8.7777	2.0878	1.4842	2.5901	2.9969	4.3609
4.	C	7.3682	8.2828	8.0633	1.4842	2.1107	3.5073	4.2735	5.5741
5.	C	6.0714	6.9874	6.8750	2.5904	3.5076	4.9108	5.6558	6.9709
6.	C	6.1026	7.0612	7.0248	2.9976	4.2744	5.6569	6.6344	7.8777
7.	C	4.9456	5.9259	5.9485	4.3618	5.5752	6.9723	7.8776	9.1597
8.	C	5.1849	6.1375	6.2333	5.4850	6.8015	8.1638	9.1791	10.4187
9.	C	3.8653	4.8448	4.8363	4.8578	5.8208	7.2212	7.8984	9.2431
10.	C	4.7702	5.6489	5.5692	3.9930	4.7095	6.0716	6.5982	7.9552
11.	C	4.7704	5.4473	5.4416	4.7948	5.1816	6.4198	6.6502	7.9998
12.	C	6.1902	6.7369	6.7911	4.5623	4.5943	5.6453	5.6319	6.9250
13.	C	3.8696	4.3987	4.4233	6.1996	6.5581	7.7632	7.8908	9.2314
14.	C	2.5201	3.1073	3.1051	7.1255	7.6390	8.9059	9.1328	10.4917
15.	C	1.5282	2.5458	2.5430	7.1979	7.9336	9.2790	9.7033	11.0763
16.	C	2.5074	3.5622	3.5911	6.2467	7.1629	8.5529	9.1591	10.5200
17.	C	0.0000	1.5399	1.5395	8.6461	9.4195	10.7696	11.2040	12.5797
18.	C	1.5399	0.0000	2.5380	9.5722	10.3532	11.6959	12.0698	13.4294
19.	C	1.5395	2.5380	0.0000	9.3853	10.0085	11.3028	11.6446	13.0193
20.	C	8.6461	9.5722	9.3853	0.0000	1.4847	2.7438	3.8992	5.0108
21.	C	9.4195	10.3532	10.0085	1.4847	0.0000	1.4083	2.4429	3.6195
22.	C	10.7696	11.6959	11.3028	2.7438	1.4083	0.0000	1.4392	2.3249
23.	C	11.2040	12.0698	11.6446	3.8992	2.4429	1.4392	0.0000	1.3786
24.	C	12.5797	13.4294	13.0193	5.0108	3.6195	2.3249	1.3786	0.0000
25.	C	13.5160	14.3055	13.8886	6.3982	4.9814	3.7771	2.5682	1.5000
26.	C	13.0915	13.9860	13.6060	4.9126	3.7281	2.3381	2.2727	1.4329
27.	C	12.0398	12.9832	12.6046	3.6259	2.6379	1.4496	2.3170	2.3571
28.	C	12.4029	13.4044	13.0063	3.8658	3.3363	2.5669	3.6764	3.6980
29.	C	11.4743	12.5444	12.0849	3.2376	3.1989	3.0479	4.4025	4.8033
30.	C	13.7504	14.7463	14.3762	5.1916	4.7352	3.8712	4.7877	4.4607
31.	C	14.9348	15.8898	15.5551	6.3239	5.6971	4.6179	5.2118	4.5196
32.	C	15.2892	16.1970	15.8694	6.7590	5.8826	4.6131	4.8124	3.8166
33.	C	14.4678	15.3510	14.9969	6.1639	5.0754	3.7080	3.5983	2.4710
34.	C	16.7786	17.6594	17.3602	8.2574	7.3671	6.0709	6.1025	4.9458
35.	C	17.6643	18.6307	18.1707	9.1718	8.2818	6.9858	7.0579	5.9217
36.	C	17.3572	18.1636	18.0518	8.7758	8.0630	6.8761	7.0281	5.9532
37.	H	7.1059	8.0640	8.0287	2.6743	4.1007	5.3905	6.5373	7.6808
38.	H	6.2797	7.2132	7.3064	5.3017	6.6994	7.9965	9.1319	10.2971
39.	H	4.9534	5.6765	6.1766	6.2316	7.5685	8.9416	9.9194	11.1604
40.	H	4.9153	6.0297	5.7759	6.1281	7.3591	8.7096	9.7029	10.9621
41.	H	4.5819	4.9003	4.9662	6.7915	6.9581	8.0500	7.9856	9.2802
42.	H	2.6245	2.8758	2.8818	8.1417	8.5692	9.7899	9.9101	11.2530
43.	H	2.5986	3.6524	3.7306	6.8041	7.8442	9.2462	9.9613	11.3076
44.	H	1.1003	2.1435	2.1429	8.7212	9.6221	11.0015	11.5633	12.9351
45.	H	10.5903	11.4191	10.9706	4.1146	2.7050	2.2162	1.0859	2.2063
46.	H	13.0363	13.7879	13.3480	6.5376	5.1009	4.0986	2.7004	2.1453
47.	H	14.2672	15.1200	14.5646	7.1176	5.6797	4.4070	3.3036	2.1661
48.	H	14.1202	14.8298	14.5726	6.8923	5.5642	4.3712	3.2799	2.1661
49.	H	13.9449	14.9734	14.5939	5.5354	5.3281	4.6709	5.7257	5.5096
50.	H	15.8089	16.7713	16.4533	7.2023	6.6914	5.6737	6.3049	5.5912
51.	H	15.0566	15.9010	15.5480	6.9706	5.7801	4.3919	3.9353	2.6065
52.	H	16.9384	17.7822	17.4864	8.5741	7.5540	6.2019	5.9768	4.6968
53.	H	2.1927	2.8159	1.0999	9.5542	10.0405	11.2827	11.4894	12.8511
54.	H	2.1928	3.5015	1.0983	8.9790	9.5743	10.8477	11.2281	12.5967
55.	H	2.1808	2.7670	1.0996	10.4049	11.0688	12.3721	12.7348	14.1099
56.	H	2.1922	1.0998	2.8165	9.7425	10.3957	11.6900	11.9354	13.2810
57.	H	2.1820	1.0996	2.7668	10.5750	11.3825	12.7331	13.1255	14.4899
58.	H	2.1933	1.0984	3.5015	9.3124	10.1854	11.5420	11.9757	13.3168
59.	H	6.3756	6.7406	6.9009	5.5977	5.5111	6.4390	6.2285	7.4528
60.	H	6.7698	7.2318	7.5449	4.0960	4.2270	5.2661	5.3458	6.5844
61.	H	6.8095	7.5178	7.2485	4.1917	3.9414	4.8957	4.7878	6.1031
62.	H	10.9180	12.0626	11.4146	3.0934	2.9193	2.9117	4.1922	4.7672
63.	H	12.1098	13.2149	12.7225	4.1538	4.2726	4.1209	5.4394	5.7237
64.	H	10.7749	11.7781	11.4940	2.4956	2.8826	3.1143	4.5482	5.1276
65.	H	18.7082	19.6529	19.2182	10.2118	9.3054	7.9902	7.9751	6.7710
66.	H	17.6668	18.6666	18.1984	9.1304	8.3802	7.1732	7.4532	6.4451
67.	H	17.4115	18.4245	17.8306	9.0854	8.0952	6.7718	6.7478	5.6142
68.	H	16.8695	17.6023	17.6186	8.3831	7.7033	6.5732	6.6925	5.6703
69.	H	17.3536	18.1871	18.0819	8.7219	8.1615	7.0684	7.4301	6.4811
70.	H	18.4169	19.2088	19.1041	9.8567	9.1096	7.8925	7.9458	6.7953

	Atom	25	26	27	28	29	30	31	32
1.	O	5.2319	5.1953	4.6248	5.6128	5.5449	6.9915	7.7917	7.6786
2.	O	7.2005	5.3800	3.9889	3.8266	2.9603	4.9716	6.1853	6.8359
3.	C	5.4838	4.8572	3.9928	4.7949	4.5626	6.1996	7.1250	7.1969
4.	C	6.7998	5.8200	4.7094	5.1821	4.5956	6.5585	7.6385	7.9322
5.	C	8.1615	7.2205	6.0720	6.4213	5.6482	7.7646	8.9060	9.2778
6.	C	9.1783	7.8993	6.6001	6.6534	5.6364	7.8942	9.1349	9.7040
7.	C	10.4176	9.2443	7.9576	8.0040	6.9311	9.2358	10.4947	11.0775
8.	C	11.7335	10.3725	9.0128	8.8688	7.6594	9.9976	11.3063	12.0232
9.	C	10.3700	9.5445	8.3836	8.6479	7.7156	9.9640	11.1612	11.5933
10.	C	9.0092	8.3821	7.3362	7.7914	7.0534	9.1576	10.2688	10.5611
11.	C	8.8630	8.6445	7.7898	8.4564	7.9147	9.8462	10.8489	10.9700

12.	C	7.6518	7.7100	7.0498	7.9124	7.6314	9.2854	10.1485	10.1040
13.	C	9.9912	9.9605	9.1562	9.8466	9.2885	11.2434	12.2406	12.3295
14.	C	11.3014	11.1594	10.2690	10.8513	10.1536	12.2427	13.3104	13.4867
15.	C	12.0202	11.5935	10.5631	10.9744	10.1111	12.3338	13.4890	13.8068
16.	C	11.5913	10.8831	9.7452	10.0196	9.0605	11.3386	12.5437	12.9692
17.	C	13.5160	13.0915	12.0398	12.4029	11.4743	13.7504	14.9348	15.2892
18.	C	14.3055	13.9860	12.9832	13.4044	12.5444	14.7463	15.8898	16.1970
19.	C	13.8886	13.6060	12.6046	13.0063	12.0849	14.3762	15.5551	15.8694
20.	C	6.3982	4.9126	3.6259	3.8658	3.2376	5.1916	6.3239	6.7590
21.	C	4.9814	3.7281	2.6379	3.3363	3.1989	4.7352	5.6971	5.8826
22.	C	3.7771	2.3381	1.4496	2.5669	3.0479	3.8712	4.6179	4.6131
23.	C	2.5682	2.2727	2.3170	3.6764	4.4025	4.7877	5.2118	4.8124
24.	C	1.5000	1.4329	2.3571	3.6980	4.8033	4.4607	4.5196	3.8166
25.	C	0.0000	2.6122	3.8144	5.0980	6.2729	5.6707	5.4447	4.4307
26.	C	2.6122	0.0000	1.4788	2.5587	3.8963	3.0838	3.0952	2.5407
27.	C	3.8144	1.4788	0.0000	1.4039	2.5107	2.5036	3.1690	3.2654
28.	C	5.0980	2.5587	1.4039	0.0000	1.5000	1.4179	2.5718	3.2679
29.	C	6.2729	3.8963	2.5107	1.5000	0.0000	2.4656	3.8287	4.7192
30.	C	5.6707	3.0838	2.5036	1.4179	2.4656	0.0000	1.3899	2.5396
31.	C	5.4447	3.0952	3.1690	2.5718	3.8287	1.3899	0.0000	1.4054
32.	C	4.4307	2.5407	3.2654	3.2679	4.7192	2.5396	1.4054	0.0000
33.	C	3.0474	1.3955	2.6067	3.2003	4.6824	3.0867	2.4708	1.3972
34.	C	5.1856	3.8652	4.7698	4.7704	6.1905	3.8697	2.5201	1.5282
35.	C	6.1317	4.8418	5.6479	5.4489	6.7402	4.4016	3.1100	2.5454
36.	C	6.2402	4.8395	5.5698	5.4399	6.7883	4.4205	3.1024	2.5435
37.	H	9.0631	7.5093	6.1308	5.9894	4.8800	7.1410	8.4172	9.1012
38.	H	11.6752	10.1016	8.6907	8.3921	7.1217	9.4250	10.7506	11.5638
39.	H	12.4461	11.1407	9.8069	9.6969	8.5380	10.8094	12.0904	12.7890
40.	H	12.2689	10.9395	9.5744	9.4077	8.1370	10.5452	11.8823	12.6163
41.	H	9.8889	10.1385	9.4751	10.2906	9.8679	11.6867	12.6001	12.5705
42.	H	11.9686	12.0029	11.1810	11.8230	11.1690	13.2230	14.2605	14.3793
43.	H	12.4429	11.5706	10.3586	10.5038	9.4374	11.7745	13.0277	13.5501
44.	H	13.9590	13.3375	12.2009	12.4419	11.4134	13.7502	14.9841	15.4358
45.	H	2.9336	3.3283	3.3528	4.6696	5.2178	5.8431	6.2976	5.8652
46.	H	1.0962	3.4935	4.4812	5.8346	6.8642	6.5654	6.4602	5.5047
47.	H	1.1002	2.9569	4.2496	5.3916	6.6018	5.8063	5.4535	4.3662
48.	H	1.1006	2.9678	4.2631	5.4962	6.7726	5.9149	5.5113	4.3707
49.	H	6.7490	4.1584	3.4190	2.1053	2.5189	1.0918	2.0868	3.4354
50.	H	6.4422	4.1750	4.2274	3.4606	4.5175	2.0883	1.0933	2.1185
51.	H	2.5885	2.0958	3.5136	4.2648	5.7304	4.1642	3.4087	2.1061
52.	H	4.6250	3.8866	5.0505	5.3343	6.8106	4.6531	3.3987	2.1231
53.	H	13.6191	13.5435	12.6369	13.1505	12.3306	14.5450	15.6686	15.8868
54.	H	13.5008	13.1438	12.1176	12.4687	11.5036	13.8280	15.0283	15.3763
55.	H	14.9849	14.6809	13.6590	14.0237	13.0609	15.3821	16.5806	16.9244
56.	H	14.0590	13.9383	13.0275	13.5579	12.7974	14.9234	16.0119	16.2248
57.	H	15.3725	15.0347	14.0103	14.3951	13.4890	15.7301	16.8963	17.2330
58.	H	14.2301	13.8129	12.7866	13.1734	12.3198	14.4825	15.6188	15.9531
59.	H	7.9992	8.3649	7.8476	8.8033	8.6212	10.1595	10.9447	10.7944
60.	H	7.3702	7.2701	6.5944	7.4359	7.2165	8.7612	9.5944	9.5660
61.	H	6.8226	6.9458	6.3364	7.2576	7.0372	8.6462	9.4879	9.4019
62.	H	6.2155	4.1014	2.7506	2.1471	1.0985	3.2532	4.5434	5.2820
63.	H	7.1544	4.6828	3.4202	2.1537	1.0952	2.5220	3.8905	5.0111
64.	H	6.6233	4.3465	2.8916	2.1653	1.1036	3.1697	4.4878	5.3365
65.	H	6.8061	5.7788	6.6750	6.5214	7.8244	5.4563	4.1291	3.4962
66.	H	6.8626	5.2237	5.7673	5.2976	6.4443	4.0789	2.8804	2.8451
67.	H	5.7589	4.6596	5.5179	5.4157	6.6740	4.5372	3.4191	2.7882
68.	H	5.9561	4.6535	5.3765	5.3956	6.7522	4.5635	3.4027	2.7827
69.	H	6.9687	5.2274	5.6942	5.2946	6.5035	4.1063	2.8773	2.8480
70.	H	6.8996	5.7745	6.6078	6.5140	7.8667	5.4728	4.1246	3.4941

Atom		33	34	35	36	37	38	39	40
1.	O	6.5749	9.0583	9.9660	9.9051	5.1950	7.4717	7.8887	7.6084
2.	O	6.4797	8.3112	9.1982	8.6717	2.3032	4.8200	5.9549	5.9492
3.	C	6.2458	8.6447	9.5705	9.3852	4.1150	6.5379	7.1171	6.8935
4.	C	7.1616	9.4173	10.3526	10.0063	2.7055	5.1013	5.6793	5.5653
5.	C	8.5516	10.7674	11.6962	11.2998	2.2164	4.0987	4.4065	4.3716
6.	C	9.1596	11.2038	12.0733	11.6424	1.0858	2.7004	3.3033	3.2804
7.	C	10.5208	12.5799	13.4340	13.0170	2.2062	2.1453	2.1660	2.1661
8.	C	11.5937	13.5181	14.3131	13.8873	2.9335	1.0962	1.1002	1.1006
9.	C	10.8825	13.0902	13.9885	13.6027	3.3282	3.4934	2.9567	2.9676
10.	C	9.7430	12.0366	12.9827	12.6005	3.3529	4.4812	4.2492	4.2632
11.	C	10.0151	12.3971	13.4005	13.0005	4.6698	5.8345	5.3911	5.4961
12.	C	9.0535	11.4656	12.5365	12.0773	5.2183	6.8642	6.6009	6.7727
13.	C	11.3341	13.7445	14.7424	14.3701	5.8433	6.5654	5.8060	5.9144
14.	C	12.5411	14.9311	15.8889	15.5502	6.2977	6.4600	5.4530	5.5108
15.	C	12.9687	15.2878	16.1996	15.8657	5.8652	5.5042	4.3652	4.3704
16.	C	12.2338	14.4671	15.3546	14.9937	4.6040	4.1120	3.0815	3.0791
17.	C	14.4678	16.7786	17.6643	17.3572	7.1059	6.2797	4.9534	4.9153
18.	C	15.3510	17.6594	18.6307	18.1636	8.0640	7.2132	5.6765	6.0297
19.	C	14.9969	17.3602	18.1707	18.0518	8.0287	7.3064	6.1766	5.7759
20.	C	6.1639	8.2574	9.1718	8.7758	2.6743	5.3017	6.2316	6.1281
21.	C	5.0754	7.3671	8.2818	8.0630	4.1007	6.6994	7.5685	7.3591
22.	C	3.7080	6.0709	6.9858	6.8761	5.3905	7.9965	8.9416	8.7096
23.	C	3.5983	6.1025	7.0579	7.0281	6.5373	9.1319	9.9194	9.7029
24.	C	2.4710	4.9458	5.9217	5.9532	7.6808	10.2971	11.1604	10.9621
25.	C	3.0474	5.1856	6.1317	6.2402	9.0631	11.6752	12.4461	12.2689
26.	C	1.3955	3.8652	4.8418	4.8395	7.5093	10.1016	11.1407	10.9395

27.	C	2.6067	4.7698	5.6479	5.5698	6.1308	8.6907	9.8069	9.5744
28.	C	3.2003	4.7704	5.4489	5.4399	5.9894	8.3921	9.6969	9.4077
29.	C	4.6824	6.1905	6.7402	6.7883	4.8800	7.1217	8.5380	8.1370
30.	C	3.0867	3.8697	4.4016	4.4205	7.1410	9.4250	10.8094	10.5452
31.	C	2.4708	2.5201	3.1100	3.1024	8.4172	10.7506	12.0904	11.8823
32.	C	1.3972	1.5282	2.5454	2.5435	9.1012	11.5638	12.7890	12.6163
33.	C	0.0000	2.5075	3.5587	3.5946	8.6921	11.2527	12.3546	12.1776
34.	C	2.5075	0.0000	1.5400	1.5394	10.5915	13.0394	14.2654	14.1267
35.	C	3.5587	1.5400	0.0000	2.5378	11.4241	13.7966	15.1240	14.8420
36.	C	3.5946	1.5394	2.5378	0.0000	10.9697	13.3475	14.5593	14.5753
37.	H	8.6921	10.5915	11.4241	10.9697	0.0000	2.6318	3.7120	3.6737
38.	H	11.2527	13.0394	13.7966	13.3475	2.6318	0.0000	1.7727	1.7722
39.	H	12.3546	14.2654	15.1240	14.5593	3.7120	1.7727	0.0000	1.7713
40.	H	12.1776	14.1267	14.8420	14.5753	3.6737	1.7722	1.7713	0.0000
41.	H	11.4946	13.9370	14.9667	14.5866	6.7500	7.6260	6.8633	7.0059
42.	H	13.3840	15.8045	16.7696	16.4479	7.3908	7.4821	6.3835	6.4434
43.	H	12.8979	15.0573	15.9069	15.5455	4.8067	3.6815	2.4664	2.4204
44.	H	14.6972	16.9408	17.7906	17.4846	6.8971	5.6926	4.3312	4.2372
45.	H	4.6041	7.1059	8.0605	8.0325	6.6182	9.1452	9.7677	9.5542
46.	H	4.1124	6.2804	7.2074	7.3134	9.1455	11.7187	12.3610	12.1822
47.	H	3.0824	4.9551	5.6704	6.1838	9.7699	12.3640	13.2144	12.9272
48.	H	3.0794	4.9155	6.0237	5.7838	9.5537	12.1813	12.9220	12.8742
49.	H	4.1493	4.5821	4.9047	4.9620	7.1387	9.2288	10.7167	10.4161
50.	H	3.4115	2.6245	2.8808	2.8767	9.1263	11.3460	12.7503	12.5480
51.	H	1.0937	2.5987	3.6469	3.7360	9.5662	12.1590	13.1872	13.0300
52.	H	2.5040	1.1004	2.1437	2.1428	11.0328	13.5522	14.6923	14.5735
53.	H	14.9388	17.3530	18.1893	18.0794	8.4704	8.0380	6.9336	6.5962
54.	H	14.5297	16.8767	17.6136	17.6221	7.6461	6.9691	6.0667	5.3636
55.	H	16.0701	18.4209	19.2175	19.1046	8.9177	7.9544	6.7497	6.3586
56.	H	15.3062	17.6619	18.6653	18.1925	8.5024	7.9473	6.4700	6.8271
57.	H	16.4019	18.7042	19.6543	19.2112	8.9513	7.8713	6.2975	6.5928
58.	H	15.1525	17.4027	18.4212	17.8195	7.7102	6.8001	5.1600	5.8228
59.	H	9.6763	12.0990	13.2044	12.7134	6.2821	7.8122	7.3887	7.6280
60.	H	8.5709	10.9074	12.0531	11.4053	4.8781	6.6866	6.4950	6.8701
61.	H	8.3086	10.7681	11.7713	11.4884	5.2609	7.1353	7.1076	7.0507
62.	H	5.0478	6.7719	7.2361	7.5439	4.7220	6.9406	8.3267	7.7414
63.	H	5.2469	6.3765	6.7455	6.8974	5.3739	7.3561	8.8988	8.4384
64.	H	5.2317	6.8078	7.5195	7.2440	3.9829	6.2780	7.6447	7.4065
65.	H	4.4361	2.1820	1.0996	2.7654	12.4806	14.8582	16.1751	15.9228
66.	H	4.0684	2.1921	1.0998	2.8173	11.2155	13.4819	14.8880	14.5793
67.	H	3.4878	2.1935	1.0984	3.5013	11.3865	13.7746	15.0974	14.7087
68.	H	3.5491	2.1929	3.5015	1.0983	10.5870	12.9877	14.1077	14.2386
69.	H	4.1062	2.1927	2.8150	1.0999	10.7387	13.0084	14.2956	14.3028
70.	H	4.4625	2.1807	2.7673	1.0997	12.0658	14.4424	15.6482	15.6745

Atom		41	42	43	44	45	46	47	48
1.	O	5.1029	6.9321	7.3885	8.7665	2.3015	4.8184	5.9549	5.9465
2.	O	7.6763	8.8497	6.9652	8.9987	5.1950	7.4719	7.8895	7.6079
3.	C	5.5348	7.2026	6.9714	8.5769	2.6730	5.3004	6.2316	6.1258
4.	C	5.3280	6.6918	5.7808	7.5559	4.0992	6.6976	7.5683	7.3559
5.	C	4.6711	5.6739	4.3920	6.2027	5.3885	7.9939	8.9412	8.7054
6.	C	5.7259	6.3050	3.9352	5.9770	6.5362	9.1306	9.9204	9.7002
7.	C	5.5097	5.5911	2.6063	4.6965	7.6794	10.2953	11.1616	10.9587
8.	C	6.7490	6.4419	2.5878	4.6238	9.0623	11.6743	12.4486	12.2666
9.	C	4.1584	4.1751	2.0958	3.8867	7.5071	10.0983	11.1408	10.9341
10.	C	3.4191	4.2276	3.5138	5.0511	6.1279	8.6866	9.8056	9.5680
11.	C	2.1053	3.4607	4.2646	5.3343	5.9855	8.3861	9.6936	9.3986
12.	C	2.5188	4.5174	5.7300	6.8101	4.8754	7.1143	8.5326	8.1261
13.	C	1.0918	2.0883	4.1641	4.6530	7.1368	9.4181	10.8058	10.5352
14.	C	2.0868	1.0933	3.4087	3.3986	8.4141	10.7450	12.0886	11.8734
15.	C	3.4353	2.1185	2.1061	2.1230	9.0992	11.5600	12.7894	12.6094
16.	C	4.1493	3.4116	1.0937	2.5038	8.6903	11.2495	12.3553	12.1718
17.	C	4.5819	2.6245	2.5986	1.1003	10.5903	13.0363	14.2672	14.1202
18.	C	4.9003	2.8758	3.6524	2.1435	11.4191	13.7879	15.1200	14.8298
19.	C	4.9662	2.8818	3.7306	2.1429	10.9706	13.3480	14.5646	14.5726
20.	C	6.7915	8.1417	6.8041	8.7212	4.1146	6.5376	7.1176	6.8923
21.	C	6.9581	8.5692	7.8442	9.6221	2.7050	5.1009	5.6797	5.5642
22.	C	8.0500	9.7899	9.2462	11.0015	2.2162	4.0986	4.4070	4.3712
23.	C	7.9856	9.9101	9.9613	11.5633	1.0859	2.7004	3.3036	3.2799
24.	C	9.2802	11.2530	11.3076	12.9351	2.2063	2.1453	2.1661	2.1661
25.	C	9.8889	11.9686	12.4429	13.9590	2.9336	1.0962	1.1002	1.1006
26.	C	10.1385	12.0029	11.5706	13.3375	3.3283	3.4935	2.9569	2.9678
27.	C	9.4751	11.1810	10.3586	12.2009	3.3528	4.4812	4.2496	4.2631
28.	C	10.2906	11.8230	10.5038	12.4419	4.6696	5.8346	5.3916	5.4962
29.	C	9.8679	11.1690	9.4374	11.4134	5.2178	6.8642	6.6018	6.7726
30.	C	11.6867	13.2230	11.7745	13.7502	5.8431	6.5654	5.8063	5.9149
31.	C	12.6001	14.2605	13.0277	14.9841	6.2976	6.4602	5.4535	5.5113
32.	C	12.5705	14.3793	13.5501	15.4358	5.8652	5.5047	4.3662	4.3707
33.	C	11.4946	13.3840	12.8979	14.6972	4.6041	4.1124	3.0824	3.0794
34.	C	13.9370	15.8045	15.0573	16.9408	7.1059	6.2804	4.9551	4.9155
35.	C	14.9667	16.7696	15.9069	17.7906	8.0605	7.2074	5.6704	6.0237
36.	C	14.5866	16.4479	15.5455	17.4846	8.0325	7.3134	6.1838	5.7838
37.	H	6.7500	7.3908	4.8067	6.8971	6.6182	9.1455	9.7699	9.5537
38.	H	7.6260	7.4821	3.6815	5.6926	9.1452	11.7187	12.3640	12.1813
39.	H	6.8633	6.3835	2.4664	4.3312	9.7677	12.3610	13.2144	12.9220
40.	H	7.0059	6.4434	2.4204	4.2372	9.5542	12.1822	12.9272	12.8742
41.	H	0.0000	2.2769	5.2114	5.4823	7.1335	9.2202	10.7112	10.4041

42.	H	2.2769	0.0000	4.2226	3.6798	9.1227	11.3397	12.7479	12.5382
43.	H	5.2114	4.2226	0.0000	2.1182	9.5649	12.1566	13.1891	13.0252
44.	H	5.4823	3.6798	2.1182	0.0000	11.0335	13.5514	14.6969	14.5690
45.	H	7.1335	9.1227	9.5649	11.0335	0.0000	2.6319	3.7126	3.6734
46.	H	9.2202	11.3397	12.1566	13.5514	2.6319	0.0000	1.7727	1.7721
47.	H	10.7112	12.7479	13.1891	14.6969	3.7126	1.7727	0.0000	1.7712
48.	H	10.4041	12.5382	13.0252	14.5690	3.6734	1.7721	1.7712	0.0000
49.	H	12.2134	13.6172	11.8415	13.8589	6.7497	7.6260	6.8633	7.0063
50.	H	13.6136	15.2302	13.8173	15.8097	7.3907	7.4823	6.3838	6.4441
51.	H	11.8337	13.8126	13.6165	15.3506	4.8070	3.6822	2.4679	2.4205
52.	H	13.8485	15.8028	15.3489	17.1697	6.8971	5.6939	4.3353	4.2363
53.	H	4.4268	2.3264	4.4785	3.0732	10.7365	13.0055	14.2967	14.2971
54.	H	5.1961	3.4119	3.6554	2.4986	10.5917	12.9935	14.1183	14.2413
55.	H	5.9755	3.7948	4.3973	2.4766	12.0670	14.4432	15.6541	15.6720
56.	H	4.3467	2.3165	4.4088	3.0731	11.2106	13.4728	14.8831	14.5672
57.	H	5.9198	3.7890	4.3333	2.4793	12.4766	14.8508	16.1727	15.9116
58.	H	5.0898	3.4050	3.5170	2.4985	11.3779	13.7612	15.0889	14.6916
59.	H	2.1027	4.3383	6.3239	7.1278	5.3686	7.3469	8.8915	8.4252
60.	H	3.3866	5.2934	6.0210	7.2984	4.7187	6.9338	8.3210	7.7304
61.	H	3.2048	5.1706	6.2582	7.3991	3.9780	6.2713	7.6403	7.3970
62.	H	9.3439	10.5920	8.9831	10.8825	4.8767	6.6863	6.4963	6.8700
63.	H	10.7983	11.9852	9.9609	11.9648	6.2814	7.8121	7.3893	7.6281
64.	H	9.2710	10.5316	8.6731	10.6951	5.2612	7.1356	7.1084	7.0502
65.	H	15.9164	17.7622	16.9689	18.8497	8.9493	7.8678	6.2942	6.5886
66.	H	15.2201	16.9307	15.7945	17.7252	8.4968	7.9398	6.4613	6.8209
67.	H	14.6834	16.4748	15.7348	17.5627	7.7047	6.7892	5.1483	5.8108
68.	H	14.0091	15.9057	15.0979	17.0231	7.6529	6.9818	6.0796	5.3778
69.	H	14.8371	16.6054	15.4216	17.4118	8.4754	8.0452	6.9395	6.6051
70.	H	15.5566	17.4564	16.6297	18.5599	8.9208	7.9604	6.7561	6.3651

Atom		49	50	51	52	53	54	55	56
1.	O	7.6766	8.8494	6.9643	8.9974	8.4720	8.2997	9.7700	9.0257
2.	O	5.1038	6.9321	7.3879	8.7633	10.1867	9.5017	10.8726	10.2487
3.	C	6.7918	8.1413	6.8030	8.7190	8.7210	8.3868	9.8589	9.1311
4.	C	6.9592	8.5689	7.8425	9.6185	8.1596	7.7039	9.1103	8.3828
5.	C	8.0526	9.7903	9.2442	10.9975	7.0656	6.5714	7.8919	7.1767
6.	C	7.9902	9.9126	9.9611	11.5611	7.4255	6.6866	7.9433	7.4585
7.	C	9.2862	11.2565	11.3075	12.9331	6.4757	5.6618	6.7915	6.4513
8.	C	9.8971	11.9743	12.4443	13.9588	6.9617	5.9437	6.8938	6.8700
9.	C	10.1436	12.0052	11.5690	13.3340	5.2232	4.6479	5.7721	5.2286
10.	C	9.4779	11.1812	10.3554	12.1957	5.6921	5.3758	6.6075	5.7703
11.	C	10.2916	11.8209	10.4982	12.4338	5.2951	5.3991	6.5153	5.2981
12.	C	9.8661	11.1640	9.4293	11.4022	6.5055	6.7579	7.8688	6.4433
13.	C	11.6883	13.2212	11.7687	13.7420	4.1084	4.5689	5.4748	4.0778
14.	C	12.6040	14.2609	13.0236	14.9780	2.8794	3.4077	4.1264	2.8791
15.	C	12.5767	14.3821	13.5483	15.4320	2.8468	2.7823	3.4937	2.8470
16.	C	11.5010	13.3872	12.8967	14.6942	4.1022	3.5430	4.4599	4.0733
17.	C	13.9449	15.8089	15.0566	16.9384	2.1927	2.1928	2.1808	2.1922
18.	C	14.9734	16.7713	15.9010	17.7822	2.8159	3.5015	2.7670	1.0998
19.	C	14.5939	16.4533	15.5480	17.4864	1.0999	1.0983	1.0996	2.8165
20.	C	5.5354	7.2023	6.9706	8.5741	9.5542	8.9790	10.4049	9.7425
21.	C	5.3281	6.6914	5.7801	7.5540	10.0405	9.5743	11.0688	10.3957
22.	C	4.6709	5.6737	4.3919	6.2019	11.2827	10.8477	12.3721	11.6900
23.	C	5.7257	6.3049	3.9353	5.9768	11.4894	11.2281	12.7348	11.9354
24.	C	5.5096	5.5912	2.6065	4.6968	12.8511	12.5967	14.1099	13.2810
25.	C	6.7490	6.4422	2.5885	4.6250	13.6191	13.5008	14.9849	14.0590
26.	C	4.1584	4.1750	2.0958	3.8866	13.5435	13.1438	14.6809	13.9383
27.	C	3.4190	4.2274	3.5136	5.0505	12.6369	12.1176	13.6590	13.0275
28.	C	2.1053	3.4606	4.2648	5.3343	13.1505	12.4687	14.0237	13.5579
29.	C	2.5189	4.5175	5.7304	6.8106	12.3306	11.5036	13.0609	12.7974
30.	C	1.0918	2.0883	4.1642	4.6531	14.5450	13.8280	15.3821	14.9234
31.	C	2.0868	1.0933	3.4087	3.3987	15.6686	15.0283	16.5806	16.0119
32.	C	3.4354	2.1185	2.1061	2.1231	15.8868	15.3763	16.9244	16.2248
33.	C	4.1493	3.4115	1.0937	2.5040	14.9388	14.5297	16.0701	15.3062
34.	C	4.5821	2.6245	2.5987	1.1004	17.3530	16.8767	18.4209	17.6619
35.	C	4.9047	2.8808	3.6469	2.1437	18.1893	17.6136	19.2175	18.6653
36.	C	4.9620	2.8767	3.7360	2.1428	18.0794	17.6221	19.1046	18.1925
37.	H	7.1387	9.1263	9.5662	11.0328	8.4704	7.6461	8.9177	8.5024
38.	H	9.2288	11.3460	12.1590	13.5522	8.0380	6.9691	7.9544	7.9473
39.	H	10.7167	12.7503	13.1872	14.6923	6.9336	6.0667	6.7497	6.4700
40.	H	10.4161	12.5480	13.0300	14.5735	6.5962	5.3636	6.3586	6.8271
41.	H	12.2134	13.6136	11.8337	13.8485	4.4268	5.1961	5.9755	4.3467
42.	H	13.6172	15.2302	13.8126	15.8028	2.3264	3.4119	3.7948	2.3165
43.	H	11.8415	13.8173	13.6165	15.3489	4.4785	3.6554	4.3973	4.4088
44.	H	13.8589	15.8097	15.3506	17.1697	3.0732	2.4986	2.4766	3.0731
45.	H	6.7497	7.3907	4.8070	6.8971	10.7365	10.5917	12.0670	11.2106
46.	H	7.6260	7.4823	3.6822	5.6939	13.0055	12.9935	14.4432	13.4728
47.	H	6.8633	6.3838	2.4679	4.3353	14.2967	14.1183	15.6541	14.8831
48.	H	7.0063	6.4441	2.4205	4.2363	14.2971	14.2413	15.6720	14.5672
49.	H	0.0000	2.2770	5.2114	5.4826	14.8406	14.0175	15.5655	15.2267
50.	H	2.2770	0.0000	4.2226	3.6798	16.6071	15.9135	17.4631	16.9324
51.	H	5.2114	4.2226	0.0000	2.1187	15.4206	15.1051	16.6329	15.7884
52.	H	5.4826	3.6798	2.1187	0.0000	17.4101	17.0301	18.5625	17.7166
53.	H	14.8406	16.6071	15.4206	17.4101	0.0000	1.7764	1.7747	2.6482
54.	H	14.0175	15.9135	15.1051	17.0301	1.7764	0.0000	1.7819	3.8325
55.	H	15.5655	17.4631	16.6329	18.5625	1.7747	1.7819	0.0000	3.1441
56.	H	15.2267	16.9324	15.7884	17.7166	2.6482	3.8325	3.1441	0.0000

57.	H	15.9235	17.7644	16.9641	18.8423	3.1412	3.7737	2.5400	1.7747
58.	H	14.6891	16.4743	15.7247	17.5494	3.8329	4.3553	3.7728	1.7764
59.	H	10.7955	11.9787	9.9508	11.9513	6.4586	6.9880	7.9506	6.2766
60.	H	9.3412	10.5856	8.9738	10.8690	7.3425	7.5451	8.6035	7.0029
61.	H	9.2693	10.5275	8.6664	10.6865	6.9560	7.0657	8.3452	7.2451
62.	H	3.3870	5.2946	6.0224	7.3013	11.6408	10.7762	12.3911	12.3007
63.	H	2.1029	4.3388	6.3245	7.1291	13.0373	12.1032	13.6608	13.5356
64.	H	3.2047	5.1695	6.2576	7.3967	11.7673	10.9802	12.4639	12.0537
65.	H	5.9225	3.7915	4.3299	2.4804	19.2170	18.6721	20.2705	19.6672
66.	H	4.3497	2.3216	4.4025	3.0731	18.2829	17.6152	19.2245	18.7657
67.	H	5.0995	3.4143	3.5073	2.4979	17.8226	17.2369	18.8765	18.4390
68.	H	5.1883	3.4036	3.6654	2.4991	17.6265	17.2481	18.6751	17.6061
69.	H	4.4227	2.3204	4.4837	3.0731	18.1761	17.6314	19.1140	18.2819
70.	H	5.9725	3.7915	4.4015	2.4761	19.1110	18.6786	20.1619	19.2168

Atom		57	58	59	60	61	62	63	64
1.	O	10.2373	9.2164	3.6568	3.1176	1.9495	4.9846	6.5902	5.3119
2.	O	10.9326	9.6172	6.5897	4.9847	5.3106	3.1151	3.6565	1.9498
3.	C	10.2121	9.0832	4.1538	3.0953	2.4947	4.0954	5.5980	4.1929
4.	C	9.3062	8.0951	4.2729	2.9210	2.8819	4.2276	5.5127	3.9433
5.	C	7.9912	6.7731	4.1214	2.9132	3.1138	5.2687	6.4427	4.8988
6.	C	7.9771	6.7527	5.4398	4.1931	4.5478	5.3498	6.2340	4.7924
7.	C	6.7736	5.6214	5.7238	4.7674	5.1274	6.5904	7.4602	6.1086
8.	C	6.8097	5.7697	7.1543	6.2153	6.6231	7.3778	8.0087	6.8292
9.	C	5.7807	4.6640	4.6828	4.1012	4.3466	7.2762	8.3720	6.9507
10.	C	6.6756	5.5179	3.4204	2.7510	2.8914	6.5985	7.8523	6.3398
11.	C	6.5202	5.4108	2.1536	2.1470	2.1655	7.4390	8.8066	7.2598
12.	C	7.8219	6.6662	1.0952	1.0985	1.1036	7.2172	8.6218	7.0374
13.	C	5.4545	4.5301	2.5217	3.2526	3.1702	8.7653	10.1637	8.6489
14.	C	4.1276	3.4128	3.8900	4.5424	4.4889	9.6009	10.9514	9.4921
15.	C	3.4964	2.7876	5.0105	5.2806	5.3377	9.5746	10.8033	9.4077
16.	C	4.4382	3.4930	5.2465	5.0466	5.2324	8.5789	9.6851	8.3144
17.	C	2.1820	2.1933	6.3756	6.7698	6.8095	10.9180	12.1098	10.7749
18.	C	1.0996	1.0984	6.7406	7.2318	7.5178	12.0626	13.2149	11.7781
19.	C	2.7668	3.5015	6.9009	7.5449	7.2485	11.4146	12.7225	11.4940
20.	C	10.5750	9.3124	5.5977	4.0960	4.1917	3.0934	4.1538	2.4956
21.	C	11.3825	10.1854	5.5111	4.2270	3.9414	2.9193	4.2726	2.8826
22.	C	12.7331	11.5420	6.4390	5.2661	4.8957	2.9117	4.1209	3.1143
23.	C	13.1255	11.9757	6.2285	5.3458	4.7878	4.1922	5.4394	4.5482
24.	C	14.4899	13.3168	7.4528	6.5844	6.1031	4.7672	5.7237	5.1276
25.	C	15.3725	14.2301	7.9992	7.3702	6.8226	6.2155	7.1544	6.6233
26.	C	15.0347	13.8129	8.3649	7.2701	6.9458	4.1014	4.6828	4.3465
27.	C	14.0103	12.7866	7.8476	6.5944	6.3364	2.7506	3.4202	2.8916
28.	C	14.3951	13.1734	8.8033	7.4359	7.2576	2.1471	2.1537	2.1653
29.	C	13.4890	12.3198	8.6212	7.2165	7.0372	1.0985	1.0952	1.1036
30.	C	15.7301	14.4825	10.1595	8.7612	8.6462	3.2532	2.5220	3.1697
31.	C	16.8963	15.6188	10.9447	9.5944	9.4879	4.5434	3.8905	4.4878
32.	C	17.2330	15.9531	10.7944	9.5660	9.4019	5.2820	5.0111	5.3365
33.	C	16.4019	15.1525	9.6763	8.5709	8.3086	5.0478	5.2469	5.2317
34.	C	18.7042	17.4027	12.0990	10.9074	10.7681	6.7719	6.3765	6.8078
35.	C	19.6543	18.4212	13.2044	12.0531	11.7713	7.2361	6.7455	7.5195
36.	C	19.2112	17.8195	12.7134	11.4053	11.4884	7.5439	6.8974	7.2440
37.	H	8.9513	7.7102	6.2821	4.8781	5.2609	4.7220	5.3739	3.9829
38.	H	7.8713	6.8001	7.8122	6.6866	7.1353	6.9406	7.3561	6.2780
39.	H	6.2975	5.1600	7.3887	6.4950	7.1076	8.3267	8.8988	7.6447
40.	H	6.5928	5.8228	7.6280	6.8701	7.0507	7.7414	8.4384	7.4065
41.	H	5.9198	5.0898	2.1027	3.3866	3.2048	9.3439	10.7983	9.2710
42.	H	3.7890	3.4050	4.3383	5.2934	5.1706	10.5920	11.9852	10.5316
43.	H	4.3333	3.5170	6.3239	6.0210	6.2582	8.9831	9.9609	8.6731
44.	H	2.4793	2.4985	7.1278	7.2984	7.3991	10.8825	11.9648	10.6951
45.	H	12.4766	11.3779	5.3686	4.7187	3.9780	4.8767	6.2814	5.2612
46.	H	14.8508	13.7612	7.3469	6.9338	6.2713	6.6863	7.8121	7.1356
47.	H	16.1727	15.0889	8.8915	8.3210	7.6403	6.4963	7.3893	7.1084
48.	H	15.9116	14.6916	8.4252	7.7304	7.3970	6.8700	7.6281	7.0502
49.	H	15.9235	14.6891	10.7955	9.3412	9.2693	3.3870	2.1029	3.2047
50.	H	17.7644	16.4743	11.9787	10.5856	10.5275	5.2946	4.3388	5.1695
51.	H	16.9641	15.7247	9.9508	8.9738	8.6664	6.0224	6.3245	6.2576
52.	H	18.8423	17.5494	11.9513	10.8690	10.6865	7.3013	7.1291	7.3967
53.	H	3.1412	3.8329	6.4586	7.3425	6.9560	11.6408	13.0373	11.7673
54.	H	3.7737	4.3553	6.9880	7.5451	7.0657	10.7762	12.1032	10.9802
55.	H	2.5400	3.7728	7.9506	8.6035	8.3452	12.3911	13.6608	12.4639
56.	H	1.7747	1.7764	6.2766	7.0029	7.2451	12.3007	13.5356	12.0537
57.	H	0.0000	1.7817	7.8111	8.3301	8.5802	12.9922	14.1224	12.7280
58.	H	1.7817	0.0000	6.7165	7.0012	7.5352	11.9270	12.9777	11.4860
59.	H	7.8111	6.7165	0.0000	1.7826	1.7893	8.2100	9.6344	8.0516
60.	H	8.3301	7.0012	1.7826	0.0000	1.7550	6.9527	8.2098	6.5353
61.	H	8.5802	7.5352	1.7893	1.7550	0.0000	6.5357	8.0519	6.5760
62.	H	12.9922	11.9270	8.2100	6.9527	6.5357	0.0000	1.7826	1.7547
63.	H	14.1224	12.9777	9.6344	8.2098	8.0519	1.7826	0.0000	1.7893
64.	H	12.7280	11.4860	8.0516	6.5353	6.5760	1.7547	1.7893	0.0000
65.	H	20.6844	19.4346	14.1115	12.9821	12.7214	8.3343	7.8150	8.5809
66.	H	19.6696	18.4379	13.5254	12.2918	12.0462	7.0039	6.2792	7.2457
67.	H	19.4398	18.2788	12.9673	11.9181	11.4798	7.0101	6.7270	7.5410
68.	H	18.6606	17.2210	12.0940	10.7659	10.9745	7.5418	6.9810	7.0579
69.	H	19.2147	17.8174	13.0321	11.6358	11.7647	7.3415	6.4554	6.9535
70.	H	20.2621	18.8634	13.6500	12.3801	12.4572	8.6032	7.9481	8.3411

	Atom	65	66	67	68	69	70
1.	O	10.9311	10.2444	9.6148	9.5037	10.1894	10.8729
2.	O	10.2376	9.0267	9.2205	8.2939	8.4724	9.7670
3.	C	10.5737	9.7392	9.3115	8.9788	9.5562	10.4042
4.	C	11.3816	10.3941	10.1866	9.5706	10.0412	11.0660
5.	C	12.7328	11.6898	11.5447	10.8422	11.2829	12.3684
6.	C	13.1280	11.9387	11.9825	11.2224	11.4906	12.7322
7.	C	14.4934	13.2856	13.3251	12.5903	12.8523	14.1071
8.	C	15.3788	14.0669	14.2422	13.4944	13.6213	14.9833
9.	C	15.0363	13.9408	13.8186	13.1370	13.5438	14.6769
10.	C	14.0092	13.0268	12.7884	12.1110	12.6363	13.6540
11.	C	14.3907	13.5539	13.1712	12.4611	13.1482	14.0166
12.	C	13.4806	12.7895	12.3125	11.4953	12.3267	13.0518
13.	C	15.7257	14.9195	14.4803	13.8202	14.5426	15.3747
14.	C	16.8949	16.0110	15.6204	15.0208	15.6673	16.5744
15.	C	17.2349	16.2275	15.9592	15.3691	15.8868	16.9198
16.	C	16.4046	15.3099	15.1598	14.5225	14.9392	16.0660
17.	C	18.7082	17.6668	17.4115	16.8695	17.3536	18.4169
18.	C	19.6529	18.6666	18.4245	17.6023	18.1871	19.2088
19.	C	19.2182	18.1984	17.8306	17.6186	18.0819	19.1041
20.	C	10.2118	9.1304	9.0854	8.3831	8.7219	9.8567
21.	C	9.3054	8.3802	8.0952	7.7033	8.1615	9.1096
22.	C	7.9902	7.1732	6.7718	6.5732	7.0684	7.8925
23.	C	7.9751	7.4532	6.7478	6.6925	7.4301	7.9458
24.	C	6.7710	6.4451	5.6142	5.6703	6.4811	6.7953
25.	C	6.8061	6.8626	5.7589	5.9561	6.9687	6.8996
26.	C	5.7788	5.2237	4.6596	4.6535	5.2274	5.7745
27.	C	6.6750	5.7673	5.5179	5.3765	5.6942	6.6078
28.	C	6.5214	5.2976	5.4157	5.3956	5.2946	6.5140
29.	C	7.8244	6.4443	6.6740	6.7522	6.5035	7.8667
30.	C	5.4563	4.0789	4.5372	4.5635	4.1063	5.4728
31.	C	4.1291	2.8804	3.4191	3.4027	2.8773	4.1246
32.	C	3.4962	2.8451	2.7882	2.7827	2.8480	3.4941
33.	C	4.4361	4.0684	3.4878	3.5491	4.1062	4.4625
34.	C	2.1820	2.1921	2.1935	2.1929	2.1927	2.1807
35.	C	1.0996	1.0998	1.0984	3.5015	2.8150	2.7673
36.	C	2.7654	2.8173	3.5013	1.0983	1.0999	1.0997
37.	H	12.4806	11.2155	11.3865	10.5870	10.7387	12.0658
38.	H	14.8582	13.4819	13.7746	12.9877	13.0084	14.4424
39.	H	16.1751	14.8880	15.0974	14.1077	14.2956	15.6482
40.	H	15.9228	14.5793	14.7087	14.2386	14.3028	15.6745
41.	H	15.9164	15.2201	14.6834	14.0091	14.8371	15.5566
42.	H	17.7622	16.9307	16.4748	15.9057	16.6054	17.4564
43.	H	16.9689	15.7945	15.7348	15.0979	15.4216	16.6297
44.	H	18.8497	17.7252	17.5627	17.0231	17.4118	18.5599
45.	H	8.9493	8.4968	7.7047	7.6529	8.4754	8.9208
46.	H	7.8678	7.9398	6.7892	6.9818	8.0452	7.9604
47.	H	6.2942	6.4613	5.1483	6.0796	6.9395	6.7561
48.	H	6.5886	6.8209	5.8108	5.3778	6.6051	6.3651
49.	H	5.9225	4.3497	5.0995	5.1883	4.4227	5.9725
50.	H	3.7915	2.3216	3.4143	3.4036	2.3204	3.7915
51.	H	4.3299	4.4025	3.5073	3.6654	4.4837	4.4015
52.	H	2.4804	3.0731	2.4979	2.4991	3.0731	2.4761
53.	H	19.2170	18.2829	17.8226	17.6265	18.1761	19.1110
54.	H	18.6721	17.6152	17.2369	17.2481	17.6314	18.6786
55.	H	20.2705	19.2245	18.8765	18.6751	19.1140	20.1619
56.	H	19.6672	18.7657	18.4390	17.6061	18.2819	19.2168
57.	H	20.6844	19.6696	19.4398	18.6606	19.2147	20.2621
58.	H	19.4346	18.4379	18.2788	17.2210	17.8174	18.8634
59.	H	14.1115	13.5254	12.9673	12.0940	13.0321	13.6500
60.	H	12.9821	12.2918	11.9181	10.7659	11.6358	12.3801
61.	H	12.7214	12.0462	11.4798	10.9745	11.7647	12.4572
62.	H	8.3343	7.0039	7.0101	7.5418	7.3415	8.6032
63.	H	7.8150	6.2792	6.7270	6.9810	6.4554	7.9481
64.	H	8.5809	7.2457	7.5410	7.0579	6.9535	8.3411
65.	H	0.0000	1.7749	1.7818	3.7730	3.1380	2.5390
66.	H	1.7749	0.0000	1.7764	3.8328	2.6484	3.1465
67.	H	1.7818	1.7764	0.0000	4.3555	3.8329	3.7724
68.	H	3.7730	3.8328	4.3555	0.0000	1.7764	1.7818
69.	H	3.1380	2.6484	3.8329	1.7764	0.0000	1.7744
70.	H	2.5390	3.1465	3.7724	1.7818	1.7744	0.0000

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	O	1	s	Ryd(3s)	1.99979	30.52830
2	O	1	s	Cor(1s)	1.70446	2.61709
3	O	1	s	Val(2s)	0.00077	8.25683
4	O	1	s	Ryd(4s)	0.00001	59.00354
5	O	1	s	Ryd(5s)	0.00000	213.85319
6	O	1	px	Ryd(3p)	1.60935	2.82777
7	O	1	px	Val(2p)	0.00193	2.30964
8	O	1	px	Ryd(4p)	0.00005	17.00460
9	O	1	py	Ryd(3p)	1.53394	2.59445
10	O	1	py	Val(2p)	0.00257	2.00719

11	O	1	py	Ryd(4p)	0.00000	13.12327
12	O	1	pz	Ryd(3p)	1.73794	2.78115
13	O	1	pz	Val(2p)	0.00263	2.43282
14	O	1	pz	Ryd(4p)	0.00003	15.03096
15	O	1	dxy	Ryd(3d)	0.00312	2.86906
16	O	1	dxz	Ryd(3d)	0.00590	4.34704
17	O	1	dyz	Ryd(3d)	0.00119	2.54960
18	O	1	dx2y2	Ryd(3d)	0.00407	3.54875
19	O	1	dz2	Ryd(3d)	0.00178	3.03158
20	O	1	f(0)	Ryd(4f)	0.00010	5.34507
21	O	1	f(c1)	Ryd(4f)	0.00018	5.96176
22	O	1	f(s1)	Ryd(4f)	0.00001	4.92611
23	O	1	f(c2)	Ryd(4f)	0.00022	5.55765
24	O	1	f(s2)	Ryd(4f)	0.00013	5.43895
25	O	1	f(c3)	Ryd(4f)	0.00011	5.40981
26	O	1	f(s3)	Ryd(4f)	0.00010	5.45213
27	O	2	s	Ryd(3s)	1.99979	30.52836
28	O	2	s	Cor(1s)	1.70444	2.61712
29	O	2	s	Val(2s)	0.00077	8.25884
30	O	2	s	Ryd(4s)	0.00001	58.99015
31	O	2	s	Ryd(5s)	0.00000	213.86181
32	O	2	px	Ryd(3p)	1.60928	2.82776
33	O	2	px	Val(2p)	0.00193	2.30974
34	O	2	px	Ryd(4p)	0.00005	17.00541
35	O	2	py	Ryd(3p)	1.53391	2.59437
36	O	2	py	Val(2p)	0.00257	2.00655
37	O	2	py	Ryd(4p)	0.00000	13.12263
38	O	2	pz	Ryd(3p)	1.73796	2.78126
39	O	2	pz	Val(2p)	0.00264	2.43384
40	O	2	pz	Ryd(4p)	0.00003	15.03201
41	O	2	dxy	Ryd(3d)	0.00312	2.86893
42	O	2	dxz	Ryd(3d)	0.00590	4.34691
43	O	2	dyz	Ryd(3d)	0.00119	2.54831
44	O	2	dx2y2	Ryd(3d)	0.00407	3.54853
45	O	2	dz2	Ryd(3d)	0.00178	3.03169
46	O	2	f(0)	Ryd(4f)	0.00010	5.34560
47	O	2	f(c1)	Ryd(4f)	0.00018	5.96162
48	O	2	f(s1)	Ryd(4f)	0.00001	4.92585
49	O	2	f(c2)	Ryd(4f)	0.00022	5.55767
50	O	2	f(s2)	Ryd(4f)	0.00013	5.43812
51	O	2	f(c3)	Ryd(4f)	0.00011	5.40995
52	O	2	f(s3)	Ryd(4f)	0.00010	5.45194
53	C	3	s	Ryd(3s)	1.99923	16.55311
54	C	3	s	Cor(1s)	0.84849	2.64828
55	C	3	s	Val(2s)	0.00768	3.05920
56	C	3	s	Ryd(4s)	0.00020	27.41369
57	C	3	s	Ryd(5s)	0.00000	100.42685
58	C	3	px	Val(2p)	0.87791	2.32678
59	C	3	px	Ryd(3p)	0.00770	4.98454
60	C	3	px	Ryd(4p)	0.00044	5.04530
61	C	3	py	Val(2p)	0.85590	1.70178
62	C	3	py	Ryd(3p)	0.00106	3.96925
63	C	3	py	Ryd(4p)	0.00027	4.25830
64	C	3	pz	Val(2p)	0.95735	2.16636
65	C	3	pz	Ryd(3p)	0.00396	4.85183
66	C	3	pz	Ryd(4p)	0.00047	5.30677
67	C	3	dxy	Ryd(3d)	0.00179	4.39854
68	C	3	dxz	Ryd(3d)	0.00110	6.41661
69	C	3	dyz	Ryd(3d)	0.00096	3.69352
70	C	3	dx2y2	Ryd(3d)	0.00095	5.78769
71	C	3	dz2	Ryd(3d)	0.00166	5.21361
72	C	3	f(0)	Ryd(4f)	0.00007	7.41156
73	C	3	f(c1)	Ryd(4f)	0.00006	7.80737
74	C	3	f(s1)	Ryd(4f)	0.00002	6.47415
75	C	3	f(c2)	Ryd(4f)	0.00009	7.11025
76	C	3	f(s2)	Ryd(4f)	0.00007	6.70256
77	C	3	f(c3)	Ryd(4f)	0.00010	7.12178
78	C	3	f(s3)	Ryd(4f)	0.00011	7.13397
79	C	4	s	Ryd(3s)	1.99905	16.57135
80	C	4	s	Cor(1s)	0.97853	2.37981
81	C	4	s	Val(2s)	0.00291	2.81424
82	C	4	s	Ryd(4s)	0.00004	29.25428
83	C	4	s	Ryd(5s)	0.00000	101.01489
84	C	4	px	Val(2p)	1.06102	2.05618
85	C	4	px	Ryd(3p)	0.00427	2.24207
86	C	4	px	Ryd(4p)	0.00029	8.30011
87	C	4	py	Ryd(3p)	0.96343	1.61195
88	C	4	py	Val(2p)	0.00392	1.57874
89	C	4	py	Ryd(4p)	0.00012	7.33032
90	C	4	pz	Val(2p)	1.06008	2.12723
91	C	4	pz	Ryd(3p)	0.00302	2.23265
92	C	4	pz	Ryd(4p)	0.00039	8.71046
93	C	4	dxy	Ryd(3d)	0.00053	4.07075
94	C	4	dxz	Ryd(3d)	0.00094	5.23283
95	C	4	dyz	Ryd(3d)	0.00087	3.97794

96	C	4	dx2y2	Ryd(3d)	0.00070	4.48092
97	C	4	dz2	Ryd(3d)	0.00101	5.47274
98	C	4	f(0)	Ryd(4f)	0.00008	7.24001
99	C	4	f(c1)	Ryd(4f)	0.00011	7.30214
100	C	4	f(s1)	Ryd(4f)	0.00009	6.65654
101	C	4	f(c2)	Ryd(4f)	0.00009	6.69527
102	C	4	f(s2)	Ryd(4f)	0.00009	6.71075
103	C	4	f(c3)	Ryd(4f)	0.00009	6.46270
104	C	4	f(s3)	Ryd(4f)	0.00007	6.62974
105	C	5	s	Ryd(3s)	1.99905	16.60051
106	C	5	s	Cor(1s)	0.90088	2.53063
107	C	5	s	Val(2s)	0.00135	2.56530
108	C	5	s	Ryd(4s)	0.00006	28.59313
109	C	5	s	Ryd(5s)	0.00000	102.38291
110	C	5	px	Ryd(3p)	1.06210	1.98871
111	C	5	px	Val(2p)	0.00357	1.87296
112	C	5	px	Ryd(4p)	0.00035	8.03199
113	C	5	py	Ryd(3p)	1.05235	1.72892
114	C	5	py	Val(2p)	0.00460	1.59662
115	C	5	py	Ryd(4p)	0.00022	7.46110
116	C	5	pz	Ryd(3p)	1.06427	2.24577
117	C	5	pz	Val(2p)	0.00377	2.15209
118	C	5	pz	Ryd(4p)	0.00044	8.36506
119	C	5	dxy	Ryd(3d)	0.00057	4.76751
120	C	5	dxz	Ryd(3d)	0.00073	5.12173
121	C	5	dyz	Ryd(3d)	0.00049	4.15377
122	C	5	dx2y2	Ryd(3d)	0.00057	3.80454
123	C	5	dz2	Ryd(3d)	0.00071	5.49596
124	C	5	f(0)	Ryd(4f)	0.00010	7.54880
125	C	5	f(c1)	Ryd(4f)	0.00006	7.30494
126	C	5	f(s1)	Ryd(4f)	0.00007	6.86155
127	C	5	f(c2)	Ryd(4f)	0.00004	6.52177
128	C	5	f(s2)	Ryd(4f)	0.00007	6.92790
129	C	5	f(c3)	Ryd(4f)	0.00009	6.39456
130	C	5	f(s3)	Ryd(4f)	0.00008	6.65734
131	C	6	s	Ryd(3s)	1.99914	16.61589
132	C	6	s	Cor(1s)	0.99204	2.31175
133	C	6	s	Val(2s)	0.00084	2.93477
134	C	6	s	Ryd(4s)	0.00008	31.98204
135	C	6	s	Ryd(5s)	0.00000	97.24173
136	C	6	px	Val(2p)	1.00064	1.86265
137	C	6	px	Ryd(3p)	0.00247	2.27481
138	C	6	px	Ryd(4p)	0.00023	7.24570
139	C	6	py	Val(2p)	0.97009	1.66758
140	C	6	py	Ryd(3p)	0.00253	1.97914
141	C	6	py	Ryd(4p)	0.00020	6.68897
142	C	6	pz	Val(2p)	1.17782	2.15216
143	C	6	pz	Ryd(3p)	0.00186	2.81462
144	C	6	pz	Ryd(4p)	0.00034	7.48127
145	C	6	dxy	Ryd(3d)	0.00069	4.58198
146	C	6	dxz	Ryd(3d)	0.00091	4.94249
147	C	6	dyz	Ryd(3d)	0.00078	4.46175
148	C	6	dx2y2	Ryd(3d)	0.00054	3.64743
149	C	6	dz2	Ryd(3d)	0.00098	5.29510
150	C	6	f(0)	Ryd(4f)	0.00010	7.55034
151	C	6	f(c1)	Ryd(4f)	0.00009	7.49519
152	C	6	f(s1)	Ryd(4f)	0.00007	7.13570
153	C	6	f(c2)	Ryd(4f)	0.00002	6.65695
154	C	6	f(s2)	Ryd(4f)	0.00008	7.07035
155	C	6	f(c3)	Ryd(4f)	0.00007	6.40755
156	C	6	f(s3)	Ryd(4f)	0.00007	6.68578
157	C	7	s	Ryd(3s)	1.99910	16.59599
158	C	7	s	Val(2s)	0.90125	2.47789
159	C	7	s	Cor(1s)	0.00090	2.42696
160	C	7	s	Ryd(4s)	0.00006	29.98709
161	C	7	s	Ryd(5s)	0.00000	100.73162
162	C	7	px	Val(2p)	1.02361	2.03354
163	C	7	px	Ryd(3p)	0.00293	2.48294
164	C	7	px	Ryd(4p)	0.00030	7.48329
165	C	7	py	Val(2p)	1.03113	1.82083
166	C	7	py	Ryd(3p)	0.00361	2.13275
167	C	7	py	Ryd(4p)	0.00024	7.15444
168	C	7	pz	Val(2p)	1.04736	2.09866
169	C	7	pz	Ryd(3p)	0.00298	2.55038
170	C	7	pz	Ryd(4p)	0.00034	8.20282
171	C	7	dxy	Ryd(3d)	0.00047	4.82904
172	C	7	dxz	Ryd(3d)	0.00084	5.17278
173	C	7	dyz	Ryd(3d)	0.00057	4.48327
174	C	7	dx2y2	Ryd(3d)	0.00060	3.77535
175	C	7	dz2	Ryd(3d)	0.00054	4.96104
176	C	7	f(0)	Ryd(4f)	0.00002	6.96751
177	C	7	f(c1)	Ryd(4f)	0.00009	7.30743
178	C	7	f(s1)	Ryd(4f)	0.00007	6.85039
179	C	7	f(c2)	Ryd(4f)	0.00002	6.67065
180	C	7	f(s2)	Ryd(4f)	0.00006	7.07234

181	C	7	f(c3)	Ryd(4f)	0.00010	6.53680
182	C	7	f(s3)	Ryd(4f)	0.00009	6.79004
183	C	8	s	Ryd(3s)	1.99943	16.60371
184	C	8	s	Cor(1s)	1.09744	2.11682
185	C	8	s	Val(2s)	0.00033	3.08825
186	C	8	s	Ryd(4s)	0.00002	24.23787
187	C	8	s	Ryd(5s)	0.00000	106.18018
188	C	8	px	Val(2p)	1.14179	1.76212
189	C	8	px	Ryd(3p)	0.00041	1.97449
190	C	8	px	Ryd(4p)	0.00013	6.35990
191	C	8	py	Val(2p)	1.17661	1.75461
192	C	8	py	Ryd(3p)	0.00052	1.98410
193	C	8	py	Ryd(4p)	0.00012	6.18759
194	C	8	pz	Val(2p)	1.23697	1.79132
195	C	8	pz	Ryd(3p)	0.00113	2.59862
196	C	8	pz	Ryd(4p)	0.00006	6.45075
197	C	8	dxy	Ryd(3d)	0.00093	4.75150
198	C	8	dxz	Ryd(3d)	0.00118	4.63915
199	C	8	dyz	Ryd(3d)	0.00055	4.06996
200	C	8	dx2y2	Ryd(3d)	0.00105	4.40905
201	C	8	dz2	Ryd(3d)	0.00120	4.72990
202	C	8	f(0)	Ryd(4f)	0.00005	7.32108
203	C	8	f(c1)	Ryd(4f)	0.00007	7.44061
204	C	8	f(s1)	Ryd(4f)	0.00000	6.90141
205	C	8	f(c2)	Ryd(4f)	0.00001	6.86018
206	C	8	f(s2)	Ryd(4f)	0.00002	7.00327
207	C	8	f(c3)	Ryd(4f)	0.00002	7.03976
208	C	8	f(s3)	Ryd(4f)	0.00007	7.34931
209	C	9	s	Ryd(3s)	1.99905	16.60893
210	C	9	s	Cor(1s)	0.90972	2.52825
211	C	9	s	Val(2s)	0.00161	2.90997
212	C	9	s	Ryd(4s)	0.00006	29.56827
213	C	9	s	Ryd(5s)	0.00000	100.25388
214	C	9	px	Ryd(3p)	1.02593	1.95084
215	C	9	px	Val(2p)	0.00348	1.91830
216	C	9	px	Ryd(4p)	0.00023	7.97418
217	C	9	py	Ryd(3p)	0.98633	1.82763
218	C	9	py	Val(2p)	0.00306	1.72484
219	C	9	py	Ryd(4p)	0.00018	7.62460
220	C	9	pz	Ryd(3p)	1.06218	2.25673
221	C	9	pz	Val(2p)	0.00365	2.21067
222	C	9	pz	Ryd(4p)	0.00041	8.29536
223	C	9	dxy	Ryd(3d)	0.00058	4.61317
224	C	9	dxz	Ryd(3d)	0.00079	5.01478
225	C	9	dyz	Ryd(3d)	0.00075	4.61174
226	C	9	dx2y2	Ryd(3d)	0.00053	3.58161
227	C	9	dz2	Ryd(3d)	0.00078	5.39039
228	C	9	f(0)	Ryd(4f)	0.00007	7.24966
229	C	9	f(c1)	Ryd(4f)	0.00009	7.24821
230	C	9	f(s1)	Ryd(4f)	0.00010	7.09212
231	C	9	f(c2)	Ryd(4f)	0.00003	6.59835
232	C	9	f(s2)	Ryd(4f)	0.00006	7.02994
233	C	9	f(c3)	Ryd(4f)	0.00007	6.36775
234	C	9	f(s3)	Ryd(4f)	0.00007	6.53717
235	C	10	s	Ryd(3s)	1.99899	16.60067
236	C	10	s	Cor(1s)	0.90885	2.53790
237	C	10	s	Val(2s)	0.00138	3.21936
238	C	10	s	Ryd(4s)	0.00006	30.19581
239	C	10	s	Ryd(5s)	0.00000	99.27604
240	C	10	px	Ryd(3p)	1.01614	1.93919
241	C	10	px	Val(2p)	0.00366	1.54891
242	C	10	px	Ryd(4p)	0.00030	8.07697
243	C	10	py	Ryd(3p)	1.00917	1.85062
244	C	10	py	Val(2p)	0.00335	1.46465
245	C	10	py	Ryd(4p)	0.00022	7.89748
246	C	10	pz	Ryd(3p)	1.05235	2.20677
247	C	10	pz	Val(2p)	0.00377	1.88396
248	C	10	pz	Ryd(4p)	0.00043	8.55251
249	C	10	dxy	Ryd(3d)	0.00062	4.97813
250	C	10	dxz	Ryd(3d)	0.00074	4.61287
251	C	10	dyz	Ryd(3d)	0.00078	4.47168
252	C	10	dx2y2	Ryd(3d)	0.00047	3.55034
253	C	10	dz2	Ryd(3d)	0.00076	5.43000
254	C	10	f(0)	Ryd(4f)	0.00009	7.39440
255	C	10	f(c1)	Ryd(4f)	0.00004	7.04808
256	C	10	f(s1)	Ryd(4f)	0.00005	6.90403
257	C	10	f(c2)	Ryd(4f)	0.00002	6.36844
258	C	10	f(s2)	Ryd(4f)	0.00010	7.00830
259	C	10	f(c3)	Ryd(4f)	0.00009	6.54523
260	C	10	f(s3)	Ryd(4f)	0.00009	6.68554
261	C	11	s	Ryd(3s)	1.99908	16.61098
262	C	11	s	Val(2s)	0.91629	2.50152
263	C	11	s	Cor(1s)	0.00053	2.44243
264	C	11	s	Ryd(4s)	0.00006	29.13523

265	C 11	s	Ryd(5s)	0.00000	101.27226
266	C 11	px	Val(2p)	0.94757	1.87270
267	C 11	px	Ryd(3p)	0.00290	2.21406
268	C 11	px	Ryd(4p)	0.00014	7.30362
269	C 11	py	Val(2p)	0.98316	1.98056
270	C 11	py	Ryd(3p)	0.00275	2.41456
271	C 11	py	Ryd(4p)	0.00017	7.47656
272	C 11	pz	Val(2p)	1.04806	2.26324
273	C 11	pz	Ryd(3p)	0.00217	2.57303
274	C 11	pz	Ryd(4p)	0.00027	8.04807
275	C 11	dxy	Ryd(3d)	0.00050	4.78133
276	C 11	dxz	Ryd(3d)	0.00069	4.55240
277	C 11	dyz	Ryd(3d)	0.00075	4.80142
278	C 11	dx2y2	Ryd(3d)	0.00044	3.61694
279	C 11	dz2	Ryd(3d)	0.00073	5.50377
280	C 11	f(0)	Ryd(4f)	0.00010	7.41583
281	C 11	f(c1)	Ryd(4f)	0.00005	7.01435
282	C 11	f(s1)	Ryd(4f)	0.00004	7.09795
283	C 11	f(c2)	Ryd(4f)	0.00001	6.45957
284	C 11	f(s2)	Ryd(4f)	0.00008	7.03974
285	C 11	f(c3)	Ryd(4f)	0.00007	6.56410
286	C 11	f(s3)	Ryd(4f)	0.00006	6.45469
287	C 12	s	Ryd(3s)	1.99941	16.61087
288	C 12	s	Cor(1s)	1.10100	2.12115
289	C 12	s	Val(2s)	0.00043	3.23622
290	C 12	s	Ryd(4s)	0.00003	24.95978
291	C 12	s	Ryd(5s)	0.00000	104.27974
292	C 12	px	Val(2p)	1.20421	1.74737
293	C 12	px	Ryd(3p)	0.00103	1.78522
294	C 12	px	Ryd(4p)	0.00010	6.89891
295	C 12	py	Val(2p)	1.13423	1.74748
296	C 12	py	Ryd(3p)	0.00096	1.79128
297	C 12	py	Ryd(4p)	0.00013	6.81311
298	C 12	pz	Val(2p)	1.22643	1.81516
299	C 12	pz	Ryd(3p)	0.00132	2.54199
300	C 12	pz	Ryd(4p)	0.00018	7.00011
301	C 12	dxy	Ryd(3d)	0.00118	4.93881
302	C 12	dxz	Ryd(3d)	0.00137	5.06869
303	C 12	dyz	Ryd(3d)	0.00124	4.87208
304	C 12	dx2y2	Ryd(3d)	0.00031	4.02483
305	C 12	dz2	Ryd(3d)	0.00042	4.13391
306	C 12	f(0)	Ryd(4f)	0.00001	6.93398
307	C 12	f(c1)	Ryd(4f)	0.00002	7.17805
308	C 12	f(s1)	Ryd(4f)	0.00002	7.08628
309	C 12	f(c2)	Ryd(4f)	0.00002	7.23787
310	C 12	f(s2)	Ryd(4f)	0.00015	8.25270
311	C 12	f(c3)	Ryd(4f)	0.00002	7.04258
312	C 12	f(s3)	Ryd(4f)	0.00000	6.88792
313	C 13	s	Ryd(3s)	1.99918	16.61139
314	C 13	s	Cor(1s)	0.97701	2.33233
315	C 13	s	Val(2s)	0.00136	2.62766
316	C 13	s	Ryd(4s)	0.00008	29.17671
317	C 13	s	Ryd(5s)	0.00000	101.06461
318	C 13	px	Val(2p)	1.07283	1.76233
319	C 13	px	Ryd(3p)	0.00329	2.31793
320	C 13	px	Ryd(4p)	0.00015	6.67873
321	C 13	py	Val(2p)	1.06938	1.85171
322	C 13	py	Ryd(3p)	0.00291	2.48971
323	C 13	py	Ryd(4p)	0.00015	6.82612
324	C 13	pz	Val(2p)	1.07126	2.18404
325	C 13	pz	Ryd(3p)	0.00229	2.87151
326	C 13	pz	Ryd(4p)	0.00021	7.58527
327	C 13	dxy	Ryd(3d)	0.00073	4.73121
328	C 13	dxz	Ryd(3d)	0.00069	4.46452
329	C 13	dyz	Ryd(3d)	0.00077	4.85843
330	C 13	dx2y2	Ryd(3d)	0.00023	3.48600
331	C 13	dz2	Ryd(3d)	0.00081	5.31199
332	C 13	f(0)	Ryd(4f)	0.00013	7.48403
333	C 13	f(c1)	Ryd(4f)	0.00006	6.98692
334	C 13	f(s1)	Ryd(4f)	0.00006	7.29861
335	C 13	f(c2)	Ryd(4f)	0.00002	6.57894
336	C 13	f(s2)	Ryd(4f)	0.00011	7.19374
337	C 13	f(c3)	Ryd(4f)	0.00007	6.53888
338	C 13	f(s3)	Ryd(4f)	0.00007	6.47914
339	C 14	s	Ryd(3s)	1.99915	16.62132
340	C 14	s	Cor(1s)	0.97503	2.34521
341	C 14	s	Val(2s)	0.00142	2.49927
342	C 14	s	Ryd(4s)	0.00008	29.63079
343	C 14	s	Ryd(5s)	0.00000	100.32710
344	C 14	px	Val(2p)	1.02229	1.88259
345	C 14	px	Ryd(3p)	0.00195	2.27700
346	C 14	px	Ryd(4p)	0.00014	7.17436
347	C 14	py	Val(2p)	1.00699	1.90047
348	C 14	py	Ryd(3p)	0.00177	2.35239
349	C 14	py	Ryd(4p)	0.00015	7.20700

350	C 14	pz	Val(2p)	1.15576	2.06552
351	C 14	pz	Ryd(3p)	0.00331	2.83767
352	C 14	pz	Ryd(4p)	0.00013	7.61636
353	C 14	dxy	Ryd(3d)	0.00072	5.14677
354	C 14	dxz	Ryd(3d)	0.00063	4.47461
355	C 14	dyz	Ryd(3d)	0.00058	4.58876
356	C 14	dx2y2	Ryd(3d)	0.00048	3.69713
357	C 14	dz2	Ryd(3d)	0.00095	4.92644
358	C 14	f(0)	Ryd(4f)	0.00007	7.14261
359	C 14	f(c1)	Ryd(4f)	0.00006	7.03672
360	C 14	f(s1)	Ryd(4f)	0.00004	6.98323
361	C 14	f(c2)	Ryd(4f)	0.00002	6.52727
362	C 14	f(s2)	Ryd(4f)	0.00012	7.12022
363	C 14	f(c3)	Ryd(4f)	0.00011	6.87955
364	C 14	f(s3)	Ryd(4f)	0.00012	6.89199
365	C 15	s	Ryd(3s)	1.99909	16.60869
366	C 15	s	Cor(1s)	0.90878	2.50103
367	C 15	s	Val(2s)	0.00174	2.93570
368	C 15	s	Ryd(4s)	0.00007	29.37127
369	C 15	s	Ryd(5s)	0.00000	101.14441
370	C 15	px	Val(2p)	1.01776	1.95956
371	C 15	px	Ryd(3p)	0.00358	1.96870
372	C 15	px	Ryd(4p)	0.00021	7.80447
373	C 15	py	Val(2p)	1.00751	1.89746
374	C 15	py	Ryd(3p)	0.00409	1.99671
375	C 15	py	Ryd(4p)	0.00017	7.82285
376	C 15	pz	Val(2p)	1.03755	2.20151
377	C 15	pz	Ryd(3p)	0.00463	2.46178
378	C 15	pz	Ryd(4p)	0.00039	9.09251
379	C 15	dxy	Ryd(3d)	0.00062	5.07460
380	C 15	dxz	Ryd(3d)	0.00063	4.85076
381	C 15	dyz	Ryd(3d)	0.00054	4.33164
382	C 15	dx2y2	Ryd(3d)	0.00037	3.72023
383	C 15	dz2	Ryd(3d)	0.00076	5.22913
384	C 15	f(0)	Ryd(4f)	0.00004	7.03762
385	C 15	f(c1)	Ryd(4f)	0.00009	7.19190
386	C 15	f(s1)	Ryd(4f)	0.00006	6.88669
387	C 15	f(c2)	Ryd(4f)	0.00002	6.55816
388	C 15	f(s2)	Ryd(4f)	0.00007	7.03548
389	C 15	f(c3)	Ryd(4f)	0.00008	6.59549
390	C 15	f(s3)	Ryd(4f)	0.00008	6.66725
391	C 16	s	Ryd(3s)	1.99909	16.62480
392	C 16	s	Cor(1s)	0.96742	2.37535
393	C 16	s	Val(2s)	0.00106	2.64614
394	C 16	s	Ryd(4s)	0.00008	30.37268
395	C 16	s	Ryd(5s)	0.00000	100.17618
396	C 16	px	Val(2p)	1.08503	1.85222
397	C 16	px	Ryd(3p)	0.00332	2.10406
398	C 16	px	Ryd(4p)	0.00015	7.25673
399	C 16	py	Val(2p)	1.04365	1.74911
400	C 16	py	Ryd(3p)	0.00338	1.95004
401	C 16	py	Ryd(4p)	0.00016	7.02544
402	C 16	pz	Val(2p)	1.05983	2.24641
403	C 16	pz	Ryd(3p)	0.00188	2.37517
404	C 16	pz	Ryd(4p)	0.00026	8.42273
405	C 16	dxy	Ryd(3d)	0.00078	4.56225
406	C 16	dxz	Ryd(3d)	0.00077	4.80613
407	C 16	dyz	Ryd(3d)	0.00073	4.51132
408	C 16	dx2y2	Ryd(3d)	0.00023	3.48831
409	C 16	dz2	Ryd(3d)	0.00095	5.55039
410	C 16	f(0)	Ryd(4f)	0.00009	7.55305
411	C 16	f(c1)	Ryd(4f)	0.00013	7.44890
412	C 16	f(s1)	Ryd(4f)	0.00012	7.25683
413	C 16	f(c2)	Ryd(4f)	0.00003	6.52954
414	C 16	f(s2)	Ryd(4f)	0.00004	6.94556
415	C 16	f(c3)	Ryd(4f)	0.00006	6.43261
416	C 16	f(s3)	Ryd(4f)	0.00008	6.54874
417	C 17	s	Ryd(3s)	1.99935	16.59424
418	C 17	s	Cor(1s)	0.98734	2.35694
419	C 17	s	Val(2s)	0.00082	3.70680
420	C 17	s	Ryd(4s)	0.00005	27.10327
421	C 17	s	Ryd(5s)	0.00000	102.99922
422	C 17	px	Val(2p)	1.09749	1.87051
423	C 17	px	Ryd(3p)	0.00287	2.32552
424	C 17	px	Ryd(4p)	0.00019	7.44525
425	C 17	py	Val(2p)	1.06776	1.87385
426	C 17	py	Ryd(3p)	0.00220	2.23889
427	C 17	py	Ryd(4p)	0.00021	7.29530
428	C 17	pz	Val(2p)	1.04542	1.91902
429	C 17	pz	Ryd(3p)	0.00165	2.64239
430	C 17	pz	Ryd(4p)	0.00032	7.65169
431	C 17	dxy	Ryd(3d)	0.00085	5.43937
432	C 17	dxz	Ryd(3d)	0.00068	4.91245
433	C 17	dyz	Ryd(3d)	0.00080	5.19765
434	C 17	dx2y2	Ryd(3d)	0.00031	4.06138

435	C 17	dz2	Ryd(3d)	0.00037	4.45113
436	C 17	f(0)	Ryd(4f)	0.00000	6.66009
437	C 17	f(c1)	Ryd(4f)	0.00001	6.80992
438	C 17	f(s1)	Ryd(4f)	0.00004	7.12290
439	C 17	f(c2)	Ryd(4f)	0.00000	6.78659
440	C 17	f(s2)	Ryd(4f)	0.00010	7.93501
441	C 17	f(c3)	Ryd(4f)	0.00000	6.82307
442	C 17	f(s3)	Ryd(4f)	0.00002	6.93409
443	C 18	s	Ryd(3s)	1.99948	16.59956
444	C 18	s	Cor(1s)	1.10520	2.07895
445	C 18	s	Val(2s)	0.00070	2.95825
446	C 18	s	Ryd(4s)	0.00002	21.02051
447	C 18	s	Ryd(5s)	0.00000	107.40165
448	C 18	px	Val(2p)	1.19752	1.74452
449	C 18	px	Ryd(3p)	0.00058	2.84371
450	C 18	px	Ryd(4p)	0.00005	5.53763
451	C 18	py	Val(2p)	1.17143	1.76419
452	C 18	py	Ryd(3p)	0.00073	2.85788
453	C 18	py	Ryd(4p)	0.00003	5.57341
454	C 18	pz	Val(2p)	1.13874	1.75637
455	C 18	pz	Ryd(3p)	0.00064	2.77620
456	C 18	pz	Ryd(4p)	0.00010	5.73847
457	C 18	dxy	Ryd(3d)	0.00163	4.95161
458	C 18	dxz	Ryd(3d)	0.00107	4.55267
459	C 18	dyz	Ryd(3d)	0.00145	4.82177
460	C 18	dx2y2	Ryd(3d)	0.00017	3.85627
461	C 18	dz2	Ryd(3d)	0.00044	4.05572
462	C 18	f(0)	Ryd(4f)	0.00001	6.77512
463	C 18	f(c1)	Ryd(4f)	0.00001	6.91646
464	C 18	f(s1)	Ryd(4f)	0.00005	7.14478
465	C 18	f(c2)	Ryd(4f)	0.00000	6.95463
466	C 18	f(s2)	Ryd(4f)	0.00017	8.07293
467	C 18	f(c3)	Ryd(4f)	0.00001	6.93745
468	C 18	f(s3)	Ryd(4f)	0.00003	7.04928
469	C 19	s	Ryd(3s)	1.99948	16.59957
470	C 19	s	Cor(1s)	1.10492	2.07937
471	C 19	s	Val(2s)	0.00070	2.96545
472	C 19	s	Ryd(4s)	0.00002	21.18948
473	C 19	s	Ryd(5s)	0.00000	107.26959
474	C 19	px	Val(2p)	1.14243	1.75878
475	C 19	px	Ryd(3p)	0.00060	2.73879
476	C 19	px	Ryd(4p)	0.00004	5.57350
477	C 19	py	Val(2p)	1.16639	1.74247
478	C 19	py	Ryd(3p)	0.00057	2.78890
479	C 19	py	Ryd(4p)	0.00008	5.64554
480	C 19	pz	Val(2p)	1.19933	1.76424
481	C 19	pz	Ryd(3p)	0.00081	3.02322
482	C 19	pz	Ryd(4p)	0.00005	5.56381
483	C 19	dxy	Ryd(3d)	0.00136	4.80962
484	C 19	dxz	Ryd(3d)	0.00111	4.57265
485	C 19	dyz	Ryd(3d)	0.00166	4.92601
486	C 19	dx2y2	Ryd(3d)	0.00017	3.90911
487	C 19	dz2	Ryd(3d)	0.00044	4.02403
488	C 19	f(0)	Ryd(4f)	0.00001	6.83114
489	C 19	f(c1)	Ryd(4f)	0.00000	6.88631
490	C 19	f(s1)	Ryd(4f)	0.00005	7.23532
491	C 19	f(c2)	Ryd(4f)	0.00001	6.99497
492	C 19	f(s2)	Ryd(4f)	0.00017	8.04305
493	C 19	f(c3)	Ryd(4f)	0.00000	6.87867
494	C 19	f(s3)	Ryd(4f)	0.00003	6.98446
495	C 20	s	Ryd(3s)	1.99923	16.55308
496	C 20	s	Cor(1s)	0.84851	2.64824
497	C 20	s	Val(2s)	0.00768	3.05986
498	C 20	s	Ryd(4s)	0.00020	27.41174
499	C 20	s	Ryd(5s)	0.00000	100.42838
500	C 20	px	Val(2p)	0.87783	2.32669
501	C 20	px	Ryd(3p)	0.00770	4.98503
502	C 20	px	Ryd(4p)	0.00044	5.04434
503	C 20	py	Val(2p)	0.85591	1.70188
504	C 20	py	Ryd(3p)	0.00106	3.97000
505	C 20	py	Ryd(4p)	0.00027	4.25536
506	C 20	pz	Val(2p)	0.95734	2.16641
507	C 20	pz	Ryd(3p)	0.00396	4.85245
508	C 20	pz	Ryd(4p)	0.00047	5.30892
509	C 20	dxy	Ryd(3d)	0.00179	4.40104
510	C 20	dxz	Ryd(3d)	0.00110	6.41680
511	C 20	dyz	Ryd(3d)	0.00096	3.69290
512	C 20	dx2y2	Ryd(3d)	0.00095	5.78653
513	C 20	dz2	Ryd(3d)	0.00166	5.21450
514	C 20	f(0)	Ryd(4f)	0.00007	7.41254
515	C 20	f(c1)	Ryd(4f)	0.00006	7.80712
516	C 20	f(s1)	Ryd(4f)	0.00002	6.47358
517	C 20	f(c2)	Ryd(4f)	0.00009	7.10929
518	C 20	f(s2)	Ryd(4f)	0.00007	6.70299
519	C 20	f(c3)	Ryd(4f)	0.00010	7.12234

520	C 20	f(s3)	Ryd(4f)	0.00011	7.13359
521	C 21	s	Ryd(3s)	1.99905	16.57136
522	C 21	s	Cor(1s)	0.97854	2.37977
523	C 21	s	Val(2s)	0.00291	2.81401
524	C 21	s	Ryd(4s)	0.00004	29.24795
525	C 21	s	Ryd(5s)	0.00000	101.01981
526	C 21	px	Val(2p)	1.06092	2.05590
527	C 21	px	Ryd(3p)	0.00427	2.24204
528	C 21	px	Ryd(4p)	0.00029	8.29902
529	C 21	py	Ryd(3p)	0.96359	1.61268
530	C 21	py	Val(2p)	0.00391	1.57925
531	C 21	py	Ryd(4p)	0.00012	7.33117
532	C 21	pz	Val(2p)	1.06004	2.12677
533	C 21	pz	Ryd(3p)	0.00302	2.23240
534	C 21	pz	Ryd(4p)	0.00039	8.71070
535	C 21	dxy	Ryd(3d)	0.00053	4.07444
536	C 21	dxz	Ryd(3d)	0.00095	5.23001
537	C 21	dyz	Ryd(3d)	0.00086	3.98167
538	C 21	dx2y2	Ryd(3d)	0.00070	4.47834
539	C 21	dz2	Ryd(3d)	0.00101	5.47054
540	C 21	f(0)	Ryd(4f)	0.00008	7.23861
541	C 21	f(c1)	Ryd(4f)	0.00011	7.29998
542	C 21	f(s1)	Ryd(4f)	0.00009	6.65807
543	C 21	f(c2)	Ryd(4f)	0.00009	6.69385
544	C 21	f(s2)	Ryd(4f)	0.00009	6.71282
545	C 21	f(c3)	Ryd(4f)	0.00009	6.46253
546	C 21	f(s3)	Ryd(4f)	0.00008	6.63125
547	C 22	s	Ryd(3s)	1.99905	16.60053
548	C 22	s	Cor(1s)	0.90088	2.53063
549	C 22	s	Val(2s)	0.00135	2.56535
550	C 22	s	Ryd(4s)	0.00006	28.59133
551	C 22	s	Ryd(5s)	0.00000	102.38392
552	C 22	px	Ryd(3p)	1.06206	1.98847
553	C 22	px	Val(2p)	0.00357	1.87253
554	C 22	px	Ryd(4p)	0.00035	8.03205
555	C 22	py	Ryd(3p)	1.05240	1.72959
556	C 22	py	Val(2p)	0.00460	1.59728
557	C 22	py	Ryd(4p)	0.00022	7.46205
558	C 22	pz	Ryd(3p)	1.06427	2.24537
559	C 22	pz	Val(2p)	0.00377	2.15171
560	C 22	pz	Ryd(4p)	0.00044	8.36501
561	C 22	dxy	Ryd(3d)	0.00057	4.76891
562	C 22	dxz	Ryd(3d)	0.00073	5.12136
563	C 22	dyz	Ryd(3d)	0.00049	4.15827
564	C 22	dx2y2	Ryd(3d)	0.00057	3.80389
565	C 22	dz2	Ryd(3d)	0.00071	5.49193
566	C 22	f(0)	Ryd(4f)	0.00010	7.54608
567	C 22	f(c1)	Ryd(4f)	0.00006	7.30294
568	C 22	f(s1)	Ryd(4f)	0.00007	6.86387
569	C 22	f(c2)	Ryd(4f)	0.00004	6.52238
570	C 22	f(s2)	Ryd(4f)	0.00007	6.93022
571	C 22	f(c3)	Ryd(4f)	0.00009	6.39485
572	C 22	f(s3)	Ryd(4f)	0.00008	6.65735
573	C 23	s	Ryd(3s)	1.99914	16.61591
574	C 23	s	Cor(1s)	0.99206	2.31173
575	C 23	s	Val(2s)	0.00084	2.93395
576	C 23	s	Ryd(4s)	0.00008	31.97821
577	C 23	s	Ryd(5s)	0.00000	97.24547
578	C 23	px	Val(2p)	1.00062	1.86228
579	C 23	px	Ryd(3p)	0.00247	2.27409
580	C 23	px	Ryd(4p)	0.00023	7.24529
581	C 23	py	Val(2p)	0.97012	1.66845
582	C 23	py	Ryd(3p)	0.00253	1.98053
583	C 23	py	Ryd(4p)	0.00020	6.69093
584	C 23	pz	Val(2p)	1.17778	2.15168
585	C 23	pz	Ryd(3p)	0.00187	2.81406
586	C 23	pz	Ryd(4p)	0.00034	7.48039
587	C 23	dxy	Ryd(3d)	0.00069	4.58300
588	C 23	dxz	Ryd(3d)	0.00091	4.94007
589	C 23	dyz	Ryd(3d)	0.00078	4.46763
590	C 23	dx2y2	Ryd(3d)	0.00054	3.64790
591	C 23	dz2	Ryd(3d)	0.00098	5.29025
592	C 23	f(0)	Ryd(4f)	0.00010	7.54791
593	C 23	f(c1)	Ryd(4f)	0.00009	7.49224
594	C 23	f(s1)	Ryd(4f)	0.00007	7.13771
595	C 23	f(c2)	Ryd(4f)	0.00002	6.65872
596	C 23	f(s2)	Ryd(4f)	0.00008	7.07170
597	C 23	f(c3)	Ryd(4f)	0.00007	6.40830
598	C 23	f(s3)	Ryd(4f)	0.00007	6.68552
599	C 24	s	Ryd(3s)	1.99910	16.59598
600	C 24	s	Val(2s)	0.90126	2.47787
601	C 24	s	Cor(1s)	0.00090	2.42702
602	C 24	s	Ryd(4s)	0.00006	29.98560
603	C 24	s	Ryd(5s)	0.00000	100.73288

604	C 24	px	Val(2p)	1.02360	2.03289
605	C 24	px	Ryd(3p)	0.00293	2.48170
606	C 24	px	Ryd(4p)	0.00030	7.48151
607	C 24	py	Val(2p)	1.03117	1.82206
608	C 24	py	Ryd(3p)	0.00361	2.13558
609	C 24	py	Ryd(4p)	0.00025	7.15781
610	C 24	pz	Val(2p)	1.04732	2.09808
611	C 24	pz	Ryd(3p)	0.00298	2.54949
612	C 24	pz	Ryd(4p)	0.00033	8.20024
613	C 24	dxy	Ryd(3d)	0.00047	4.83089
614	C 24	dxz	Ryd(3d)	0.00084	5.17035
615	C 24	dyz	Ryd(3d)	0.00057	4.48854
616	C 24	dx2y2	Ryd(3d)	0.00060	3.77530
617	C 24	dz2	Ryd(3d)	0.00054	4.95621
618	C 24	f(0)	Ryd(4f)	0.00002	6.96502
619	C 24	f(c1)	Ryd(4f)	0.00009	7.30535
620	C 24	f(s1)	Ryd(4f)	0.00007	6.85172
621	C 24	f(c2)	Ryd(4f)	0.00002	6.67188
622	C 24	f(s2)	Ryd(4f)	0.00006	7.07286
623	C 24	f(c3)	Ryd(4f)	0.00010	6.53832
624	C 24	f(s3)	Ryd(4f)	0.00009	6.78960
625	C 25	s	Ryd(3s)	1.99943	16.60371
626	C 25	s	Cor(1s)	1.09744	2.11680
627	C 25	s	Val(2s)	0.00033	3.08877
628	C 25	s	Ryd(4s)	0.00002	24.23098
629	C 25	s	Ryd(5s)	0.00000	106.18564
630	C 25	px	Val(2p)	1.14194	1.76213
631	C 25	px	Ryd(3p)	0.00041	1.97475
632	C 25	px	Ryd(4p)	0.00013	6.36008
633	C 25	py	Val(2p)	1.17649	1.75471
634	C 25	py	Ryd(3p)	0.00052	1.98467
635	C 25	py	Ryd(4p)	0.00012	6.18713
636	C 25	pz	Val(2p)	1.23696	1.79117
637	C 25	pz	Ryd(3p)	0.00113	2.59766
638	C 25	pz	Ryd(4p)	0.00006	6.45040
639	C 25	dxy	Ryd(3d)	0.00092	4.75107
640	C 25	dxz	Ryd(3d)	0.00119	4.64282
641	C 25	dyz	Ryd(3d)	0.00054	4.06432
642	C 25	dx2y2	Ryd(3d)	0.00105	4.41018
643	C 25	dz2	Ryd(3d)	0.00120	4.73074
644	C 25	f(0)	Ryd(4f)	0.00005	7.31915
645	C 25	f(c1)	Ryd(4f)	0.00007	7.44611
646	C 25	f(s1)	Ryd(4f)	0.00000	6.90003
647	C 25	f(c2)	Ryd(4f)	0.00001	6.85950
648	C 25	f(s2)	Ryd(4f)	0.00002	6.99941
649	C 25	f(c3)	Ryd(4f)	0.00002	7.04229
650	C 25	f(s3)	Ryd(4f)	0.00007	7.34833
651	C 26	s	Ryd(3s)	1.99905	16.60894
652	C 26	s	Cor(1s)	0.90973	2.52823
653	C 26	s	Val(2s)	0.00161	2.90979
654	C 26	s	Ryd(4s)	0.00006	29.56738
655	C 26	s	Ryd(5s)	0.00000	100.25493
656	C 26	px	Ryd(3p)	1.02583	1.95015
657	C 26	px	Val(2p)	0.00348	1.91726
658	C 26	px	Ryd(4p)	0.00023	7.97260
659	C 26	py	Ryd(3p)	0.98650	1.82949
660	C 26	py	Val(2p)	0.00306	1.72666
661	C 26	py	Ryd(4p)	0.00018	7.62831
662	C 26	pz	Ryd(3p)	1.06203	2.25556
663	C 26	pz	Val(2p)	0.00365	2.20936
664	C 26	pz	Ryd(4p)	0.00041	8.29256
665	C 26	dxy	Ryd(3d)	0.00058	4.61503
666	C 26	dxz	Ryd(3d)	0.00079	5.01055
667	C 26	dyz	Ryd(3d)	0.00075	4.62072
668	C 26	dx2y2	Ryd(3d)	0.00053	3.58334
669	C 26	dz2	Ryd(3d)	0.00078	5.38255
670	C 26	f(0)	Ryd(4f)	0.00006	7.24484
671	C 26	f(c1)	Ryd(4f)	0.00009	7.24407
672	C 26	f(s1)	Ryd(4f)	0.00010	7.09551
673	C 26	f(c2)	Ryd(4f)	0.00003	6.60070
674	C 26	f(s2)	Ryd(4f)	0.00006	7.03013
675	C 26	f(c3)	Ryd(4f)	0.00007	6.37086
676	C 26	f(s3)	Ryd(4f)	0.00007	6.53721
677	C 27	s	Ryd(3s)	1.99899	16.60070
678	C 27	s	Cor(1s)	0.90881	2.53798
679	C 27	s	Val(2s)	0.00138	3.21939
680	C 27	s	Ryd(4s)	0.00006	30.19524
681	C 27	s	Ryd(5s)	0.00000	99.27713
682	C 27	px	Ryd(3p)	1.01617	1.93894
683	C 27	px	Val(2p)	0.00366	1.54856
684	C 27	px	Ryd(4p)	0.00030	8.07599
685	C 27	py	Ryd(3p)	1.00913	1.85100
686	C 27	py	Val(2p)	0.00336	1.46554
687	C 27	py	Ryd(4p)	0.00022	7.90007
688	C 27	pz	Ryd(3p)	1.05243	2.20677

689	C 27	pz	Val(2p)	0.00377	1.88322
690	C 27	pz	Ryd(4p)	0.00043	8.55186
691	C 27	dxy	Ryd(3d)	0.00062	4.97829
692	C 27	dxz	Ryd(3d)	0.00074	4.61361
693	C 27	dyz	Ryd(3d)	0.00078	4.47414
694	C 27	dx2y2	Ryd(3d)	0.00047	3.54932
695	C 27	dz2	Ryd(3d)	0.00076	5.42850
696	C 27	f(0)	Ryd(4f)	0.00009	7.39334
697	C 27	f(c1)	Ryd(4f)	0.00004	7.04922
698	C 27	f(s1)	Ryd(4f)	0.00005	6.90499
699	C 27	f(c2)	Ryd(4f)	0.00002	6.36886
700	C 27	f(s2)	Ryd(4f)	0.00010	7.00817
701	C 27	f(c3)	Ryd(4f)	0.00008	6.54579
702	C 27	f(s3)	Ryd(4f)	0.00009	6.68454
703	C 28	s	Ryd(3s)	1.99908	16.61099
704	C 28	s	Val(2s)	0.91628	2.50155
705	C 28	s	Cor(1s)	0.00053	2.44252
706	C 28	s	Ryd(4s)	0.00006	29.13735
707	C 28	s	Ryd(5s)	0.00000	101.27046
708	C 28	px	Val(2p)	0.94757	1.87260
709	C 28	px	Ryd(3p)	0.00289	2.21409
710	C 28	px	Ryd(4p)	0.00014	7.30263
711	C 28	py	Val(2p)	0.98327	1.98090
712	C 28	py	Ryd(3p)	0.00275	2.41685
713	C 28	py	Ryd(4p)	0.00017	7.47772
714	C 28	pz	Val(2p)	1.04802	2.26311
715	C 28	pz	Ryd(3p)	0.00217	2.57334
716	C 28	pz	Ryd(4p)	0.00027	8.04601
717	C 28	dxy	Ryd(3d)	0.00050	4.77966
718	C 28	dxz	Ryd(3d)	0.00069	4.55429
719	C 28	dyz	Ryd(3d)	0.00076	4.80344
720	C 28	dx2y2	Ryd(3d)	0.00044	3.61802
721	C 28	dz2	Ryd(3d)	0.00073	5.50137
722	C 28	f(0)	Ryd(4f)	0.00010	7.41395
723	C 28	f(c1)	Ryd(4f)	0.00005	7.01549
724	C 28	f(s1)	Ryd(4f)	0.00004	7.09917
725	C 28	f(c2)	Ryd(4f)	0.00001	6.46125
726	C 28	f(s2)	Ryd(4f)	0.00008	7.03858
727	C 28	f(c3)	Ryd(4f)	0.00007	6.56402
728	C 28	f(s3)	Ryd(4f)	0.00006	6.45442
729	C 29	s	Ryd(3s)	1.99941	16.61087
730	C 29	s	Cor(1s)	1.10099	2.12112
731	C 29	s	Val(2s)	0.00043	3.23637
732	C 29	s	Ryd(4s)	0.00003	24.96255
733	C 29	s	Ryd(5s)	0.00000	104.27573
734	C 29	px	Val(2p)	1.20426	1.74722
735	C 29	px	Ryd(3p)	0.00103	1.78620
736	C 29	px	Ryd(4p)	0.00010	6.89638
737	C 29	py	Val(2p)	1.13403	1.74753
738	C 29	py	Ryd(3p)	0.00096	1.79215
739	C 29	py	Ryd(4p)	0.00013	6.81231
740	C 29	pz	Val(2p)	1.22656	1.81531
741	C 29	pz	Ryd(3p)	0.00132	2.54430
742	C 29	pz	Ryd(4p)	0.00018	7.00072
743	C 29	dxy	Ryd(3d)	0.00118	4.93786
744	C 29	dxz	Ryd(3d)	0.00137	5.06795
745	C 29	dyz	Ryd(3d)	0.00124	4.87003
746	C 29	dx2y2	Ryd(3d)	0.00031	4.02626
747	C 29	dz2	Ryd(3d)	0.00043	4.13609
748	C 29	f(0)	Ryd(4f)	0.00001	6.93546
749	C 29	f(c1)	Ryd(4f)	0.00002	7.17948
750	C 29	f(s1)	Ryd(4f)	0.00002	7.08686
751	C 29	f(c2)	Ryd(4f)	0.00002	7.23729
752	C 29	f(s2)	Ryd(4f)	0.00015	8.24845
753	C 29	f(c3)	Ryd(4f)	0.00002	7.04400
754	C 29	f(s3)	Ryd(4f)	0.00000	6.88785
755	C 30	s	Ryd(3s)	1.99918	16.61142
756	C 30	s	Cor(1s)	0.97700	2.33234
757	C 30	s	Val(2s)	0.00136	2.62824
758	C 30	s	Ryd(4s)	0.00008	29.17364
759	C 30	s	Ryd(5s)	0.00000	101.06791
760	C 30	px	Val(2p)	1.07252	1.76121
761	C 30	px	Ryd(3p)	0.00329	2.31689
762	C 30	px	Ryd(4p)	0.00015	6.67562
763	C 30	py	Val(2p)	1.06956	1.85373
764	C 30	py	Ryd(3p)	0.00290	2.49285
765	C 30	py	Ryd(4p)	0.00015	6.82994
766	C 30	pz	Val(2p)	1.07140	2.18318
767	C 30	pz	Ryd(3p)	0.00229	2.87058
768	C 30	pz	Ryd(4p)	0.00021	7.58328
769	C 30	dxy	Ryd(3d)	0.00073	4.73043
770	C 30	dxz	Ryd(3d)	0.00069	4.45945
771	C 30	dyz	Ryd(3d)	0.00077	4.86498
772	C 30	dx2y2	Ryd(3d)	0.00023	3.48970
773	C 30	dz2	Ryd(3d)	0.00081	5.30785

774	C	30	f(0)	Ryd(4f)	0.00013	7.48025
775	C	30	f(c1)	Ryd(4f)	0.00006	6.98286
776	C	30	f(s1)	Ryd(4f)	0.00006	7.30172
777	C	30	f(c2)	Ryd(4f)	0.00002	6.58213
778	C	30	f(s2)	Ryd(4f)	0.00011	7.19307
779	C	30	f(c3)	Ryd(4f)	0.00007	6.54092
780	C	30	f(s3)	Ryd(4f)	0.00007	6.47949
781	C	31	s	Ryd(3s)	1.99915	16.62132
782	C	31	s	Cor(1s)	0.97504	2.34516
783	C	31	s	Val(2s)	0.00142	2.49919
784	C	31	s	Ryd(4s)	0.00008	29.63414
785	C	31	s	Ryd(5s)	0.00000	100.32345
786	C	31	px	Val(2p)	1.02205	1.88070
787	C	31	px	Ryd(3p)	0.00195	2.27448
788	C	31	px	Ryd(4p)	0.00014	7.16897
789	C	31	py	Val(2p)	1.00735	1.90316
790	C	31	py	Ryd(3p)	0.00177	2.35706
791	C	31	py	Ryd(4p)	0.00015	7.21449
792	C	31	pz	Val(2p)	1.15565	2.06467
793	C	31	pz	Ryd(3p)	0.00331	2.83569
794	C	31	pz	Ryd(4p)	0.00013	7.61428
795	C	31	dxy	Ryd(3d)	0.00072	5.14689
796	C	31	dxz	Ryd(3d)	0.00063	4.47000
797	C	31	dyz	Ryd(3d)	0.00058	4.59482
798	C	31	dx2y2	Ryd(3d)	0.00048	3.69914
799	C	31	dz2	Ryd(3d)	0.00095	4.92255
800	C	31	f(0)	Ryd(4f)	0.00007	7.14066
801	C	31	f(c1)	Ryd(4f)	0.00006	7.03294
802	C	31	f(s1)	Ryd(4f)	0.00004	6.98579
803	C	31	f(c2)	Ryd(4f)	0.00002	6.52900
804	C	31	f(s2)	Ryd(4f)	0.00012	7.11929
805	C	31	f(c3)	Ryd(4f)	0.00011	6.88361
806	C	31	f(s3)	Ryd(4f)	0.00012	6.88986
807	C	32	s	Ryd(3s)	1.99909	16.60868
808	C	32	s	Cor(1s)	0.90880	2.50100
809	C	32	s	Val(2s)	0.00174	2.93569
810	C	32	s	Ryd(4s)	0.00007	29.37063
811	C	32	s	Ryd(5s)	0.00000	101.14383
812	C	32	px	Val(2p)	1.01762	1.95816
813	C	32	px	Ryd(3p)	0.00359	1.96642
814	C	32	px	Ryd(4p)	0.00021	7.80298
815	C	32	py	Val(2p)	1.00771	1.89989
816	C	32	py	Ryd(3p)	0.00408	2.00091
817	C	32	py	Ryd(4p)	0.00018	7.82693
818	C	32	pz	Val(2p)	1.03744	2.20044
819	C	32	pz	Ryd(3p)	0.00463	2.45933
820	C	32	pz	Ryd(4p)	0.00039	9.08808
821	C	32	dxy	Ryd(3d)	0.00063	5.07374
822	C	32	dxz	Ryd(3d)	0.00063	4.85127
823	C	32	dyz	Ryd(3d)	0.00054	4.33741
824	C	32	dx2y2	Ryd(3d)	0.00037	3.72137
825	C	32	dz2	Ryd(3d)	0.00076	5.22197
826	C	32	f(0)	Ryd(4f)	0.00004	7.03512
827	C	32	f(c1)	Ryd(4f)	0.00009	7.18880
828	C	32	f(s1)	Ryd(4f)	0.00006	6.88775
829	C	32	f(c2)	Ryd(4f)	0.00002	6.56216
830	C	32	f(s2)	Ryd(4f)	0.00007	7.03554
831	C	32	f(c3)	Ryd(4f)	0.00008	6.59785
832	C	32	f(s3)	Ryd(4f)	0.00008	6.66490
833	C	33	s	Ryd(3s)	1.99909	16.62480
834	C	33	s	Cor(1s)	0.96742	2.37533
835	C	33	s	Val(2s)	0.00106	2.64611
836	C	33	s	Ryd(4s)	0.00008	30.37052
837	C	33	s	Ryd(5s)	0.00000	100.17767
838	C	33	px	Val(2p)	1.08465	1.85141
839	C	33	px	Ryd(3p)	0.00331	2.10237
840	C	33	px	Ryd(4p)	0.00015	7.25416
841	C	33	py	Val(2p)	1.04422	1.75124
842	C	33	py	Ryd(3p)	0.00338	1.95303
843	C	33	py	Ryd(4p)	0.00016	7.03006
844	C	33	pz	Val(2p)	1.05963	2.24508
845	C	33	pz	Ryd(3p)	0.00188	2.37354
846	C	33	pz	Ryd(4p)	0.00026	8.41927
847	C	33	dxy	Ryd(3d)	0.00078	4.56387
848	C	33	dxz	Ryd(3d)	0.00077	4.80419
849	C	33	dyz	Ryd(3d)	0.00073	4.51999
850	C	33	dx2y2	Ryd(3d)	0.00023	3.48956
851	C	33	dz2	Ryd(3d)	0.00095	5.54062
852	C	33	f(0)	Ryd(4f)	0.00009	7.54590
853	C	33	f(c1)	Ryd(4f)	0.00013	7.44549
854	C	33	f(s1)	Ryd(4f)	0.00012	7.26032
855	C	33	f(c2)	Ryd(4f)	0.00003	6.53338
856	C	33	f(s2)	Ryd(4f)	0.00004	6.94645
857	C	33	f(c3)	Ryd(4f)	0.00006	6.43476
858	C	33	f(s3)	Ryd(4f)	0.00008	6.54847

859	C 34	s	Ryd(3s)	1.99935	16.59423
860	C 34	s	Cor(1s)	0.98736	2.35691
861	C 34	s	Val(2s)	0.00082	3.70683
862	C 34	s	Ryd(4s)	0.00005	27.10266
863	C 34	s	Ryd(5s)	0.00000	102.99953
864	C 34	px	Val(2p)	1.09640	1.87082
865	C 34	px	Ryd(3p)	0.00284	2.32560
866	C 34	px	Ryd(4p)	0.00019	7.43720
867	C 34	py	Val(2p)	1.06857	1.87364
868	C 34	py	Ryd(3p)	0.00222	2.23881
869	C 34	py	Ryd(4p)	0.00021	7.30433
870	C 34	pz	Val(2p)	1.04572	1.91889
871	C 34	pz	Ryd(3p)	0.00166	2.64228
872	C 34	pz	Ryd(4p)	0.00032	7.65130
873	C 34	dxy	Ryd(3d)	0.00085	5.44039
874	C 34	dxz	Ryd(3d)	0.00069	4.91672
875	C 34	dyz	Ryd(3d)	0.00080	5.20173
876	C 34	dx2y2	Ryd(3d)	0.00030	4.05751
877	C 34	dz2	Ryd(3d)	0.00037	4.44526
878	C 34	f(0)	Ryd(4f)	0.00000	6.65807
879	C 34	f(c1)	Ryd(4f)	0.00001	6.80837
880	C 34	f(s1)	Ryd(4f)	0.00003	7.12146
881	C 34	f(c2)	Ryd(4f)	0.00000	6.78846
882	C 34	f(s2)	Ryd(4f)	0.00010	7.94229
883	C 34	f(c3)	Ryd(4f)	0.00000	6.82131
884	C 34	f(s3)	Ryd(4f)	0.00002	6.93143
885	C 35	s	Ryd(3s)	1.99948	16.59954
886	C 35	s	Cor(1s)	1.10527	2.07880
887	C 35	s	Val(2s)	0.00071	2.95826
888	C 35	s	Ryd(4s)	0.00002	21.01525
889	C 35	s	Ryd(5s)	0.00000	107.40773
890	C 35	px	Val(2p)	1.19686	1.74462
891	C 35	px	Ryd(3p)	0.00058	2.84280
892	C 35	px	Ryd(4p)	0.00005	5.53941
893	C 35	py	Val(2p)	1.17202	1.76410
894	C 35	py	Ryd(3p)	0.00073	2.85806
895	C 35	py	Ryd(4p)	0.00003	5.57194
896	C 35	pz	Val(2p)	1.13864	1.75614
897	C 35	pz	Ryd(3p)	0.00064	2.77543
898	C 35	pz	Ryd(4p)	0.00010	5.73573
899	C 35	dxy	Ryd(3d)	0.00163	4.94877
900	C 35	dxz	Ryd(3d)	0.00106	4.55153
901	C 35	dyz	Ryd(3d)	0.00145	4.82379
902	C 35	dx2y2	Ryd(3d)	0.00017	3.85852
903	C 35	dz2	Ryd(3d)	0.00044	4.05416
904	C 35	f(0)	Ryd(4f)	0.00001	6.77472
905	C 35	f(c1)	Ryd(4f)	0.00001	6.91569
906	C 35	f(s1)	Ryd(4f)	0.00005	7.14351
907	C 35	f(c2)	Ryd(4f)	0.00000	6.95850
908	C 35	f(s2)	Ryd(4f)	0.00017	8.07198
909	C 35	f(c3)	Ryd(4f)	0.00001	6.93660
910	C 35	f(s3)	Ryd(4f)	0.00003	7.04957
911	C 36	s	Ryd(3s)	1.99948	16.59960
912	C 36	s	Cor(1s)	1.10485	2.07952
913	C 36	s	Val(2s)	0.00070	2.96622
914	C 36	s	Ryd(4s)	0.00002	21.19726
915	C 36	s	Ryd(5s)	0.00000	107.26200
916	C 36	px	Val(2p)	1.14179	1.75893
917	C 36	px	Ryd(3p)	0.00060	2.73738
918	C 36	px	Ryd(4p)	0.00004	5.57673
919	C 36	py	Val(2p)	1.16724	1.74251
920	C 36	py	Ryd(3p)	0.00057	2.79024
921	C 36	py	Ryd(4p)	0.00008	5.64548
922	C 36	pz	Val(2p)	1.19928	1.76427
923	C 36	pz	Ryd(3p)	0.00081	3.02191
924	C 36	pz	Ryd(4p)	0.00005	5.56658
925	C 36	dxy	Ryd(3d)	0.00137	4.81269
926	C 36	dxz	Ryd(3d)	0.00112	4.57965
927	C 36	dyz	Ryd(3d)	0.00166	4.92602
928	C 36	dx2y2	Ryd(3d)	0.00017	3.90461
929	C 36	dz2	Ryd(3d)	0.00043	4.01893
930	C 36	f(0)	Ryd(4f)	0.00001	6.82916
931	C 36	f(c1)	Ryd(4f)	0.00000	6.88722
932	C 36	f(s1)	Ryd(4f)	0.00005	7.22980
933	C 36	f(c2)	Ryd(4f)	0.00001	6.99347
934	C 36	f(s2)	Ryd(4f)	0.00017	8.05487
935	C 36	f(c3)	Ryd(4f)	0.00000	6.87685
936	C 36	f(s3)	Ryd(4f)	0.00003	6.98213
937	H 37	s	Val(1s)	0.75120	1.38792
938	H 37	s	Ryd(3s)	0.00098	2.99861
939	H 37	s	Ryd(2s)	0.00050	2.92314
940	H 37	px	Ryd(2p)	0.00021	2.38335
941	H 37	py	Ryd(2p)	0.00023	1.84394
942	H 37	pz	Ryd(2p)	0.00077	5.11604

943	H 37	dxy	Ryd(3d)	0.00001	3.89092
944	H 37	dxz	Ryd(3d)	0.00002	5.65588
945	H 37	dyz	Ryd(3d)	0.00000	5.18089
946	H 37	dx2y2	Ryd(3d)	0.00001	3.79597
947	H 37	dz2	Ryd(3d)	0.00003	6.59269
948	H 38	s	Val(1s)	0.76951	1.29481
949	H 38	s	Ryd(3s)	0.00058	2.69428
950	H 38	s	Ryd(2s)	0.00014	2.32620
951	H 38	px	Ryd(2p)	0.00012	2.23273
952	H 38	py	Ryd(2p)	0.00008	1.83405
953	H 38	pz	Ryd(2p)	0.00027	4.09607
954	H 38	dxy	Ryd(3d)	0.00001	3.90265
955	H 38	dxz	Ryd(3d)	0.00002	5.64435
956	H 38	dyz	Ryd(3d)	0.00000	5.12487
957	H 38	dx2y2	Ryd(3d)	0.00001	3.87369
958	H 38	dz2	Ryd(3d)	0.00003	6.18440
959	H 39	s	Val(1s)	0.77818	1.26333
960	H 39	s	Ryd(2s)	0.00099	2.19827
961	H 39	s	Ryd(3s)	0.00017	2.37948
962	H 39	px	Ryd(2p)	0.00036	3.34116
963	H 39	py	Ryd(2p)	0.00018	2.20376
964	H 39	pz	Ryd(2p)	0.00016	2.75885
965	H 39	dxy	Ryd(3d)	0.00001	4.89300
966	H 39	dxz	Ryd(3d)	0.00003	5.67465
967	H 39	dyz	Ryd(3d)	0.00001	4.58563
968	H 39	dx2y2	Ryd(3d)	0.00001	4.89988
969	H 39	dz2	Ryd(3d)	0.00000	4.79456
970	H 40	s	Val(1s)	0.77906	1.26125
971	H 40	s	Ryd(2s)	0.00104	2.17238
972	H 40	s	Ryd(3s)	0.00018	2.41532
973	H 40	px	Ryd(2p)	0.00023	2.00603
974	H 40	py	Ryd(2p)	0.00038	4.23552
975	H 40	pz	Ryd(2p)	0.00009	2.10095
976	H 40	dxy	Ryd(3d)	0.00001	5.31596
977	H 40	dxz	Ryd(3d)	0.00001	3.86938
978	H 40	dyz	Ryd(3d)	0.00001	5.48178
979	H 40	dx2y2	Ryd(3d)	0.00003	5.66983
980	H 40	dz2	Ryd(3d)	0.00001	4.51721
981	H 41	s	Val(1s)	0.78493	1.30470
982	H 41	s	Ryd(2s)	0.00136	2.29358
983	H 41	s	Ryd(3s)	0.00036	2.88328
984	H 41	px	Ryd(2p)	0.00057	3.07586
985	H 41	py	Ryd(2p)	0.00048	2.92505
986	H 41	pz	Ryd(2p)	0.00029	2.89411
987	H 41	dxy	Ryd(3d)	0.00003	5.74726
988	H 41	dxz	Ryd(3d)	0.00002	5.08536
989	H 41	dyz	Ryd(3d)	0.00002	4.84858
990	H 41	dx2y2	Ryd(3d)	0.00000	4.90525
991	H 41	dz2	Ryd(3d)	0.00001	4.77395
992	H 42	s	Val(1s)	0.78668	1.31896
993	H 42	s	Ryd(2s)	0.00167	2.10176
994	H 42	s	Ryd(3s)	0.00036	3.20187
995	H 42	px	Ryd(2p)	0.00035	2.26576
996	H 42	py	Ryd(2p)	0.00028	1.94901
997	H 42	pz	Ryd(2p)	0.00064	4.73402
998	H 42	dxy	Ryd(3d)	0.00001	4.01386
999	H 42	dxz	Ryd(3d)	0.00002	5.70099
1000	H 42	dyz	Ryd(3d)	0.00000	5.24868
1001	H 42	dx2y2	Ryd(3d)	0.00001	3.89503
1002	H 42	dz2	Ryd(3d)	0.00004	6.62048
1003	H 43	s	Val(1s)	0.78719	1.31665
1004	H 43	s	Ryd(2s)	0.00187	2.12314
1005	H 43	s	Ryd(3s)	0.00044	3.59117
1006	H 43	px	Ryd(2p)	0.00056	3.79591
1007	H 43	py	Ryd(2p)	0.00049	3.07281
1008	H 43	pz	Ryd(2p)	0.00017	2.27688
1009	H 43	dxy	Ryd(3d)	0.00004	6.33257
1010	H 43	dxz	Ryd(3d)	0.00001	4.81052
1011	H 43	dyz	Ryd(3d)	0.00001	4.43195
1012	H 43	dx2y2	Ryd(3d)	0.00000	5.30090
1013	H 43	dz2	Ryd(3d)	0.00002	4.54968
1014	H 44	s	Val(1s)	0.78463	1.25744
1015	H 44	s	Ryd(2s)	0.00274	2.53507
1016	H 44	s	Ryd(3s)	0.00031	2.77884
1017	H 44	px	Ryd(2p)	0.00042	3.28107
1018	H 44	py	Ryd(2p)	0.00034	2.85555
1019	H 44	pz	Ryd(2p)	0.00015	2.32889
1020	H 44	dxy	Ryd(3d)	0.00005	5.72578
1021	H 44	dxz	Ryd(3d)	0.00003	4.94552
1022	H 44	dyz	Ryd(3d)	0.00002	4.57301
1023	H 44	dx2y2	Ryd(3d)	0.00001	5.03022

1024	H 44	dz2	Ryd(3d)	0.00002	4.52441
1025	H 45	s	Val(1s)	0.75115	1.38801
1026	H 45	s	Ryd(3s)	0.00098	3.00085
1027	H 45	s	Ryd(2s)	0.00050	2.92262
1028	H 45	px	Ryd(2p)	0.00021	2.38413
1029	H 45	py	Ryd(2p)	0.00023	1.84454
1030	H 45	pz	Ryd(2p)	0.00077	5.11613
1031	H 45	dxy	Ryd(3d)	0.00001	3.89050
1032	H 45	dxz	Ryd(3d)	0.00002	5.65661
1033	H 45	dyz	Ryd(3d)	0.00000	5.18126
1034	H 45	dx2y2	Ryd(3d)	0.00001	3.79627
1035	H 45	dz2	Ryd(3d)	0.00003	6.59179
1036	H 46	s	Val(1s)	0.76949	1.29480
1037	H 46	s	Ryd(3s)	0.00058	2.69381
1038	H 46	s	Ryd(2s)	0.00014	2.32570
1039	H 46	px	Ryd(2p)	0.00012	2.23411
1040	H 46	py	Ryd(2p)	0.00008	1.83352
1041	H 46	pz	Ryd(2p)	0.00027	4.09545
1042	H 46	dxy	Ryd(3d)	0.00001	3.90273
1043	H 46	dxz	Ryd(3d)	0.00002	5.64600
1044	H 46	dyz	Ryd(3d)	0.00000	5.12438
1045	H 46	dx2y2	Ryd(3d)	0.00001	3.87429
1046	H 46	dz2	Ryd(3d)	0.00003	6.18306
1047	H 47	s	Val(1s)	0.77817	1.26331
1048	H 47	s	Ryd(2s)	0.00099	2.19782
1049	H 47	s	Ryd(3s)	0.00017	2.38004
1050	H 47	px	Ryd(2p)	0.00036	3.34078
1051	H 47	py	Ryd(2p)	0.00018	2.19890
1052	H 47	pz	Ryd(2p)	0.00016	2.76331
1053	H 47	dxy	Ryd(3d)	0.00001	4.88714
1054	H 47	dxz	Ryd(3d)	0.00003	5.68058
1055	H 47	dyz	Ryd(3d)	0.00001	4.58437
1056	H 47	dx2y2	Ryd(3d)	0.00001	4.89738
1057	H 47	dz2	Ryd(3d)	0.00000	4.79777
1058	H 48	s	Val(1s)	0.77906	1.26127
1059	H 48	s	Ryd(2s)	0.00104	2.17330
1060	H 48	s	Ryd(3s)	0.00018	2.41468
1061	H 48	px	Ryd(2p)	0.00023	2.00730
1062	H 48	py	Ryd(2p)	0.00038	4.23879
1063	H 48	pz	Ryd(2p)	0.00008	2.09627
1064	H 48	dxy	Ryd(3d)	0.00001	5.32043
1065	H 48	dxz	Ryd(3d)	0.00001	3.86699
1066	H 48	dyz	Ryd(3d)	0.00001	5.47637
1067	H 48	dx2y2	Ryd(3d)	0.00003	5.67399
1068	H 48	dz2	Ryd(3d)	0.00001	4.51649
1069	H 49	s	Val(1s)	0.78494	1.30474
1070	H 49	s	Ryd(2s)	0.00136	2.29478
1071	H 49	s	Ryd(3s)	0.00036	2.88278
1072	H 49	px	Ryd(2p)	0.00057	3.06980
1073	H 49	py	Ryd(2p)	0.00048	2.92756
1074	H 49	pz	Ryd(2p)	0.00029	2.89777
1075	H 49	dxy	Ryd(3d)	0.00003	5.74284
1076	H 49	dxz	Ryd(3d)	0.00002	5.08599
1077	H 49	dyz	Ryd(3d)	0.00002	4.85219
1078	H 49	dx2y2	Ryd(3d)	0.00000	4.90321
1079	H 49	dz2	Ryd(3d)	0.00001	4.77594
1080	H 50	s	Val(1s)	0.78668	1.31892
1081	H 50	s	Ryd(2s)	0.00167	2.10118
1082	H 50	s	Ryd(3s)	0.00036	3.20213
1083	H 50	px	Ryd(2p)	0.00036	2.26320
1084	H 50	py	Ryd(2p)	0.00027	1.95233
1085	H 50	pz	Ryd(2p)	0.00064	4.73356
1086	H 50	dxy	Ryd(3d)	0.00001	4.01309
1087	H 50	dxz	Ryd(3d)	0.00002	5.70211
1088	H 50	dyz	Ryd(3d)	0.00000	5.24917
1089	H 50	dx2y2	Ryd(3d)	0.00001	3.89508
1090	H 50	dz2	Ryd(3d)	0.00004	6.61908
1091	H 51	s	Val(1s)	0.78716	1.31666
1092	H 51	s	Ryd(2s)	0.00186	2.12299
1093	H 51	s	Ryd(3s)	0.00044	3.58910
1094	H 51	px	Ryd(2p)	0.00056	3.78792
1095	H 51	py	Ryd(2p)	0.00049	3.08114
1096	H 51	pz	Ryd(2p)	0.00017	2.27533
1097	H 51	dxy	Ryd(3d)	0.00004	6.33365
1098	H 51	dxz	Ryd(3d)	0.00001	4.80750
1099	H 51	dyz	Ryd(3d)	0.00001	4.43688
1100	H 51	dx2y2	Ryd(3d)	0.00000	5.29951
1101	H 51	dz2	Ryd(3d)	0.00002	4.54863
1102	H 52	s	Val(1s)	0.78461	1.25742
1103	H 52	s	Ryd(2s)	0.00274	2.53419

1104	H 52	s	Ryd(3s)	0.00031	2.77839
1105	H 52	px	Ryd(2p)	0.00042	3.26004
1106	H 52	py	Ryd(2p)	0.00035	2.87175
1107	H 52	pz	Ryd(2p)	0.00015	2.33315
1108	H 52	dxy	Ryd(3d)	0.00005	5.72368
1109	H 52	dxz	Ryd(3d)	0.00003	4.93694
1110	H 52	dyz	Ryd(3d)	0.00002	4.58951
1111	H 52	dx2y2	Ryd(3d)	0.00000	5.02318
1112	H 52	dz2	Ryd(3d)	0.00002	4.52516
1113	H 53	s	Val(1s)	0.79346	1.26652
1114	H 53	s	Ryd(2s)	0.00112	1.94880
1115	H 53	s	Ryd(3s)	0.00018	2.50285
1116	H 53	px	Ryd(2p)	0.00034	3.54703
1117	H 53	py	Ryd(2p)	0.00015	2.62379
1118	H 53	pz	Ryd(2p)	0.00011	2.45203
1119	H 53	dxy	Ryd(3d)	0.00003	5.36056
1120	H 53	dxz	Ryd(3d)	0.00002	5.16558
1121	H 53	dyz	Ryd(3d)	0.00001	4.45946
1122	H 53	dx2y2	Ryd(3d)	0.00000	5.11820
1123	H 53	dz2	Ryd(3d)	0.00001	4.56534
1124	H 54	s	Val(1s)	0.77769	1.28683
1125	H 54	s	Ryd(2s)	0.00062	2.16383
1126	H 54	s	Ryd(3s)	0.00018	2.42186
1127	H 54	px	Ryd(2p)	0.00013	2.29045
1128	H 54	py	Ryd(2p)	0.00016	2.87324
1129	H 54	pz	Ryd(2p)	0.00025	3.02239
1130	H 54	dxy	Ryd(3d)	0.00001	4.73433
1131	H 54	dxz	Ryd(3d)	0.00001	4.87910
1132	H 54	dyz	Ryd(3d)	0.00004	5.39992
1133	H 54	dx2y2	Ryd(3d)	0.00001	4.56467
1134	H 54	dz2	Ryd(3d)	0.00000	5.08671
1135	H 55	s	Val(1s)	0.78576	1.27719
1136	H 55	s	Ryd(3s)	0.00074	2.44369
1137	H 55	s	Ryd(2s)	0.00015	2.39211
1138	H 55	px	Ryd(2p)	0.00010	2.25206
1139	H 55	py	Ryd(2p)	0.00012	2.82431
1140	H 55	pz	Ryd(2p)	0.00017	3.20118
1141	H 55	dxy	Ryd(3d)	0.00001	4.51985
1142	H 55	dxz	Ryd(3d)	0.00001	4.90273
1143	H 55	dyz	Ryd(3d)	0.00003	5.54295
1144	H 55	dx2y2	Ryd(3d)	0.00000	4.50191
1145	H 55	dz2	Ryd(3d)	0.00001	5.14595
1146	H 56	s	Val(1s)	0.79370	1.26673
1147	H 56	s	Ryd(2s)	0.00112	1.95024
1148	H 56	s	Ryd(3s)	0.00017	2.50253
1149	H 56	px	Ryd(2p)	0.00019	3.10319
1150	H 56	py	Ryd(2p)	0.00025	2.96366
1151	H 56	pz	Ryd(2p)	0.00016	2.55881
1152	H 56	dxy	Ryd(3d)	0.00003	5.38785
1153	H 56	dxz	Ryd(3d)	0.00002	4.87215
1154	H 56	dyz	Ryd(3d)	0.00002	4.80133
1155	H 56	dx2y2	Ryd(3d)	0.00000	5.04222
1156	H 56	dz2	Ryd(3d)	0.00001	4.56342
1157	H 57	s	Val(1s)	0.78576	1.27757
1158	H 57	s	Ryd(3s)	0.00074	2.43272
1159	H 57	s	Ryd(2s)	0.00015	2.38076
1160	H 57	px	Ryd(2p)	0.00007	2.34415
1161	H 57	py	Ryd(2p)	0.00013	2.65594
1162	H 57	pz	Ryd(2p)	0.00021	3.26384
1163	H 57	dxy	Ryd(3d)	0.00001	4.50371
1164	H 57	dxz	Ryd(3d)	0.00002	5.05085
1165	H 57	dyz	Ryd(3d)	0.00003	5.36949
1166	H 57	dx2y2	Ryd(3d)	0.00000	4.49737
1167	H 57	dz2	Ryd(3d)	0.00001	5.18627
1168	H 58	s	Val(1s)	0.77939	1.28544
1169	H 58	s	Ryd(2s)	0.00063	2.16294
1170	H 58	s	Ryd(3s)	0.00017	2.42802
1171	H 58	px	Ryd(2p)	0.00019	3.29017
1172	H 58	py	Ryd(2p)	0.00018	2.73118
1173	H 58	pz	Ryd(2p)	0.00016	2.17898
1174	H 58	dxy	Ryd(3d)	0.00003	5.61443
1175	H 58	dxz	Ryd(3d)	0.00002	4.87833
1176	H 58	dyz	Ryd(3d)	0.00001	4.51697
1177	H 58	dx2y2	Ryd(3d)	0.00000	5.15911
1178	H 58	dz2	Ryd(3d)	0.00001	4.49155
1179	H 59	s	Val(1s)	0.78813	1.27197
1180	H 59	s	Ryd(2s)	0.00063	2.46442
1181	H 59	s	Ryd(3s)	0.00019	2.60527
1182	H 59	px	Ryd(2p)	0.00018	2.37774
1183	H 59	py	Ryd(2p)	0.00022	2.86259
1184	H 59	pz	Ryd(2p)	0.00019	3.50343

1185	H 59	dxy	Ryd(3d)	0.00001	4.70740
1186	H 59	dxz	Ryd(3d)	0.00002	5.05343
1187	H 59	dyz	Ryd(3d)	0.00002	5.44485
1188	H 59	dx2y2	Ryd(3d)	0.00001	4.48058
1189	H 59	dz2	Ryd(3d)	0.00001	5.37813
1190	H 60	s	Val(1s)	0.76088	1.26344
1191	H 60	s	Ryd(2s)	0.00097	1.65543
1192	H 60	s	Ryd(3s)	0.00022	2.81965
1193	H 60	px	Ryd(2p)	0.00019	2.70096
1194	H 60	py	Ryd(2p)	0.00036	2.90630
1195	H 60	pz	Ryd(2p)	0.00028	2.69510
1196	H 60	dxy	Ryd(3d)	0.00002	5.18593
1197	H 60	dxz	Ryd(3d)	0.00002	4.98117
1198	H 60	dyz	Ryd(3d)	0.00003	5.28318
1199	H 60	dx2y2	Ryd(3d)	0.00000	4.87364
1200	H 60	dz2	Ryd(3d)	0.00000	4.78640
1201	H 61	s	Val(1s)	0.72274	1.34421
1202	H 61	s	Ryd(3s)	0.00121	3.48277
1203	H 61	s	Ryd(2s)	0.00040	2.51781
1204	H 61	px	Ryd(2p)	0.00050	3.59626
1205	H 61	py	Ryd(2p)	0.00018	2.11926
1206	H 61	pz	Ryd(2p)	0.00045	3.12191
1207	H 61	dxy	Ryd(3d)	0.00001	4.79796
1208	H 61	dxz	Ryd(3d)	0.00004	5.86305
1209	H 61	dyz	Ryd(3d)	0.00001	4.48675
1210	H 61	dx2y2	Ryd(3d)	0.00002	4.82584
1211	H 61	dz2	Ryd(3d)	0.00001	4.98610
1212	H 62	s	Val(1s)	0.76091	1.26354
1213	H 62	s	Ryd(2s)	0.00097	1.65635
1214	H 62	s	Ryd(3s)	0.00022	2.81915
1215	H 62	px	Ryd(2p)	0.00019	2.70086
1216	H 62	py	Ryd(2p)	0.00036	2.90808
1217	H 62	pz	Ryd(2p)	0.00028	2.69343
1218	H 62	dxy	Ryd(3d)	0.00002	5.18737
1219	H 62	dxz	Ryd(3d)	0.00002	4.97996
1220	H 62	dyz	Ryd(3d)	0.00003	5.28345
1221	H 62	dx2y2	Ryd(3d)	0.00000	4.87475
1222	H 62	dz2	Ryd(3d)	0.00000	4.78569
1223	H 63	s	Val(1s)	0.78810	1.27206
1224	H 63	s	Ryd(2s)	0.00063	2.46786
1225	H 63	s	Ryd(3s)	0.00019	2.60293
1226	H 63	px	Ryd(2p)	0.00018	2.37586
1227	H 63	py	Ryd(2p)	0.00022	2.85961
1228	H 63	pz	Ryd(2p)	0.00019	3.50741
1229	H 63	dxy	Ryd(3d)	0.00001	4.70366
1230	H 63	dxz	Ryd(3d)	0.00002	5.05532
1231	H 63	dyz	Ryd(3d)	0.00002	5.44555
1232	H 63	dx2y2	Ryd(3d)	0.00001	4.47806
1233	H 63	dz2	Ryd(3d)	0.00001	5.38207
1234	H 64	s	Val(1s)	0.72271	1.34408
1235	H 64	s	Ryd(3s)	0.00121	3.48278
1236	H 64	s	Ryd(2s)	0.00040	2.51643
1237	H 64	px	Ryd(2p)	0.00050	3.59720
1238	H 64	py	Ryd(2p)	0.00018	2.11689
1239	H 64	pz	Ryd(2p)	0.00045	3.12243
1240	H 64	dxy	Ryd(3d)	0.00001	4.79710
1241	H 64	dxz	Ryd(3d)	0.00004	5.86520
1242	H 64	dyz	Ryd(3d)	0.00001	4.48495
1243	H 64	dx2y2	Ryd(3d)	0.00002	4.82649
1244	H 64	dz2	Ryd(3d)	0.00001	4.98761
1245	H 65	s	Val(1s)	0.78579	1.27765
1246	H 65	s	Ryd(3s)	0.00074	2.43114
1247	H 65	s	Ryd(2s)	0.00015	2.38032
1248	H 65	px	Ryd(2p)	0.00007	2.33546
1249	H 65	py	Ryd(2p)	0.00013	2.66715
1250	H 65	pz	Ryd(2p)	0.00021	3.26124
1251	H 65	dxy	Ryd(3d)	0.00001	4.50477
1252	H 65	dxz	Ryd(3d)	0.00002	5.03910
1253	H 65	dyz	Ryd(3d)	0.00003	5.38002
1254	H 65	dx2y2	Ryd(3d)	0.00000	4.50008
1255	H 65	dz2	Ryd(3d)	0.00001	5.18385
1256	H 66	s	Val(1s)	0.79360	1.26668
1257	H 66	s	Ryd(2s)	0.00112	1.95091
1258	H 66	s	Ryd(3s)	0.00017	2.50105
1259	H 66	px	Ryd(2p)	0.00019	3.08115
1260	H 66	py	Ryd(2p)	0.00026	2.98213
1261	H 66	pz	Ryd(2p)	0.00016	2.55837
1262	H 66	dxy	Ryd(3d)	0.00003	5.38713
1263	H 66	dxz	Ryd(3d)	0.00002	4.85724
1264	H 66	dyz	Ryd(3d)	0.00002	4.81764
1265	H 66	dx2y2	Ryd(3d)	0.00000	5.03947

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1266    H 66  dz2    Ryd( 3d)         0.00001           4.56368

1267    H 67  s      Val( 1s)         0.77947           1.28534
1268    H 67  s      Ryd( 2s)         0.00063           2.16404
1269    H 67  s      Ryd( 3s)         0.00017           2.42813
1270    H 67  px     Ryd( 2p)         0.00019           3.30962
1271    H 67  py     Ryd( 2p)         0.00018           2.71144
1272    H 67  pz     Ryd( 2p)         0.00016           2.17956
1273    H 67  dxy    Ryd( 3d)         0.00003           5.61021
1274    H 67  dxz    Ryd( 3d)         0.00002           4.89276
1275    H 67  dyz    Ryd( 3d)         0.00001           4.50322
1276    H 67  dx2y2  Ryd( 3d)         0.00001           5.16240
1277    H 67  dz2    Ryd( 3d)         0.00001           4.49184

1278    H 68  s      Val( 1s)         0.77763           1.28687
1279    H 68  s      Ryd( 2s)         0.00062           2.16265
1280    H 68  s      Ryd( 3s)         0.00018           2.42283
1281    H 68  px     Ryd( 2p)         0.00014           2.30511
1282    H 68  py     Ryd( 2p)         0.00015           2.85798
1283    H 68  pz     Ryd( 2p)         0.00025           3.02194
1284    H 68  dxy    Ryd( 3d)         0.00001           4.73733
1285    H 68  dxz    Ryd( 3d)         0.00001           4.89363
1286    H 68  dyz    Ryd( 3d)         0.00004           5.38481
1287    H 68  dx2y2  Ryd( 3d)         0.00001           4.56224
1288    H 68  dz2    Ryd( 3d)         0.00000           5.08667

1289    H 69  s      Val( 1s)         0.79354           1.26659
1290    H 69  s      Ryd( 2s)         0.00112           1.94819
1291    H 69  s      Ryd( 3s)         0.00018           2.50473
1292    H 69  px     Ryd( 2p)         0.00034           3.52682
1293    H 69  py     Ryd( 2p)         0.00015           2.63831
1294    H 69  pz     Ryd( 2p)         0.00011           2.46246
1295    H 69  dxy    Ryd( 3d)         0.00003           5.35699
1296    H 69  dxz    Ryd( 3d)         0.00002           5.15932
1297    H 69  dyz    Ryd( 3d)         0.00001           4.47694
1298    H 69  dx2y2  Ryd( 3d)         0.00000           5.10921
1299    H 69  dz2    Ryd( 3d)         0.00001           4.56861

1300    H 70  s      Val( 1s)         0.78571           1.27718
1301    H 70  s      Ryd( 3s)         0.00074           2.44378
1302    H 70  s      Ryd( 2s)         0.00015           2.39343
1303    H 70  px     Ryd( 2p)         0.00010           2.24770
1304    H 70  py     Ryd( 2p)         0.00013           2.83786
1305    H 70  pz     Ryd( 2p)         0.00017           3.19226
1306    H 70  dxy    Ryd( 3d)         0.00001           4.52579
1307    H 70  dxz    Ryd( 3d)         0.00001           4.89061
1308    H 70  dyz    Ryd( 3d)         0.00003           5.54994
1309    H 70  dx2y2  Ryd( 3d)         0.00000           4.50964
1310    H 70  dz2    Ryd( 3d)         0.00001           5.13817

   1 low occupancy (<1.9990e) core orbital  found on  O  1
   1 low occupancy (<1.9990e) core orbital  found on  O  2
   1 low occupancy (<1.9990e) core orbital  found on  C  3
   1 low occupancy (<1.9990e) core orbital  found on  C  4
   1 low occupancy (<1.9990e) core orbital  found on  C  5
   1 low occupancy (<1.9990e) core orbital  found on  C  6
   1 low occupancy (<1.9990e) core orbital  found on  C  7
   1 low occupancy (<1.9990e) core orbital  found on  C  8
   1 low occupancy (<1.9990e) core orbital  found on  C  9
   1 low occupancy (<1.9990e) core orbital  found on  C 10
   1 low occupancy (<1.9990e) core orbital  found on  C 11
   1 low occupancy (<1.9990e) core orbital  found on  C 12
   1 low occupancy (<1.9990e) core orbital  found on  C 13
   1 low occupancy (<1.9990e) core orbital  found on  C 14
   1 low occupancy (<1.9990e) core orbital  found on  C 15
   1 low occupancy (<1.9990e) core orbital  found on  C 16
   1 low occupancy (<1.9990e) core orbital  found on  C 17
   1 low occupancy (<1.9990e) core orbital  found on  C 18
   1 low occupancy (<1.9990e) core orbital  found on  C 19
   1 low occupancy (<1.9990e) core orbital  found on  C 20
   1 low occupancy (<1.9990e) core orbital  found on  C 21
   1 low occupancy (<1.9990e) core orbital  found on  C 22
   1 low occupancy (<1.9990e) core orbital  found on  C 23
   1 low occupancy (<1.9990e) core orbital  found on  C 24
   1 low occupancy (<1.9990e) core orbital  found on  C 25
   1 low occupancy (<1.9990e) core orbital  found on  C 26
   1 low occupancy (<1.9990e) core orbital  found on  C 27
   1 low occupancy (<1.9990e) core orbital  found on  C 28
   1 low occupancy (<1.9990e) core orbital  found on  C 29
   1 low occupancy (<1.9990e) core orbital  found on  C 30
   1 low occupancy (<1.9990e) core orbital  found on  C 31
   1 low occupancy (<1.9990e) core orbital  found on  C 32
   1 low occupancy (<1.9990e) core orbital  found on  C 33
   1 low occupancy (<1.9990e) core orbital  found on  C 34
   1 low occupancy (<1.9990e) core orbital  found on  C 35
   1 low occupancy (<1.9990e) core orbital  found on  C 36

     Population inversion found on atom  O  1
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    Population inversion found on atom  O  2
    Population inversion found on atom  C  3
    Population inversion found on atom  C  4
    Population inversion found on atom  C  5
    Population inversion found on atom  C  6
    Population inversion found on atom  C  7
    Population inversion found on atom  C  8
    Population inversion found on atom  C  9
    Population inversion found on atom  C 10
    Population inversion found on atom  C 11
    Population inversion found on atom  C 12
    Population inversion found on atom  C 13
    Population inversion found on atom  C 14
    Population inversion found on atom  C 15
    Population inversion found on atom  C 16
    Population inversion found on atom  C 17
    Population inversion found on atom  C 18
    Population inversion found on atom  C 19
    Population inversion found on atom  C 20
    Population inversion found on atom  C 21
    Population inversion found on atom  C 22
    Population inversion found on atom  C 23
    Population inversion found on atom  C 24
    Population inversion found on atom  C 25
    Population inversion found on atom  C 26
    Population inversion found on atom  C 27
    Population inversion found on atom  C 28
    Population inversion found on atom  C 29
    Population inversion found on atom  C 30
    Population inversion found on atom  C 31
    Population inversion found on atom  C 32
    Population inversion found on atom  C 33
    Population inversion found on atom  C 34
    Population inversion found on atom  C 35
    Population inversion found on atom  C 36
    Population inversion found on atom  H 37
    Population inversion found on atom  H 38
    Population inversion found on atom  H 45
    Population inversion found on atom  H 46
    Population inversion found on atom  H 55
    Population inversion found on atom  H 57
    Population inversion found on atom  H 61
    Population inversion found on atom  H 64
    Population inversion found on atom  H 65
    Population inversion found on atom  H 70
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Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
O 1	-0.61037	1.70446	0.00789	6.89802	8.61037
O 2	-0.61028	1.70444	0.00790	6.89794	8.61028
C 3	0.43236	0.84849	2.69883	2.02031	5.56764
C 4	-0.08174	0.97853	2.12793	2.97528	6.08174
C 5	-0.09661	0.90088	0.01330	5.18243	6.09661
C 6	-0.15268	0.99204	3.14939	2.01124	6.15268
C 7	-0.01727	0.00090	4.00335	2.01302	6.01727
C 8	-0.66010	1.09744	3.55570	2.00696	6.66010
C 9	0.00022	0.90972	0.01179	5.07827	5.99978
C 10	-0.00251	0.90885	0.01216	5.08150	6.00251
C 11	0.09333	0.00053	3.89509	2.01105	5.90667
C 12	-0.67422	1.10100	3.56529	2.00793	6.67422
C 13	-0.20385	0.97701	3.21483	2.01200	6.20385
C 14	-0.17207	0.97503	3.18647	2.01057	6.17207
C 15	0.01107	0.90878	3.06456	2.01558	5.98893
C 16	-0.16930	0.96742	3.18957	2.01232	6.16930
C 17	-0.20886	0.98734	3.21150	2.01002	6.20886
C 18	-0.62024	1.10520	3.50839	2.00666	6.62024
C 19	-0.62044	1.10492	3.50885	2.00666	6.62044
C 20	0.43242	0.84851	2.69876	2.02031	5.56758
C 21	-0.08176	0.97854	2.12779	2.97543	6.08176
C 22	-0.09662	0.90088	0.01329	5.18245	6.09662
C 23	-0.15265	0.99206	3.14935	2.01124	6.15265
C 24	-0.01728	0.00090	4.00336	2.01302	6.01728
C 25	-0.66012	1.09744	3.55572	2.00696	6.66012
C 26	0.00028	0.90973	0.01179	5.07819	5.99972
C 27	-0.00255	0.90881	0.01217	5.08157	6.00255
C 28	0.09329	0.00053	3.89513	2.01105	5.90671
C 29	-0.67421	1.10099	3.56528	2.00793	6.67421
C 30	-0.20383	0.97700	3.21483	2.01200	6.20383
C 31	-0.17207	0.97504	3.18646	2.01057	6.17207
C 32	0.01110	0.90880	3.06451	2.01558	5.98890
C 33	-0.16930	0.96742	3.18956	2.01231	6.16930
C 34	-0.20889	0.98736	3.21150	2.01002	6.20889
C 35	-0.62016	1.10527	3.50823	2.00665	6.62016

C 36	-0.62053	1.10485	3.50900	2.00667	6.62053
H 37	0.24605	0.00000	0.75120	0.00276	0.75395
H 38	0.22923	0.00000	0.76951	0.00126	0.77077
H 39	0.21990	0.00000	0.77818	0.00192	0.78010
H 40	0.21895	0.00000	0.77906	0.00198	0.78105
H 41	0.21195	0.00000	0.78493	0.00312	0.78805
H 42	0.20994	0.00000	0.78668	0.00338	0.79006
H 43	0.20921	0.00000	0.78719	0.00361	0.79079
H 44	0.21128	0.00000	0.78463	0.00408	0.78872
H 45	0.24609	0.00000	0.75115	0.00276	0.75391
H 46	0.22925	0.00000	0.76949	0.00126	0.77075
H 47	0.21990	0.00000	0.77817	0.00192	0.78010
H 48	0.21895	0.00000	0.77906	0.00198	0.78105
H 49	0.21194	0.00000	0.78494	0.00312	0.78806
H 50	0.20994	0.00000	0.78668	0.00338	0.79006
H 51	0.20923	0.00000	0.78716	0.00360	0.79077
H 52	0.21130	0.00000	0.78461	0.00408	0.78870
H 53	0.20457	0.00000	0.79346	0.00197	0.79543
H 54	0.22091	0.00000	0.77769	0.00141	0.77909
H 55	0.21289	0.00000	0.78576	0.00135	0.78711
H 56	0.20432	0.00000	0.79370	0.00198	0.79568
H 57	0.21288	0.00000	0.78576	0.00136	0.78712
H 58	0.21919	0.00000	0.77939	0.00142	0.78081
H 59	0.21039	0.00000	0.78813	0.00148	0.78961
H 60	0.23703	0.00000	0.76088	0.00209	0.76297
H 61	0.27444	0.00000	0.72274	0.00282	0.72556
H 62	0.23700	0.00000	0.76091	0.00209	0.76300
H 63	0.21042	0.00000	0.78810	0.00148	0.78958
H 64	0.27447	0.00000	0.72271	0.00282	0.72553
H 65	0.21285	0.00000	0.78579	0.00136	0.78715
H 66	0.20442	0.00000	0.79360	0.00198	0.79558
H 67	0.21912	0.00000	0.77947	0.00141	0.78088
H 68	0.22096	0.00000	0.77763	0.00141	0.77904
H 69	0.20448	0.00000	0.79354	0.00197	0.79552
H 70	0.21294	0.00000	0.78571	0.00135	0.78706
* Total *	0.00000	32.93713	118.26714	102.79573	254.00000

Natural Population

Core	32.93713 (45.7460% of 72)
Valence	118.26714 (64.9819% of 182)
Natural Minimal Basis	151.20427 (59.5292% of 254)
Natural Rydberg Basis	102.79573 (40.4708% of 254)

Atom No	Natural Electron Configuration
O 1	[core]2p(0.01)3s(2.00)3p(4.88)3d(0.02)
O 2	[core]2p(0.01)3s(2.00)3p(4.88)3d(0.02)
C 3	[core]2s(0.01)2p(2.69)3s(2.00)3p(0.01)3d(0.01)
C 4	[core]2p(2.13)3s(2.00)3p(0.97)
C 5	[core]2p(0.01)3s(2.00)3p(3.18)
C 6	[core]2p(3.15)3s(2.00)3p(0.01)
C 7	[core]2s(0.90)2p(3.10)3s(2.00)3p(0.01)
C 8	[core]2p(3.56)3s(2.00)
C 9	[core]2p(0.01)3s(2.00)3p(3.07)
C 10	[core]2p(0.01)3s(2.00)3p(3.08)
C 11	[core]2s(0.92)2p(2.98)3s(2.00)3p(0.01)
C 12	[core]2p(3.56)3s(2.00)
C 13	[core]2p(3.21)3s(2.00)3p(0.01)
C 14	[core]2p(3.19)3s(2.00)3p(0.01)
C 15	[core]2p(3.06)3s(2.00)3p(0.01)
C 16	[core]2p(3.19)3s(2.00)3p(0.01)
C 17	[core]2p(3.21)3s(2.00)3p(0.01)
C 18	[core]2p(3.51)3s(2.00)
C 19	[core]2p(3.51)3s(2.00)
C 20	[core]2s(0.01)2p(2.69)3s(2.00)3p(0.01)3d(0.01)
C 21	[core]2p(2.12)3s(2.00)3p(0.97)
C 22	[core]2p(0.01)3s(2.00)3p(3.18)
C 23	[core]2p(3.15)3s(2.00)3p(0.01)
C 24	[core]2s(0.90)2p(3.10)3s(2.00)3p(0.01)
C 25	[core]2p(3.56)3s(2.00)
C 26	[core]2p(0.01)3s(2.00)3p(3.07)
C 27	[core]2p(0.01)3s(2.00)3p(3.08)
C 28	[core]2s(0.92)2p(2.98)3s(2.00)3p(0.01)
C 29	[core]2p(3.56)3s(2.00)
C 30	[core]2p(3.21)3s(2.00)3p(0.01)
C 31	[core]2p(3.19)3s(2.00)3p(0.01)
C 32	[core]2p(3.06)3s(2.00)3p(0.01)
C 33	[core]2p(3.19)3s(2.00)3p(0.01)
C 34	[core]2p(3.21)3s(2.00)3p(0.01)
C 35	[core]2p(3.51)3s(2.00)
C 36	[core]2p(3.51)3s(2.00)
H 37	1s(0.75)
H 38	1s(0.77)
H 39	1s(0.78)
H 40	1s(0.78)

H	41	1s(0.78)
H	42	1s(0.79)
H	43	1s(0.79)
H	44	1s(0.78)
H	45	1s(0.75)
H	46	1s(0.77)
H	47	1s(0.78)
H	48	1s(0.78)
H	49	1s(0.78)
H	50	1s(0.79)
H	51	1s(0.79)
H	52	1s(0.78)
H	53	1s(0.79)
H	54	1s(0.78)
H	55	1s(0.79)
H	56	1s(0.79)
H	57	1s(0.79)
H	58	1s(0.78)
H	59	1s(0.79)
H	60	1s(0.76)
H	61	1s(0.72)
H	62	1s(0.76)
H	63	1s(0.79)
H	64	1s(0.72)
H	65	1s(0.79)
H	66	1s(0.79)
H	67	1s(0.78)
H	68	1s(0.78)
H	69	1s(0.79)
H	70	1s(0.79)

Wiberg bond index matrix in the NAO basis:

	Atom	1	2	3	4	5	6	7	8	9
1.	O	0.0000	0.0443	1.5942	0.1054	0.0037	0.0056	0.0004	0.0002	0.0029
2.	O	0.0443	0.0000	0.0605	0.0992	0.0043	0.0110	0.0013	0.0002	0.0018
3.	C	1.5942	0.0605	0.0000	1.0729	0.0091	0.0172	0.0009	0.0006	0.0020
4.	C	0.1054	0.0992	1.0729	0.0000	1.3064	0.0118	0.0369	0.0006	0.0261
5.	C	0.0037	0.0043	0.0091	1.3064	0.0000	1.2115	0.0142	0.0109	0.0299
6.	C	0.0056	0.0110	0.0172	0.0118	1.2115	0.0000	1.4907	0.0085	0.0158
7.	C	0.0004	0.0013	0.0009	0.0369	0.0142	1.4907	0.0000	1.0430	1.2375
8.	C	0.0002	0.0002	0.0006	0.0006	0.0109	0.0085	1.0430	0.0000	0.0076
9.	C	0.0029	0.0018	0.0020	0.0261	0.0299	0.0158	1.2375	0.0076	0.0000
10.	C	0.0073	0.0048	0.0082	0.0131	1.2130	0.0144	0.0316	0.0109	1.0986
11.	C	0.0049	0.0009	0.0006	0.0082	0.0082	0.0605	0.0241	0.0005	0.0305
12.	C	0.0144	0.0002	0.0024	0.0029	0.0040	0.0029	0.0019	0.0006	0.0155
13.	C	0.0037	0.0032	0.0025	0.0042	0.0473	0.0015	0.0196	0.0001	0.0042
14.	C	0.0020	0.0000	0.0003	0.0009	0.0015	0.0374	0.0021	0.0001	0.0469
15.	C	0.0033	0.0025	0.0020	0.0064	0.0230	0.0015	0.0469	0.0007	0.0104
16.	C	0.0023	0.0007	0.0012	0.0008	0.0199	0.0717	0.0093	0.0017	1.3825
17.	C	0.0000	0.0000	0.0000	0.0001	0.0003	0.0003	0.0005	0.0002	0.0104
18.	C	0.0001	0.0001	0.0001	0.0004	0.0009	0.0002	0.0016	0.0000	0.0008
19.	C	0.0001	0.0001	0.0001	0.0003	0.0009	0.0002	0.0015	0.0000	0.0007
20.	C	0.0605	1.5944	0.0552	1.0656	0.0085	0.0077	0.0011	0.0001	0.0023
21.	C	0.0992	0.1055	1.0656	0.0922	0.0587	0.0112	0.0135	0.0004	0.0174
22.	C	0.0043	0.0037	0.0085	0.0587	0.0013	0.0044	0.0005	0.0000	0.0032
23.	C	0.0111	0.0056	0.0077	0.0112	0.0044	0.0017	0.0018	0.0000	0.0026
24.	C	0.0013	0.0004	0.0011	0.0135	0.0005	0.0018	0.0003	0.0000	0.0017
25.	C	0.0002	0.0002	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0018	0.0029	0.0023	0.0174	0.0032	0.0026	0.0017	0.0000	0.0037
27.	C	0.0048	0.0073	0.0172	0.0165	0.0078	0.0028	0.0031	0.0001	0.0052
28.	C	0.0009	0.0049	0.0002	0.0012	0.0001	0.0001	0.0000	0.0000	0.0000
29.	C	0.0002	0.0144	0.0008	0.0011	0.0002	0.0001	0.0000	0.0000	0.0000
30.	C	0.0032	0.0037	0.0038	0.0136	0.0050	0.0024	0.0026	0.0001	0.0045
31.	C	0.0000	0.0020	0.0002	0.0010	0.0003	0.0001	0.0001	0.0000	0.0002
32.	C	0.0025	0.0033	0.0026	0.0148	0.0042	0.0025	0.0023	0.0001	0.0044
33.	C	0.0007	0.0023	0.0013	0.0008	0.0016	0.0002	0.0006	0.0000	0.0006
34.	C	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0001	0.0001	0.0001	0.0007	0.0002	0.0001	0.0001	0.0000	0.0002
36.	C	0.0001	0.0001	0.0001	0.0006	0.0002	0.0001	0.0001	0.0000	0.0002
37.	H	0.0004	0.0065	0.0006	0.0011	0.0019	0.9025	0.0031	0.0015	0.0120
38.	H	0.0000	0.0000	0.0000	0.0000	0.0006	0.0030	0.0025	0.9305	0.0091
39.	H	0.0000	0.0000	0.0000	0.0018	0.0004	0.0147	0.0029	0.9208	0.0054
40.	H	0.0000	0.0000	0.0001	0.0015	0.0005	0.0157	0.0029	0.9206	0.0056
41.	H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0005	0.0003	0.0000	0.0003
42.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0003	0.0000	0.0003
43.	H	0.0000	0.0001	0.0000	0.0005	0.0003	0.0012	0.0044	0.0016	0.0038
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0008
45.	H	0.0066	0.0004	0.0004	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0008	0.0000	0.0001	0.0000	0.0000	0.0001
48.	H	0.0000	0.0000	0.0001	0.0006	0.0000	0.0001	0.0000	0.0000	0.0001
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000	0.0003
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
57.	H	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000	0.0003
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0001	0.0001	0.0002	0.0001	0.0005	0.0002	0.0003	0.0001	0.0006
60.	H	0.0013	0.0001	0.0002	0.0011	0.0003	0.0013	0.0005	0.0000	0.0018
61.	H	0.0346	0.0002	0.0008	0.0013	0.0001	0.0023	0.0005	0.0000	0.0024
62.	H	0.0001	0.0013	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0002	0.0346	0.0003	0.0030	0.0000	0.0001	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		10	11	12	13	14	15	16	17	18
1.	O	0.0073	0.0049	0.0144	0.0037	0.0020	0.0033	0.0023	0.0000	0.0001
2.	O	0.0048	0.0009	0.0002	0.0032	0.0000	0.0025	0.0007	0.0000	0.0001
3.	C	0.0082	0.0006	0.0024	0.0025	0.0003	0.0020	0.0012	0.0000	0.0001
4.	C	0.0131	0.0082	0.0029	0.0042	0.0009	0.0064	0.0008	0.0001	0.0004
5.	C	1.2130	0.0082	0.0040	0.0473	0.0015	0.0230	0.0199	0.0003	0.0009
6.	C	0.0144	0.0605	0.0029	0.0015	0.0374	0.0015	0.0717	0.0003	0.0002
7.	C	0.0316	0.0241	0.0019	0.0196	0.0021	0.0469	0.0093	0.0005	0.0016
8.	C	0.0109	0.0005	0.0006	0.0001	0.0001	0.0007	0.0017	0.0002	0.0000
9.	C	1.0986	0.0305	0.0155	0.0042	0.0469	0.0104	1.3825	0.0104	0.0008
10.	C	0.0000	1.3746	0.0126	0.0120	0.0503	0.0082	0.0231	0.0005	0.0004
11.	C	1.3746	0.0000	1.0542	1.3213	0.0152	0.0434	0.0172	0.0004	0.0019
12.	C	0.0126	1.0542	0.0000	0.0094	0.0122	0.0018	0.0011	0.0003	0.0001
13.	C	0.0120	1.3213	0.0094	0.0000	1.4652	0.0110	0.0571	0.0112	0.0010
14.	C	0.0503	0.0152	0.0122	1.4652	0.0000	1.3466	0.0155	0.0079	0.0070
15.	C	0.0082	0.0434	0.0018	0.0110	1.3466	0.0000	1.3944	0.9963	0.0092
16.	C	0.0231	0.0172	0.0011	0.0571	0.0155	1.3944	0.0000	0.0078	0.0111
17.	C	0.0005	0.0004	0.0003	0.0112	0.0079	0.9963	0.0078	0.0000	1.0020
18.	C	0.0004	0.0019	0.0001	0.0010	0.0070	0.0092	0.0111	1.0020	0.0000
19.	C	0.0004	0.0017	0.0001	0.0010	0.0066	0.0094	0.0114	1.0027	0.0071
20.	C	0.0172	0.0002	0.0008	0.0038	0.0002	0.0026	0.0013	0.0000	0.0001
21.	C	0.0165	0.0012	0.0011	0.0136	0.0010	0.0148	0.0008	0.0001	0.0007
22.	C	0.0078	0.0001	0.0002	0.0050	0.0003	0.0042	0.0016	0.0000	0.0002
23.	C	0.0028	0.0001	0.0001	0.0024	0.0001	0.0025	0.0002	0.0000	0.0001
24.	C	0.0031	0.0000	0.0000	0.0026	0.0001	0.0023	0.0006	0.0000	0.0001
25.	C	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
26.	C	0.0052	0.0000	0.0000	0.0045	0.0002	0.0044	0.0006	0.0000	0.0002
27.	C	0.0056	0.0001	0.0001	0.0052	0.0003	0.0055	0.0004	0.0000	0.0003
28.	C	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000
29.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	C	0.0052	0.0001	0.0000	0.0051	0.0002	0.0052	0.0004	0.0000	0.0002
31.	C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000
32.	C	0.0055	0.0000	0.0000	0.0052	0.0003	0.0051	0.0005	0.0000	0.0002
33.	C	0.0004	0.0001	0.0000	0.0004	0.0000	0.0005	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0003	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000
36.	C	0.0002	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000
37.	H	0.0088	0.0002	0.0001	0.0005	0.0001	0.0006	0.0003	0.0001	0.0000
38.	H	0.0002	0.0003	0.0001	0.0000	0.0001	0.0001	0.0011	0.0001	0.0000
39.	H	0.0012	0.0010	0.0001	0.0009	0.0002	0.0012	0.0005	0.0001	0.0001
40.	H	0.0012	0.0009	0.0001	0.0010	0.0002	0.0013	0.0005	0.0001	0.0001
41.	H	0.0109	0.0029	0.0046	0.9154	0.0035	0.0114	0.0002	0.0005	0.0001
42.	H	0.0002	0.0113	0.0005	0.0035	0.9130	0.0031	0.0119	0.0052	0.0006
43.	H	0.0143	0.0002	0.0005	0.0004	0.0129	0.0036	0.9087	0.0046	0.0004
44.	H	0.0001	0.0001	0.0000	0.0003	0.0079	0.0023	0.0030	0.9059	0.0025
45.	H	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0002	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000
48.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0001	0.0000	0.0000	0.0003	0.0005	0.0017	0.0006	0.0032	0.0015
54.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0013	0.0002	0.0017	0.0105
55.	H	0.0002	0.0003	0.0000	0.0003	0.0009	0.0103	0.0010	0.0018	0.0015
56.	H	0.0001	0.0001	0.0000	0.0002	0.0005	0.0017	0.0006	0.0032	0.9386
57.	H	0.0002	0.0003	0.0000	0.0002	0.0010	0.0103	0.0010	0.0018	0.9350
58.	H	0.0000	0.0000	0.0000	0.0000	0.0002	0.0013	0.0002	0.0017	0.9357
59.	H	0.0086	0.0020	0.9379	0.0035	0.0010	0.0002	0.0001	0.0000	0.0000
60.	H	0.0078	0.0037	0.9101	0.0105	0.0011	0.0021	0.0012	0.0000	0.0001
61.	H	0.0080	0.0048	0.8514	0.0096	0.0014	0.0027	0.0014	0.0000	0.0001
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0001	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000

	Atom	19	20	21	22	23	24	25	26	27
1.	O	0.0001	0.0605	0.0992	0.0043	0.0111	0.0013	0.0002	0.0018	0.0048
2.	O	0.0001	1.5944	0.1055	0.0037	0.0056	0.0004	0.0002	0.0029	0.0073
3.	C	0.0001	0.0552	1.0656	0.0085	0.0077	0.0011	0.0001	0.0023	0.0172
4.	C	0.0003	1.0656	0.0922	0.0587	0.0112	0.0135	0.0004	0.0174	0.0165
5.	C	0.0009	0.0085	0.0587	0.0013	0.0044	0.0005	0.0000	0.0032	0.0078
6.	C	0.0002	0.0077	0.0112	0.0044	0.0017	0.0018	0.0000	0.0026	0.0028
7.	C	0.0015	0.0011	0.0135	0.0005	0.0018	0.0003	0.0000	0.0017	0.0031
8.	C	0.0000	0.0001	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
9.	C	0.0007	0.0023	0.0174	0.0032	0.0026	0.0017	0.0000	0.0037	0.0052
10.	C	0.0004	0.0172	0.0165	0.0078	0.0028	0.0031	0.0001	0.0052	0.0056
11.	C	0.0017	0.0002	0.0012	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001
12.	C	0.0001	0.0008	0.0011	0.0002	0.0001	0.0000	0.0000	0.0000	0.0001
13.	C	0.0010	0.0038	0.0136	0.0050	0.0024	0.0026	0.0001	0.0045	0.0052
14.	C	0.0066	0.0002	0.0010	0.0003	0.0001	0.0001	0.0000	0.0002	0.0003
15.	C	0.0094	0.0026	0.0148	0.0042	0.0025	0.0023	0.0001	0.0044	0.0055
16.	C	0.0114	0.0013	0.0008	0.0016	0.0002	0.0006	0.0000	0.0006	0.0004
17.	C	1.0027	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0071	0.0001	0.0007	0.0002	0.0001	0.0001	0.0000	0.0002	0.0003
19.	C	0.0000	0.0001	0.0006	0.0002	0.0001	0.0001	0.0000	0.0002	0.0002
20.	C	0.0001	0.0000	1.0727	0.0091	0.0172	0.0009	0.0006	0.0020	0.0081
21.	C	0.0006	1.0727	0.0000	1.3066	0.0118	0.0369	0.0006	0.0261	0.0131
22.	C	0.0002	0.0091	1.3066	0.0000	1.2114	0.0142	0.0109	0.0299	1.2129
23.	C	0.0001	0.0172	0.0118	1.2114	0.0000	1.4908	0.0085	0.0158	0.0144
24.	C	0.0001	0.0009	0.0369	0.0142	1.4908	0.0000	1.0430	1.2373	0.0316
25.	C	0.0000	0.0006	0.0006	0.0109	0.0085	1.0430	0.0000	0.0076	0.0109
26.	C	0.0002	0.0020	0.0261	0.0299	0.0158	1.2373	0.0076	0.0000	1.0987
27.	C	0.0002	0.0081	0.0131	1.2129	0.0144	0.0316	0.0109	1.0987	0.0000
28.	C	0.0000	0.0006	0.0082	0.0082	0.0605	0.0241	0.0005	0.0304	1.3746
29.	C	0.0000	0.0024	0.0029	0.0040	0.0029	0.0019	0.0006	0.0155	0.0126
30.	C	0.0002	0.0025	0.0042	0.0473	0.0015	0.0196	0.0001	0.0042	0.0120
31.	C	0.0000	0.0003	0.0009	0.0015	0.0374	0.0021	0.0001	0.0469	0.0503
32.	C	0.0002	0.0020	0.0064	0.0230	0.0015	0.0469	0.0007	0.0104	0.0082
33.	C	0.0000	0.0012	0.0008	0.0200	0.0717	0.0093	0.0017	1.3826	0.0231
34.	C	0.0000	0.0000	0.0001	0.0003	0.0003	0.0005	0.0002	0.0104	0.0005
35.	C	0.0000	0.0001	0.0004	0.0009	0.0002	0.0016	0.0000	0.0008	0.0004
36.	C	0.0000	0.0001	0.0003	0.0008	0.0002	0.0014	0.0000	0.0007	0.0004
37.	H	0.0000	0.0004	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0001	0.0000	0.0008	0.0000	0.0001	0.0000	0.0000	0.0001	0.0002
40.	H	0.0001	0.0001	0.0006	0.0000	0.0001	0.0000	0.0000	0.0001	0.0001
41.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0005	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0025	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0006	0.0011	0.0019	0.9025	0.0031	0.0015	0.0120	0.0088
46.	H	0.0000	0.0000	0.0000	0.0006	0.0030	0.0025	0.9305	0.0091	0.0002
47.	H	0.0000	0.0000	0.0018	0.0004	0.0147	0.0029	0.9209	0.0054	0.0012
48.	H	0.0000	0.0001	0.0015	0.0005	0.0157	0.0029	0.9206	0.0056	0.0012
49.	H	0.0000	0.0000	0.0000	0.0004	0.0005	0.0003	0.0000	0.0003	0.0109
50.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0003	0.0000	0.0003	0.0002
51.	H	0.0000	0.0000	0.0005	0.0003	0.0012	0.0044	0.0016	0.0038	0.0143
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0008	0.0001
53.	H	0.9386	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.9350	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.9350	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
56.	H	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0016	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
58.	H	0.0105	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0001	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0001	0.0003	0.0030	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001
62.	H	0.0000	0.0002	0.0011	0.0003	0.0013	0.0005	0.0000	0.0018	0.0078
63.	H	0.0000	0.0002	0.0001	0.0005	0.0002	0.0003	0.0001	0.0006	0.0086
64.	H	0.0000	0.0008	0.0013	0.0001	0.0023	0.0005	0.0000	0.0024	0.0080
65.	H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000	0.0003	0.0002
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
70.	H	0.0000	0.0000	0.0001	0.0002	0.0000	0.0002	0.0000	0.0003	0.0002

	Atom	28	29	30	31	32	33	34	35	36
1.	O	0.0009	0.0002	0.0032	0.0000	0.0025	0.0007	0.0000	0.0001	0.0001
2.	O	0.0049	0.0144	0.0037	0.0020	0.0033	0.0023	0.0000	0.0001	0.0001
3.	C	0.0002	0.0008	0.0038	0.0002	0.0026	0.0013	0.0000	0.0001	0.0001
4.	C	0.0012	0.0011	0.0136	0.0010	0.0148	0.0008	0.0001	0.0007	0.0006
5.	C	0.0001	0.0002	0.0050	0.0003	0.0042	0.0016	0.0000	0.0002	0.0002
6.	C	0.0001	0.0001	0.0024	0.0001	0.0025	0.0002	0.0000	0.0001	0.0001
7.	C	0.0000	0.0000	0.0026	0.0001	0.0023	0.0006	0.0000	0.0001	0.0001
8.	C	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0045	0.0002	0.0044	0.0006	0.0000	0.0002	0.0002

10.	C	0.0001	0.0001	0.0052	0.0003	0.0055	0.0004	0.0000	0.0003	0.0002
11.	C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0001	0.0000	0.0051	0.0002	0.0052	0.0004	0.0000	0.0002	0.0002
14.	C	0.0000	0.0000	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0052	0.0003	0.0051	0.0005	0.0000	0.0002	0.0002
16.	C	0.0001	0.0000	0.0004	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
20.	C	0.0006	0.0024	0.0025	0.0003	0.0020	0.0012	0.0000	0.0001	0.0001
21.	C	0.0082	0.0029	0.0042	0.0009	0.0064	0.0008	0.0001	0.0004	0.0003
22.	C	0.0082	0.0040	0.0473	0.0015	0.0230	0.0200	0.0003	0.0009	0.0008
23.	C	0.0605	0.0029	0.0015	0.0374	0.0015	0.0717	0.0003	0.0002	0.0002
24.	C	0.0241	0.0019	0.0196	0.0021	0.0469	0.0093	0.0005	0.0016	0.0014
25.	C	0.0005	0.0006	0.0001	0.0001	0.0007	0.0017	0.0002	0.0000	0.0000
26.	C	0.0304	0.0155	0.0042	0.0469	0.0104	1.3826	0.0104	0.0008	0.0007
27.	C	1.3746	0.0126	0.0120	0.0503	0.0082	0.0231	0.0005	0.0004	0.0004
28.	C	0.0000	1.0542	1.3213	0.0152	0.0434	0.0172	0.0004	0.0020	0.0017
29.	C	1.0542	0.0000	0.0094	0.0122	0.0018	0.0011	0.0003	0.0001	0.0001
30.	C	1.3213	0.0094	0.0000	1.4652	0.0110	0.0571	0.0112	0.0010	0.0010
31.	C	0.0152	0.0122	1.4652	0.0000	1.3466	0.0155	0.0079	0.0070	0.0065
32.	C	0.0434	0.0018	0.0110	1.3466	0.0000	1.3943	0.9963	0.0092	0.0094
33.	C	0.0172	0.0011	0.0571	0.0155	1.3943	0.0000	0.0078	0.0111	0.0114
34.	C	0.0004	0.0003	0.0112	0.0079	0.9963	0.0078	0.0000	1.0019	1.0029
35.	C	0.0020	0.0001	0.0010	0.0070	0.0092	0.0111	1.0019	0.0000	0.0071
36.	C	0.0017	0.0001	0.0010	0.0065	0.0094	0.0114	1.0029	0.0071	0.0000
37.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0002	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0002	0.0001	0.0005	0.0001	0.0006	0.0003	0.0001	0.0000	0.0000
46.	H	0.0003	0.0001	0.0000	0.0001	0.0001	0.0011	0.0001	0.0000	0.0000
47.	H	0.0010	0.0001	0.0009	0.0002	0.0011	0.0005	0.0001	0.0001	0.0001
48.	H	0.0009	0.0001	0.0010	0.0002	0.0013	0.0005	0.0001	0.0001	0.0001
49.	H	0.0029	0.0046	0.9154	0.0035	0.0114	0.0002	0.0005	0.0001	0.0001
50.	H	0.0113	0.0005	0.0035	0.9130	0.0031	0.0119	0.0052	0.0005	0.0006
51.	H	0.0002	0.0005	0.0004	0.0129	0.0036	0.9087	0.0046	0.0004	0.0005
52.	H	0.0001	0.0000	0.0003	0.0079	0.0023	0.0030	0.9059	0.0025	0.0025
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0036	0.9101	0.0105	0.0011	0.0021	0.0012	0.0000	0.0001	0.0001
63.	H	0.0020	0.9379	0.0035	0.0010	0.0002	0.0001	0.0000	0.0000	0.0000
64.	H	0.0048	0.8514	0.0096	0.0014	0.0027	0.0014	0.0000	0.0001	0.0001
65.	H	0.0003	0.0000	0.0002	0.0010	0.0103	0.0010	0.0018	0.9350	0.0016
66.	H	0.0001	0.0000	0.0002	0.0005	0.0017	0.0006	0.0032	0.9386	0.0014
67.	H	0.0000	0.0000	0.0000	0.0002	0.0013	0.0002	0.0017	0.9358	0.0105
68.	H	0.0000	0.0000	0.0000	0.0002	0.0013	0.0002	0.0017	0.0105	0.9350
69.	H	0.0000	0.0000	0.0003	0.0005	0.0017	0.0006	0.0032	0.0015	0.9386
70.	H	0.0003	0.0000	0.0003	0.0009	0.0103	0.0010	0.0018	0.0015	0.9349

Atom	37	38	39	40	41	42	43	44	45
1. O	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066
2. O	0.0065	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0004
3. C	0.0006	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0004
4. C	0.0011	0.0000	0.0018	0.0015	0.0000	0.0000	0.0005	0.0000	0.0011
5. C	0.0019	0.0006	0.0004	0.0005	0.0004	0.0003	0.0003	0.0000	0.0000
6. C	0.9025	0.0030	0.0147	0.0157	0.0005	0.0001	0.0012	0.0000	0.0000
7. C	0.0031	0.0025	0.0029	0.0029	0.0003	0.0003	0.0044	0.0001	0.0000
8. C	0.0015	0.9305	0.9208	0.9206	0.0000	0.0000	0.0016	0.0001	0.0000
9. C	0.0120	0.0091	0.0054	0.0056	0.0003	0.0003	0.0038	0.0008	0.0000
10. C	0.0088	0.0002	0.0012	0.0012	0.0109	0.0002	0.0143	0.0001	0.0000
11. C	0.0002	0.0003	0.0010	0.0009	0.0029	0.0113	0.0002	0.0001	0.0000
12. C	0.0001	0.0001	0.0001	0.0001	0.0046	0.0005	0.0005	0.0000	0.0001
13. C	0.0005	0.0000	0.0009	0.0010	0.9154	0.0035	0.0004	0.0003	0.0000
14. C	0.0001	0.0001	0.0002	0.0002	0.0035	0.9130	0.0129	0.0079	0.0000
15. C	0.0006	0.0001	0.0012	0.0013	0.0114	0.0031	0.0036	0.0023	0.0000
16. C	0.0003	0.0011	0.0005	0.0005	0.0002	0.0119	0.9087	0.0030	0.0000
17. C	0.0001	0.0001	0.0001	0.0001	0.0005	0.0052	0.0046	0.9059	0.0000
18. C	0.0000	0.0000	0.0001	0.0001	0.0001	0.0006	0.0004	0.0025	0.0000
19. C	0.0000	0.0000	0.0001	0.0001	0.0001	0.0006	0.0005	0.0025	0.0000
20. C	0.0004	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0006
21. C	0.0011	0.0000	0.0008	0.0006	0.0000	0.0000	0.0001	0.0000	0.0011
22. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019
23. C	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.9025
24. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0031

25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015
26.	C	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0120
27.	C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0088
28.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
29.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
30.	C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0005
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
32.	C	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0006
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000
38.	H	0.0001	0.0000	0.0004	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0001	0.0004	0.0000	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
40.	H	0.0000	0.0004	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000
41.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0061	0.0003	0.0004	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0061	0.0000	0.0006	0.0009	0.0000
43.	H	0.0001	0.0000	0.0001	0.0001	0.0003	0.0006	0.0000	0.0008	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0009	0.0008	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0123	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0023	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0001	0.0124	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0023	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0006	0.0001	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	46	47	48	49	50	51	52	53	54
1. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
2. O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3. C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4. C	0.0000	0.0008	0.0006	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
5. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6. C	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9. C	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
10. C	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13. C	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
14. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0002
15. C	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000	0.0000	0.0017	0.0013
16. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0002
17. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0032	0.0017
18. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015	0.0105
19. C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9386	0.9350
20. C	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21. C	0.0000	0.0018	0.0015	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000
22. C	0.0006	0.0004	0.0005	0.0004	0.0003	0.0003	0.0000	0.0000	0.0000
23. C	0.0030	0.0147	0.0157	0.0005	0.0001	0.0012	0.0000	0.0000	0.0000
24. C	0.0025	0.0029	0.0029	0.0003	0.0003	0.0044	0.0001	0.0000	0.0000
25. C	0.9305	0.9209	0.9206	0.0000	0.0000	0.0016	0.0001	0.0000	0.0000
26. C	0.0091	0.0054	0.0056	0.0003	0.0003	0.0038	0.0008	0.0000	0.0000
27. C	0.0002	0.0012	0.0012	0.0109	0.0002	0.0143	0.0001	0.0000	0.0000
28. C	0.0003	0.0010	0.0009	0.0029	0.0113	0.0002	0.0001	0.0000	0.0000
29. C	0.0001	0.0001	0.0001	0.0046	0.0005	0.0005	0.0000	0.0000	0.0000
30. C	0.0000	0.0009	0.0010	0.9154	0.0035	0.0004	0.0003	0.0000	0.0000
31. C	0.0001	0.0002	0.0002	0.0035	0.9130	0.0129	0.0079	0.0000	0.0000
32. C	0.0001	0.0011	0.0013	0.0114	0.0031	0.0036	0.0023	0.0000	0.0000
33. C	0.0011	0.0005	0.0005	0.0002	0.0119	0.9087	0.0030	0.0000	0.0000
34. C	0.0001	0.0001	0.0001	0.0005	0.0052	0.0046	0.9059	0.0000	0.0000
35. C	0.0000	0.0001	0.0001	0.0001	0.0005	0.0004	0.0025	0.0000	0.0000
36. C	0.0000	0.0001	0.0001	0.0001	0.0006	0.0005	0.0025	0.0000	0.0000
37. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39. H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0123	0.0017
45.	H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000
46.	H	0.0000	0.0004	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0004	0.0000	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
48.	H	0.0004	0.0003	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0061	0.0003	0.0004	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0061	0.0000	0.0006	0.0009	0.0000	0.0000
51.	H	0.0000	0.0001	0.0001	0.0003	0.0006	0.0000	0.0008	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0004	0.0009	0.0008	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0003
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0001
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0011
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0006	0.0001	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0023	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0124	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0004	0.0001	0.0123	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002	0.0023	0.0000	0.0000

Atom		55	56	57	58	59	60	61	62	63
1.	O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0013	0.0346	0.0001	0.0001
2.	O	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0013	0.0001
3.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0008	0.0002	0.0000
4.	C	0.0001	0.0000	0.0001	0.0000	0.0001	0.0011	0.0013	0.0003	0.0000
5.	C	0.0002	0.0000	0.0002	0.0000	0.0005	0.0003	0.0001	0.0000	0.0000
6.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0013	0.0023	0.0000	0.0000
7.	C	0.0002	0.0000	0.0002	0.0000	0.0003	0.0005	0.0005	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
9.	C	0.0003	0.0001	0.0003	0.0000	0.0006	0.0018	0.0024	0.0000	0.0000
10.	C	0.0002	0.0001	0.0002	0.0000	0.0086	0.0078	0.0080	0.0000	0.0000
11.	C	0.0003	0.0001	0.0003	0.0000	0.0020	0.0037	0.0048	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.9379	0.9101	0.8514	0.0000	0.0000
13.	C	0.0003	0.0002	0.0002	0.0000	0.0035	0.0105	0.0096	0.0000	0.0000
14.	C	0.0009	0.0005	0.0010	0.0002	0.0010	0.0011	0.0014	0.0000	0.0000
15.	C	0.0103	0.0017	0.0103	0.0013	0.0002	0.0021	0.0027	0.0000	0.0000
16.	C	0.0010	0.0006	0.0010	0.0002	0.0001	0.0012	0.0014	0.0000	0.0000
17.	C	0.0018	0.0032	0.0018	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0015	0.9386	0.9350	0.9357	0.0000	0.0001	0.0001	0.0000	0.0000
19.	C	0.9350	0.0015	0.0016	0.0105	0.0000	0.0001	0.0001	0.0000	0.0000
20.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0003	0.0002	0.0002
21.	C	0.0001	0.0000	0.0001	0.0000	0.0000	0.0003	0.0030	0.0011	0.0001
22.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0005
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0013	0.0002
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0003
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
26.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0018	0.0006
27.	C	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0078	0.0086
28.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.0020
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9101	0.9379
30.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0105	0.0035
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011	0.0010
32.	C	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0021	0.0002
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0012	0.0001
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0006	0.0003	0.0000	0.0000	0.0000
42.	H	0.0001	0.0005	0.0001	0.0000	0.0001	0.0001	0.0001	0.0000	0.0000
43.	H	0.0002	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0023	0.0124	0.0023	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0006
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0002	0.0003	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0003	0.0001	0.0002	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000

55.	H	0.0000	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	0.0002	0.0000	0.0002	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0002	0.0002	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0002	0.0003	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0010	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0013	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0010	0.0013	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013	0.0010
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	Atom	64	65	66	67	68	69	70
1.	O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	O	0.0346	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0030	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
14.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0013	0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
22.	C	0.0001	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002
23.	C	0.0023	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0005	0.0002	0.0000	0.0000	0.0000	0.0000	0.0002
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0024	0.0003	0.0001	0.0000	0.0000	0.0001	0.0003
27.	C	0.0080	0.0002	0.0001	0.0000	0.0000	0.0001	0.0002
28.	C	0.0048	0.0003	0.0001	0.0000	0.0000	0.0000	0.0003
29.	C	0.8514	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	C	0.0096	0.0002	0.0002	0.0000	0.0000	0.0003	0.0003
31.	C	0.0014	0.0010	0.0005	0.0002	0.0002	0.0005	0.0009
32.	C	0.0027	0.0103	0.0017	0.0013	0.0013	0.0017	0.0103
33.	C	0.0014	0.0010	0.0006	0.0002	0.0002	0.0006	0.0010
34.	C	0.0000	0.0018	0.0032	0.0017	0.0017	0.0032	0.0018
35.	C	0.0001	0.9350	0.9386	0.9358	0.0105	0.0015	0.0015
36.	C	0.0001	0.0016	0.0014	0.0105	0.9350	0.9386	0.9349
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0001	0.0001	0.0004	0.0000	0.0000	0.0004	0.0001
51.	H	0.0000	0.0002	0.0001	0.0000	0.0000	0.0001	0.0002
52.	H	0.0000	0.0023	0.0124	0.0017	0.0017	0.0123	0.0023
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0002	0.0003	0.0002	0.0002	0.0002
66.	H	0.0000	0.0002	0.0000	0.0003	0.0001	0.0003	0.0001
67.	H	0.0000	0.0003	0.0003	0.0000	0.0011	0.0001	0.0002
68.	H	0.0000	0.0002	0.0001	0.0011	0.0000	0.0003	0.0003
69.	H	0.0000	0.0002	0.0003	0.0001	0.0003	0.0000	0.0002

70. H	0.0000	0.0002	0.0001	0.0002	0.0003	0.0002	0.0000	

Wiberg bond index, Totals by atom:

Atom		1
1.	O	2.0297
2.	O	2.0299
3.	C	3.9446
4.	C	4.0198
5.	C	4.0115
6.	C	3.9429
7.	C	4.0103
8.	C	3.8630
9.	C	4.0139
10.	C	4.0169
11.	C	3.9982
12.	C	3.8445
13.	C	3.9712
14.	C	3.9657
15.	C	4.0203
16.	C	3.9680
17.	C	3.9711
18.	C	3.8730
19.	C	3.8723
20.	C	3.9446
21.	C	4.0198
22.	C	4.0114
23.	C	3.9428
24.	C	4.0103
25.	C	3.8630
26.	C	4.0139
27.	C	4.0169
28.	C	3.9982
29.	C	3.8445
30.	C	3.9712
31.	C	3.9657
32.	C	4.0203
33.	C	3.9680
34.	C	3.9711
35.	C	3.8731
36.	C	3.8723
37.	H	0.9425
38.	H	0.9489
39.	H	0.9541
40.	H	0.9546
41.	H	0.9591
42.	H	0.9602
43.	H	0.9608
44.	H	0.9606
45.	H	0.9425
46.	H	0.9489
47.	H	0.9541
48.	H	0.9546
49.	H	0.9591
50.	H	0.9602
51.	H	0.9608
52.	H	0.9606
53.	H	0.9606
54.	H	0.9528
55.	H	0.9564
56.	H	0.9607
57.	H	0.9565
58.	H	0.9536
59.	H	0.9575
60.	H	0.9462
61.	H	0.9278
62.	H	0.9462
63.	H	0.9575
64.	H	0.9278
65.	H	0.9565
66.	H	0.9607
67.	H	0.9536
68.	H	0.9528
69.	H	0.9606
70.	H	0.9564

Atom-atom overlap-weighted NAO bond order:

Atom		1	2	3	4	5	6	7	8	9
1.	O	0.0000	0.0003	1.2549	-0.0432	-0.0022	-0.0004	-0.0001	0.0000	-0.0002
2.	O	0.0003	0.0000	0.0008	-0.0440	-0.0054	-0.0039	-0.0002	0.0002	-0.0005
3.	C	1.2549	0.0008	0.0000	0.9212	0.0005	0.0046	0.0002	0.0000	0.0009
4.	C	-0.0432	-0.0440	0.9212	0.0000	1.0943	0.0085	-0.0028	-0.0004	0.0020
5.	C	-0.0022	-0.0054	0.0005	1.0943	0.0000	0.9953	-0.0282	0.0073	-0.0510

6.	C	-0.0004	-0.0039	0.0046	0.0085	0.9953	0.0000	1.1652	0.0104	-0.0021
7.	C	-0.0001	-0.0002	0.0002	-0.0028	-0.0282	1.1652	0.0000	0.9001	1.0126
8.	C	0.0000	0.0002	0.0000	-0.0004	0.0073	0.0104	0.9001	0.0000	0.0076
9.	C	-0.0002	-0.0005	0.0009	0.0020	-0.0510	-0.0021	1.0126	0.0076	0.0000
10.	C	0.0034	-0.0013	-0.0121	0.0081	0.9956	-0.0263	-0.0435	0.0073	0.9114
11.	C	-0.0024	-0.0001	-0.0040	-0.0202	-0.0022	-0.0032	0.0002	-0.0002	0.0220
12.	C	-0.0249	0.0000	-0.0082	-0.0007	-0.0197	0.0011	0.0003	0.0001	0.0095
13.	C	0.0002	0.0000	0.0002	-0.0004	0.0026	-0.0006	0.0018	0.0000	-0.0202
14.	C	0.0001	0.0000	-0.0002	-0.0002	-0.0005	0.0008	0.0000	-0.0003	-0.0334
15.	C	0.0000	0.0000	-0.0001	0.0002	0.0023	-0.0011	0.0001	0.0004	-0.0045
16.	C	-0.0001	-0.0001	0.0000	-0.0004	0.0025	-0.0048	-0.0012	-0.0083	1.1178
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	-0.0007	0.0000	0.0079
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0006
19.	C	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	-0.0006
20.	C	0.0008	1.2550	0.0716	0.9094	-0.0100	-0.0271	0.0014	-0.0002	0.0003
21.	C	-0.0440	-0.0432	0.9095	0.0184	-0.0008	-0.0021	0.0009	0.0000	0.0006
22.	C	-0.0054	-0.0022	-0.0100	-0.0009	0.0002	0.0005	0.0000	0.0000	0.0000
23.	C	-0.0040	-0.0004	-0.0271	-0.0021	0.0005	0.0001	0.0000	0.0000	0.0000
24.	C	-0.0002	-0.0001	0.0014	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0002	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	-0.0005	-0.0002	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000
27.	C	-0.0013	0.0034	0.0065	-0.0020	0.0003	-0.0001	0.0000	0.0000	0.0000
28.	C	-0.0001	-0.0024	-0.0003	-0.0009	-0.0001	-0.0001	0.0000	0.0000	0.0000
29.	C	0.0000	-0.0248	0.0002	-0.0016	0.0003	0.0003	0.0000	0.0000	0.0000
30.	C	0.0000	0.0002	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	-0.0001	-0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0002	0.0132	0.0000	-0.0046	0.0116	0.7903	0.0173	-0.0020	0.0077
38.	H	0.0000	0.0001	0.0000	0.0002	0.0000	-0.0035	0.0107	0.7703	0.0008
39.	H	0.0000	0.0000	0.0000	-0.0001	0.0009	-0.0003	0.0111	0.7714	-0.0034
40.	H	0.0000	0.0000	0.0000	-0.0003	0.0008	-0.0007	0.0113	0.7718	-0.0035
41.	H	0.0000	0.0000	0.0000	0.0000	0.0006	-0.0001	-0.0001	0.0000	0.0017
42.	H	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0001	-0.0002	0.0000	0.0016
43.	H	0.0000	0.0000	0.0000	-0.0002	0.0016	0.0000	-0.0058	0.0063	0.0166
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0003	-0.0002	0.0003
45.	H	0.0133	0.0002	0.0003	-0.0008	0.0001	-0.0001	0.0000	0.0000	0.0000
46.	H	0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
59.	H	-0.0005	0.0000	0.0002	0.0004	0.0006	-0.0001	-0.0002	0.0000	0.0006
60.	H	-0.0013	0.0001	0.0010	0.0041	0.0024	0.0004	0.0003	0.0000	0.0005
61.	H	0.0467	0.0000	0.0013	-0.0007	0.0005	0.0001	0.0001	0.0000	0.0000
62.	H	0.0001	-0.0013	0.0004	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	-0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0467	-0.0001	-0.0016	0.0002	0.0004	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom	10	11	12	13	14	15	16	17	18
1. O	0.0034	-0.0024	-0.0249	0.0002	0.0001	0.0000	-0.0001	0.0000	0.0000
2. O	-0.0013	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000
3. C	-0.0121	-0.0040	-0.0082	0.0002	-0.0002	-0.0001	0.0000	0.0000	0.0000
4. C	0.0081	-0.0202	-0.0007	-0.0004	-0.0002	0.0002	-0.0004	0.0000	0.0000
5. C	0.9956	-0.0022	-0.0197	0.0026	-0.0005	0.0023	0.0025	0.0000	0.0000
6. C	-0.0263	-0.0032	0.0011	-0.0006	0.0008	-0.0011	-0.0048	0.0001	0.0000
7. C	-0.0435	0.0002	0.0003	0.0018	0.0000	0.0001	-0.0012	-0.0007	0.0000
8. C	0.0073	-0.0002	0.0001	0.0000	-0.0003	0.0004	-0.0083	0.0000	0.0000
9. C	0.9114	0.0220	0.0095	-0.0202	-0.0334	-0.0045	1.1178	0.0079	-0.0006
10. C	0.0000	1.1075	-0.0113	-0.0010	-0.0305	-0.0176	0.0138	0.0005	-0.0001
11. C	1.1075	0.0000	0.8655	1.0746	0.0053	-0.0275	-0.0189	-0.0004	0.0000
12. C	-0.0113	0.8655	0.0000	-0.0035	0.0064	0.0000	-0.0005	0.0000	0.0000
13. C	-0.0010	1.0746	-0.0035	0.0000	1.1640	-0.0074	-0.0350	0.0059	-0.0001
14. C	-0.0305	0.0053	0.0064	1.1640	0.0000	1.0973	0.0043	-0.0056	-0.0094
15. C	-0.0176	-0.0275	0.0000	-0.0074	1.0973	0.0000	1.1217	0.8122	0.0022
16. C	0.0138	-0.0189	-0.0005	-0.0350	0.0043	1.1217	0.0000	-0.0017	-0.0035
17. C	0.0005	-0.0004	0.0000	0.0059	-0.0056	0.8122	-0.0017	0.0000	0.8420
18. C	-0.0001	0.0000	0.0000	-0.0001	-0.0094	0.0022	-0.0035	0.8420	0.0000
19. C	0.0000	-0.0002	0.0000	-0.0001	-0.0091	0.0026	-0.0033	0.8427	0.0067
20. C	0.0065	-0.0003	0.0002	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000

21.	C	-0.0020	-0.0009	-0.0016	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0003	-0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23.	C	-0.0001	-0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0069	0.0006	0.0002	-0.0001	0.0000	-0.0001	0.0008	0.0000	0.0000
38.	H	0.0006	-0.0001	0.0000	0.0000	0.0000	-0.0001	0.0007	0.0000	0.0000
39.	H	0.0002	-0.0001	0.0000	0.0002	0.0001	0.0001	0.0003	0.0000	0.0001
40.	H	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0002	0.0000	-0.0001
41.	H	0.0038	0.0159	-0.0024	0.7960	0.0202	0.0037	0.0009	0.0010	0.0000
42.	H	0.0010	0.0040	0.0009	0.0177	0.7927	0.0155	0.0054	-0.0023	0.0028
43.	H	0.0051	0.0014	-0.0001	0.0018	0.0057	0.0182	0.7900	-0.0045	0.0007
44.	H	-0.0002	0.0000	0.0000	0.0009	0.0018	0.0082	0.0004	0.7874	0.0140
45.	H	0.0001	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0001	-0.0002	0.0000	0.0003	0.0021	-0.0042	0.0006	0.0048	-0.0011
54.	H	0.0000	0.0000	0.0000	0.0003	-0.0010	-0.0029	0.0008	0.0099	-0.0008
55.	H	0.0000	0.0000	0.0000	-0.0001	0.0004	0.0032	0.0008	0.0110	-0.0015
56.	H	0.0001	-0.0002	0.0000	0.0003	0.0021	-0.0043	0.0006	0.0047	0.7821
57.	H	0.0000	0.0000	0.0000	-0.0001	0.0005	0.0032	0.0008	0.0108	0.7771
58.	H	-0.0001	0.0000	0.0000	0.0003	-0.0011	-0.0030	0.0009	0.0099	0.7755
59.	H	0.0016	0.0094	0.7822	-0.0026	0.0002	-0.0002	0.0002	0.0000	0.0000
60.	H	-0.0069	0.0160	0.7666	0.0000	0.0010	-0.0002	0.0001	0.0000	0.0000
61.	H	-0.0029	0.0169	0.7345	-0.0013	0.0001	0.0001	0.0001	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		19	20	21	22	23	24	25	26	27
1.	O	0.0000	0.0008	-0.0440	-0.0054	-0.0040	-0.0002	0.0002	-0.0005	-0.0013
2.	O	0.0000	1.2550	-0.0432	-0.0022	-0.0004	-0.0001	0.0000	-0.0002	0.0034
3.	C	0.0000	0.0716	0.9095	-0.0100	-0.0271	0.0014	-0.0002	0.0003	0.0065
4.	C	0.0000	0.9094	0.0184	-0.0009	-0.0021	0.0009	0.0000	0.0006	-0.0020
5.	C	-0.0001	-0.0100	-0.0008	0.0002	0.0005	0.0000	0.0000	0.0000	0.0003
6.	C	0.0000	-0.0271	-0.0021	0.0005	0.0001	0.0000	0.0000	0.0000	-0.0001
7.	C	0.0000	0.0014	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	-0.0006	0.0003	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0065	-0.0020	0.0003	-0.0001	0.0000	0.0000	0.0000	0.0001
11.	C	-0.0002	-0.0003	-0.0009	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0002	-0.0016	0.0003	0.0003	0.0000	0.0000	0.0000	0.0000
13.	C	-0.0001	0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	-0.0091	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	-0.0033	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.8427	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0067	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0000	0.0000	0.9210	0.0005	0.0046	0.0002	0.0000	0.0009	-0.0121
21.	C	0.0000	0.9210	0.0000	1.0945	0.0085	-0.0028	-0.0004	0.0020	0.0081
22.	C	0.0000	0.0005	1.0945	0.0000	0.9952	-0.0282	0.0073	-0.0510	0.9956
23.	C	0.0000	0.0046	0.0085	0.9952	0.0000	1.1653	0.0104	-0.0020	-0.0263
24.	C	0.0000	0.0002	-0.0028	-0.0282	1.1653	0.0000	0.9001	1.0125	-0.0435
25.	C	0.0000	0.0000	-0.0004	0.0073	0.0104	0.9001	0.0000	0.0076	0.0073
26.	C	0.0000	0.0009	0.0020	-0.0510	-0.0020	1.0125	0.0076	0.0000	0.9115
27.	C	0.0000	-0.0121	0.0081	0.9956	-0.0263	-0.0435	0.0073	0.9115	0.0000
28.	C	0.0000	-0.0040	-0.0202	-0.0022	-0.0032	0.0002	-0.0002	0.0220	1.1075
29.	C	0.0000	-0.0082	-0.0007	-0.0197	0.0011	0.0003	0.0001	0.0095	-0.0113
30.	C	0.0000	0.0002	-0.0004	0.0026	-0.0006	0.0018	0.0000	-0.0202	-0.0010
31.	C	0.0000	-0.0002	-0.0002	-0.0005	0.0008	0.0000	-0.0003	-0.0335	-0.0305
32.	C	0.0000	-0.0001	0.0002	0.0023	-0.0011	0.0001	0.0004	-0.0045	-0.0176
33.	C	0.0000	0.0000	-0.0004	0.0025	-0.0048	-0.0012	-0.0083	1.1178	0.0138
34.	C	0.0000	0.0000	0.0000	0.0000	0.0001	-0.0007	0.0000	0.0079	0.0005
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0006	-0.0001

36.	C	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	-0.0006	0.0000
37.	H	0.0000	0.0003	-0.0008	0.0001	-0.0001	0.0000	0.0000	0.0000	0.0001
38.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0029	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0140	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	-0.0046	0.0116	0.7903	0.0173	-0.0020	0.0077	0.0069
46.	H	0.0000	0.0000	0.0002	0.0000	-0.0035	0.0107	0.7703	0.0008	0.0006
47.	H	0.0000	0.0000	-0.0001	0.0009	-0.0003	0.0111	0.7714	-0.0034	0.0002
48.	H	0.0000	0.0000	-0.0003	0.0008	-0.0007	0.0113	0.7718	-0.0035	0.0001
49.	H	0.0000	0.0000	0.0000	0.0006	-0.0001	-0.0001	0.0000	0.0017	0.0038
50.	H	0.0000	0.0000	0.0000	-0.0002	0.0001	-0.0002	0.0000	0.0016	0.0010
51.	H	0.0000	0.0000	-0.0002	0.0016	0.0000	-0.0058	0.0063	0.0167	0.0051
52.	H	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0003	-0.0002	0.0003	-0.0002
53.	H	0.7820	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.7749	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.7772	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	-0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	-0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	-0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0004	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	-0.0001	-0.0016	0.0002	0.0004	0.0000	0.0000	0.0000	-0.0001
62.	H	0.0000	0.0010	0.0041	0.0024	0.0004	0.0003	0.0000	0.0005	-0.0069
63.	H	0.0000	0.0002	0.0004	0.0006	-0.0001	-0.0002	0.0000	0.0006	0.0016
64.	H	0.0000	0.0013	-0.0007	0.0005	0.0001	0.0001	0.0000	0.0000	-0.0029
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	-0.0001
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000

Atom	28	29	30	31	32	33	34	35	36
1.	O	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000
2.	O	-0.0024	-0.0248	0.0002	0.0001	0.0000	-0.0001	0.0000	0.0000	0.0000
3.	C	-0.0003	0.0002	0.0002	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
4.	C	-0.0009	-0.0016	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	-0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	-0.0001	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	-0.0040	-0.0082	0.0002	-0.0002	-0.0001	0.0000	0.0000	0.0000	0.0000
21.	C	-0.0202	-0.0007	-0.0004	-0.0002	0.0002	-0.0004	0.0000	0.0000	0.0000
22.	C	-0.0022	-0.0197	0.0026	-0.0005	0.0023	0.0025	0.0000	0.0000	-0.0001
23.	C	-0.0032	0.0011	-0.0006	0.0008	-0.0011	-0.0048	0.0001	0.0000	0.0000
24.	C	0.0002	0.0003	0.0018	0.0000	0.0001	-0.0012	-0.0007	0.0000	0.0000
25.	C	-0.0002	0.0001	0.0000	-0.0003	0.0004	-0.0083	0.0000	0.0000	0.0000
26.	C	0.0220	0.0095	-0.0202	-0.0335	-0.0045	1.1178	0.0079	-0.0006	-0.0006
27.	C	1.1075	-0.0113	-0.0010	-0.0305	-0.0176	0.0138	0.0005	-0.0001	0.0000
28.	C	0.0000	0.8655	1.0747	0.0053	-0.0274	-0.0189	-0.0004	0.0000	-0.0002
29.	C	0.8655	0.0000	-0.0035	0.0064	0.0000	-0.0005	0.0000	0.0000	0.0000
30.	C	1.0747	-0.0035	0.0000	1.1640	-0.0074	-0.0350	0.0059	-0.0001	-0.0001
31.	C	0.0053	0.0064	1.1640	0.0000	1.0973	0.0043	-0.0056	-0.0093	-0.0092
32.	C	-0.0274	0.0000	-0.0074	1.0973	0.0000	1.1217	0.8122	0.0022	0.0025
33.	C	-0.0189	-0.0005	-0.0350	0.0043	1.1217	0.0000	-0.0017	-0.0035	-0.0032
34.	C	-0.0004	0.0000	0.0059	-0.0056	0.8122	-0.0017	0.0000	0.8418	0.8429
35.	C	0.0000	0.0000	-0.0001	-0.0093	0.0022	-0.0035	0.8418	0.0000	0.0067
36.	C	-0.0002	0.0000	-0.0001	-0.0092	0.0025	-0.0032	0.8429	0.0067	0.0000
37.	H	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0006	0.0002	-0.0001	0.0000	-0.0001	0.0008	0.0000	0.0000	0.0000
46.	H	-0.0001	0.0000	0.0000	0.0000	-0.0001	0.0007	0.0000	0.0000	0.0000
47.	H	-0.0001	0.0000	0.0002	0.0001	0.0001	0.0002	0.0000	0.0001	-0.0001
48.	H	0.0001	0.0000	0.0001	0.0000	0.0001	0.0002	0.0000	-0.0001	0.0001
49.	H	0.0159	-0.0024	0.7960	0.0202	0.0037	0.0009	0.0010	0.0000	0.0000
50.	H	0.0040	0.0009	0.0177	0.7927	0.0155	0.0054	-0.0023	0.0028	0.0030

51.	H	0.0014	-0.0001	0.0018	0.0057	0.0182	0.7900	-0.0045	0.0007	0.0008
52.	H	0.0000	0.0000	0.0009	0.0018	0.0082	0.0004	0.7874	0.0140	0.0140
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0160	0.7666	0.0000	0.0010	-0.0002	0.0001	0.0000	0.0000	0.0000
63.	H	0.0094	0.7821	-0.0026	0.0002	-0.0002	0.0002	0.0000	0.0000	0.0000
64.	H	0.0169	0.7345	-0.0013	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	-0.0001	0.0005	0.0032	0.0008	0.0108	0.7772	-0.0014
66.	H	-0.0002	0.0000	0.0003	0.0022	-0.0043	0.0006	0.0047	0.7820	-0.0011
67.	H	0.0000	0.0000	0.0003	-0.0011	-0.0030	0.0009	0.0099	0.7755	-0.0008
68.	H	0.0000	0.0000	0.0003	-0.0010	-0.0029	0.0008	0.0099	-0.0008	0.7749
69.	H	-0.0002	0.0000	0.0003	0.0021	-0.0042	0.0006	0.0048	-0.0011	0.7821
70.	H	0.0000	0.0000	-0.0001	0.0005	0.0032	0.0008	0.0110	-0.0015	0.7772

Atom		37	38	39	40	41	42	43	44	45
1.	O	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0133
2.	O	0.0132	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
3.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
4.	C	-0.0046	0.0002	-0.0001	-0.0003	0.0000	0.0000	-0.0002	0.0000	-0.0008
5.	C	0.0116	0.0000	0.0009	0.0008	0.0006	-0.0002	0.0016	0.0000	0.0001
6.	C	0.7903	-0.0035	-0.0003	-0.0007	-0.0001	0.0001	0.0000	-0.0001	-0.0001
7.	C	0.0173	0.0107	0.0111	0.0113	-0.0001	-0.0002	-0.0058	0.0003	0.0000
8.	C	-0.0020	0.7703	0.7714	0.7718	0.0000	0.0000	0.0063	-0.0002	0.0000
9.	C	0.0077	0.0008	-0.0034	-0.0035	0.0017	0.0016	0.0166	0.0003	0.0000
10.	C	0.0069	0.0006	0.0002	0.0001	0.0038	0.0010	0.0051	-0.0002	0.0001
11.	C	0.0006	-0.0001	-0.0001	0.0001	0.0159	0.0040	0.0014	0.0000	0.0000
12.	C	0.0002	0.0000	0.0000	0.0000	-0.0024	0.0009	-0.0001	0.0000	-0.0001
13.	C	-0.0001	0.0000	0.0002	0.0001	0.7960	0.0177	0.0018	0.0009	0.0000
14.	C	0.0000	0.0000	0.0001	0.0000	0.0202	0.7927	0.0057	0.0018	0.0000
15.	C	-0.0001	-0.0001	0.0001	0.0001	0.0037	0.0155	0.0182	0.0082	0.0000
16.	C	0.0008	0.0007	0.0003	0.0002	0.0009	0.0054	0.7900	0.0004	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0010	-0.0023	-0.0045	0.7874	0.0000
18.	C	0.0000	0.0000	0.0001	-0.0001	0.0000	0.0028	0.0007	0.0140	0.0000
19.	C	0.0000	0.0000	-0.0001	0.0001	0.0000	0.0029	0.0008	0.0140	0.0000
20.	C	0.0003	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	-0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0046
22.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0116
23.	C	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7903
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0173
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0020
26.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0077
27.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0069
28.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
29.	C	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
30.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	-0.0010	-0.0004	-0.0003	0.0000	0.0000	0.0001	0.0000	0.0000
38.	H	-0.0010	0.0000	0.0058	0.0059	0.0000	0.0000	-0.0001	0.0000	0.0000
39.	H	-0.0004	0.0058	0.0000	0.0076	0.0000	0.0000	0.0002	0.0001	0.0000
40.	H	-0.0003	0.0059	0.0076	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0058	-0.0001	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	-0.0058	0.0000	0.0009	-0.0016	0.0000
43.	H	0.0001	-0.0001	0.0002	0.0003	-0.0001	0.0009	0.0000	0.0008	0.0000
44.	H	0.0000	0.0000	0.0001	0.0001	0.0000	-0.0016	0.0008	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0010
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0004
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0003
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	-0.0001	-0.0065	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0003	-0.0003	-0.0014	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	-0.0016	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	-0.0001	-0.0066	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	-0.0016	0.0000
58.	H	0.0000	0.0000	0.0001	0.0000	0.0000	-0.0003	-0.0004	-0.0014	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0019	0.0003	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	-0.0005	-0.0001	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		46	47	48	49	50	51	52	53	54
1.	O	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
10.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003
14.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0021	-0.0010
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0042	-0.0029
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0008
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0048	0.0099
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0011	-0.0008
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7820	0.7749
20.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	0.0002	-0.0001	-0.0003	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000
22.	C	0.0000	0.0009	0.0008	0.0006	-0.0002	0.0016	0.0000	0.0000	0.0000
23.	C	-0.0035	-0.0003	-0.0007	-0.0001	0.0001	0.0000	-0.0001	0.0000	0.0000
24.	C	0.0107	0.0111	0.0113	-0.0001	-0.0002	-0.0058	0.0003	0.0000	0.0000
25.	C	0.7703	0.7714	0.7718	0.0000	0.0000	0.0063	-0.0002	0.0000	0.0000
26.	C	0.0008	-0.0034	-0.0035	0.0017	0.0016	0.0167	0.0003	0.0000	0.0000
27.	C	0.0006	0.0002	0.0001	0.0038	0.0010	0.0051	-0.0002	0.0000	0.0000
28.	C	-0.0001	-0.0001	0.0001	0.0159	0.0040	0.0014	0.0000	0.0000	0.0000
29.	C	0.0000	0.0000	0.0000	-0.0024	0.0009	-0.0001	0.0000	0.0000	0.0000
30.	C	0.0000	0.0002	0.0001	0.7960	0.0177	0.0018	0.0009	0.0000	0.0000
31.	C	0.0000	0.0001	0.0000	0.0202	0.7927	0.0057	0.0018	0.0000	0.0000
32.	C	-0.0001	0.0001	0.0001	0.0037	0.0155	0.0182	0.0082	0.0000	0.0000
33.	C	0.0007	0.0002	0.0002	0.0009	0.0054	0.7900	0.0004	0.0000	0.0000
34.	C	0.0000	0.0000	0.0000	0.0010	-0.0023	-0.0045	0.7874	0.0000	0.0000
35.	C	0.0000	0.0001	-0.0001	0.0000	0.0028	0.0007	0.0140	0.0000	0.0000
36.	C	0.0000	-0.0001	0.0001	0.0000	0.0030	0.0008	0.0140	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	-0.0003
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0003
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0065	-0.0014
45.	H	-0.0010	-0.0004	-0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
46.	H	0.0000	0.0058	0.0059	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000
47.	H	0.0058	0.0000	0.0076	0.0000	0.0000	0.0002	0.0001	0.0000	0.0000
48.	H	0.0059	0.0076	0.0000	0.0000	0.0000	0.0003	0.0001	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	-0.0058	-0.0001	0.0000	0.0000	0.0000
50.	H	0.0000	0.0000	0.0000	-0.0058	0.0000	0.0009	-0.0016	0.0000	0.0000
51.	H	-0.0001	0.0002	0.0003	-0.0001	0.0009	0.0000	0.0008	0.0000	0.0000
52.	H	0.0000	0.0001	0.0001	0.0000	-0.0016	0.0008	0.0000	0.0000	0.0000
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0047
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0047	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0043
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0017	-0.0003
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0004
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0008
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0000	0.0000	0.0000	0.0019	0.0003	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	-0.0005	-0.0001	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	-0.0016	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0002	-0.0001	-0.0066	0.0000	0.0000
67.	H	0.0000	0.0001	0.0000	0.0000	-0.0003	-0.0004	-0.0014	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	-0.0003	-0.0003	-0.0014	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0002	-0.0001	-0.0065	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0003	0.0003	-0.0016	0.0000	0.0000

Atom		55	56	57	58	59	60	61	62	63
1.	O	0.0000	0.0000	0.0000	0.0000	-0.0005	-0.0013	0.0467	0.0001	0.0000
2.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0013	-0.0005
3.	C	0.0000	0.0000	0.0000	0.0000	0.0002	0.0010	0.0013	0.0004	0.0000
4.	C	0.0000	0.0000	0.0000	0.0000	0.0004	0.0041	-0.0007	0.0009	0.0000
5.	C	0.0000	0.0000	0.0000	0.0000	0.0006	0.0024	0.0005	0.0000	0.0000
6.	C	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0004	0.0001	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0003	0.0001	0.0000	0.0000

8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	-0.0002	0.0000	-0.0002	0.0003	0.0006	0.0005	0.0000	0.0000	0.0000
10.	C	0.0000	0.0001	0.0000	-0.0001	0.0016	-0.0069	-0.0029	0.0000	0.0000
11.	C	0.0000	-0.0002	0.0000	0.0000	0.0094	0.0160	0.0169	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.7822	0.7666	0.7345	0.0000	0.0000
13.	C	-0.0001	0.0003	-0.0001	0.0003	-0.0026	0.0000	-0.0013	0.0000	0.0000
14.	C	0.0004	0.0021	0.0005	-0.0011	0.0002	0.0010	0.0001	0.0000	0.0000
15.	C	0.0032	-0.0043	0.0032	-0.0030	-0.0002	-0.0002	0.0001	0.0000	0.0000
16.	C	0.0008	0.0006	0.0008	0.0009	0.0002	0.0001	0.0001	0.0000	0.0000
17.	C	0.0110	0.0047	0.0108	0.0099	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	-0.0015	0.7821	0.7771	0.7755	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.7772	-0.0011	-0.0014	-0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	-0.0001	0.0010	0.0002
21.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	-0.0016	0.0041	0.0004
22.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0024	0.0006
23.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0004	-0.0001
24.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	-0.0002
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0005	0.0006
27.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0069	0.0016
28.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0160	0.0094
29.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7666	0.7821
30.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0026
31.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0010	0.0002
32.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	-0.0002
33.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0002
34.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0019	-0.0012	-0.0005	0.0000	0.0000
42.	H	0.0003	0.0003	0.0003	-0.0003	0.0003	0.0000	-0.0001	0.0000	0.0000
43.	H	0.0003	-0.0001	0.0003	-0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	-0.0016	-0.0066	-0.0016	-0.0014	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0019
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
51.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53.	H	0.0045	-0.0017	-0.0001	-0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0043	-0.0003	-0.0004	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	-0.0001	-0.0006	-0.0004	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	-0.0001	0.0000	0.0045	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	-0.0006	0.0045	0.0000	0.0043	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	-0.0004	0.0047	0.0043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0064	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000	0.0072	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0064	0.0072	0.0000	0.0000	0.0000
62.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054
63.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0064
65.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Atom		64	65	66	67	68	69	70
1.	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.	O	0.0467	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.	C	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	-0.0016	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.	C	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	C	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
14.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
16.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
20.	C	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21.	C	-0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22.	C	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

23.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
24.	C	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
25.	C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26.	C	0.0000	-0.0002	0.0000	0.0003	0.0003	0.0000	-0.0002
27.	C	-0.0029	0.0000	0.0001	-0.0001	0.0000	0.0001	0.0000
28.	C	0.0169	0.0000	-0.0002	0.0000	0.0000	-0.0002	0.0000
29.	C	0.7345	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30.	C	-0.0013	-0.0001	0.0003	0.0003	0.0003	0.0003	-0.0001
31.	C	0.0001	0.0005	0.0022	-0.0011	-0.0010	0.0021	0.0005
32.	C	0.0001	0.0032	-0.0043	-0.0030	-0.0029	-0.0042	0.0032
33.	C	0.0001	0.0008	0.0006	0.0009	0.0008	0.0006	0.0008
34.	C	0.0000	0.0108	0.0047	0.0099	0.0099	0.0048	0.0110
35.	C	0.0000	0.7772	0.7820	0.7755	-0.0008	-0.0011	-0.0015
36.	C	0.0000	-0.0014	-0.0011	-0.0008	0.7749	0.7821	0.7772
37.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
38.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
40.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
47.	H	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000
48.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
49.	H	-0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50.	H	-0.0001	0.0003	0.0002	-0.0003	-0.0003	0.0002	0.0003
51.	H	0.0000	0.0003	-0.0001	-0.0004	-0.0003	-0.0001	0.0003
52.	H	0.0000	-0.0016	-0.0066	-0.0014	-0.0014	-0.0065	-0.0016
53.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
56.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
57.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
59.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
60.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
61.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
62.	H	0.0072	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
63.	H	0.0064	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
64.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
65.	H	0.0000	0.0000	0.0044	0.0043	-0.0004	-0.0001	-0.0006
66.	H	0.0000	0.0044	0.0000	0.0047	-0.0003	-0.0017	-0.0001
67.	H	0.0000	0.0043	0.0047	0.0000	0.0008	-0.0003	-0.0004
68.	H	0.0000	-0.0004	-0.0003	0.0008	0.0000	0.0047	0.0043
69.	H	0.0000	-0.0001	-0.0017	-0.0003	0.0047	0.0000	0.0045
70.	H	0.0000	-0.0006	-0.0001	-0.0004	0.0043	0.0045	0.0000

Atom-atom overlap-weighted NAO bond order, Totals by atom:

Atom		1
1.	O	1.1894
2.	O	1.1895
3.	C	3.1141
4.	C	2.8409
5.	C	3.0005
6.	C	2.9016
7.	C	3.0510
8.	C	3.2417
9.	C	3.0027
10.	C	2.9179
11.	C	3.0579
12.	C	3.0952
13.	C	2.9951
14.	C	3.0140
15.	C	3.0180
16.	C	2.9860
17.	C	3.3359
18.	C	3.1860
19.	C	3.1871
20.	C	3.1141
21.	C	2.8410
22.	C	3.0006
23.	C	2.9015
24.	C	3.0511
25.	C	3.2417
26.	C	3.0028
27.	C	2.9179
28.	C	3.0580
29.	C	3.0952
30.	C	2.9951
31.	C	3.0140
32.	C	3.0180
33.	C	2.9860
34.	C	3.3358

35.	C	3.1857
36.	C	3.1872
37.	H	0.8401
38.	H	0.7906
39.	H	0.7937
40.	H	0.7936
41.	H	0.8355
42.	H	0.8363
43.	H	0.8396
44.	H	0.8070
45.	H	0.8401
46.	H	0.7906
47.	H	0.7937
48.	H	0.7936
49.	H	0.8355
50.	H	0.8363
51.	H	0.8396
52.	H	0.8070
53.	H	0.7851
54.	H	0.7887
55.	H	0.7976
56.	H	0.7852
57.	H	0.7973
58.	H	0.7890
59.	H	0.8059
60.	H	0.7968
61.	H	0.8073
62.	H	0.7969
63.	H	0.8059
64.	H	0.8072
65.	H	0.7973
66.	H	0.7850
67.	H	0.7890
68.	H	0.7887
69.	H	0.7852
70.	H	0.7976

MO bond order:

Atom		1	2	3	4	5	6	7	8	9
1.	O	0.0000	0.2433	0.0668	0.0077	0.0493	0.0448	0.0018	-0.0030	-0.0213
2.	O	0.2433	0.0000	-0.1692	0.0529	0.0397	0.0408	-0.0287	0.0118	0.0019
3.	C	0.0668	-0.1692	0.0000	0.1142	-0.1428	0.0296	0.0130	0.0136	0.0245
4.	C	0.0077	0.0529	0.1142	0.0000	0.7946	0.1360	0.0098	0.0136	0.0902
5.	C	0.0493	0.0397	-0.1428	0.7946	0.0000	-1.3396	-0.1928	-0.0643	0.0219
6.	C	0.0448	0.0408	0.0296	0.1360	-1.3396	0.0000	0.5044	0.2282	-0.0943
7.	C	0.0018	-0.0287	0.0130	0.0098	-0.1928	0.5044	0.0000	-0.9071	-1.1105
8.	C	-0.0030	0.0118	0.0136	0.0136	-0.0643	0.2282	-0.9071	0.0000	-0.0726
9.	C	-0.0213	0.0019	0.0245	0.0902	0.0219	-0.0943	-1.1105	-0.0726	0.0000
10.	C	0.0277	0.0083	-0.0026	-0.0370	0.0610	-0.1288	-0.1124	-0.0703	-0.0972
11.	C	0.0389	-0.0055	-0.0054	0.0042	-0.0417	-0.1130	-0.0927	0.0210	-0.0732
12.	C	-0.0517	0.0101	0.0184	0.0101	0.1392	0.0015	0.0142	-0.0181	-0.0885
13.	C	-0.0033	0.0008	0.0261	-0.0056	-0.0391	0.0265	0.0373	-0.0035	0.0150
14.	C	0.0058	0.0030	-0.0033	0.0028	0.0078	0.0451	0.0390	0.0099	-0.0051
15.	C	0.0173	0.0167	-0.0064	0.0177	0.0024	0.0082	-0.1184	-0.0282	0.0099
16.	C	-0.0104	-0.0054	0.0058	0.0016	0.0575	0.0545	0.1189	0.0565	0.8471
17.	C	-0.0029	-0.0008	0.0026	-0.0001	0.0078	0.0135	-0.0193	0.0221	0.0205
18.	C	0.0043	0.0036	-0.0019	0.0018	0.0046	-0.0080	-0.0057	0.0016	0.0317
19.	C	0.0015	0.0021	-0.0014	0.0011	0.0006	0.0151	0.0108	0.0028	0.0074
20.	C	-0.1407	-0.3692	-0.2241	-0.3236	0.0841	-0.0430	-0.0091	-0.0014	0.0294
21.	C	0.0356	0.0470	-0.0079	0.1528	-0.0367	-0.0508	0.0615	-0.0204	0.0392
22.	C	0.0185	0.0265	-0.1257	-0.1171	0.0342	0.0099	-0.0076	0.0026	-0.0061
23.	C	-0.1166	0.0294	0.0329	-0.0936	0.0099	-0.0095	-0.0044	-0.0042	-0.0090
24.	C	-0.0009	0.0136	-0.0045	0.0537	-0.0070	-0.0012	0.0046	0.0024	0.0081
25.	C	0.0102	-0.0013	0.0142	-0.0021	-0.0019	-0.0004	0.0003	-0.0007	-0.0020
26.	C	-0.0169	-0.0190	0.0482	0.0165	-0.0072	-0.0072	0.0087	-0.0024	0.0047
27.	C	0.0119	0.0405	-0.0058	-0.0650	0.0292	-0.0148	0.0012	-0.0036	-0.0006
28.	C	-0.0073	0.0111	0.0059	0.0094	0.0049	0.0087	0.0015	0.0018	0.0033
29.	C	0.0130	0.0252	0.0007	0.0196	-0.0037	0.0122	-0.0014	0.0038	0.0025
30.	C	-0.0030	0.0093	0.0114	0.0218	-0.0046	-0.0006	0.0065	-0.0002	0.0051
31.	C	-0.0038	-0.0056	0.0028	0.0029	0.0001	0.0006	-0.0006	0.0005	-0.0005
32.	C	0.0083	0.0166	-0.0030	-0.0314	0.0116	0.0006	-0.0055	0.0002	-0.0047
33.	C	-0.0099	-0.0137	0.0030	0.0088	-0.0083	0.0019	0.0071	-0.0008	0.0048
34.	C	0.0005	0.0006	-0.0026	-0.0012	0.0003	-0.0002	0.0002	-0.0003	-0.0002
35.	C	0.0109	0.0159	-0.0087	-0.0239	0.0092	0.0021	-0.0054	0.0007	-0.0042
36.	C	-0.0094	-0.0104	0.0077	0.0178	-0.0064	0.0002	0.0044	0.0000	0.0034
37.	H	-0.0043	-0.0303	0.0000	0.0094	-0.0131	-0.5078	0.0676	-0.0342	-0.0595
38.	H	0.0001	0.0015	0.0011	-0.0030	-0.0240	-0.0246	-0.0686	-0.6381	-0.0499
39.	H	-0.0039	-0.0013	-0.0034	0.0297	-0.0041	-0.0235	-0.0609	0.6062	-0.0098
40.	H	0.0030	0.0004	-0.0018	-0.0167	-0.0010	0.0563	-0.0900	0.0268	0.0244
41.	H	-0.0047	0.0019	0.0094	0.0062	-0.0139	0.0246	0.0210	0.0010	0.0043
42.	H	-0.0020	-0.0007	0.0014	0.0036	0.0188	0.0061	0.0306	0.0090	-0.0046
43.	H	-0.0027	0.0015	0.0035	0.0141	-0.0303	0.0127	-0.0967	0.0622	-0.0579
44.	H	-0.0004	0.0008	-0.0001	0.0004	0.0064	0.0041	-0.0075	-0.0034	0.0287
45.	H	0.0165	0.0045	0.0196	0.0111	0.0012	0.0080	0.0009	0.0004	0.0004
46.	H	-0.0032	0.0003	0.0054	-0.0007	0.0017	0.0020	-0.0006	0.0001	-0.0004

47.	H	-0.0028	-0.0009	0.0105	0.0296	-0.0063	-0.0003	0.0044	0.0001	0.0043
48.	H	0.0045	0.0025	-0.0029	-0.0281	0.0043	-0.0009	-0.0029	-0.0006	-0.0044
49.	H	-0.0023	0.0026	-0.0014	0.0014	-0.0011	0.0021	0.0000	0.0006	0.0002
50.	H	0.0001	0.0015	-0.0013	0.0000	0.0002	0.0005	0.0000	0.0002	-0.0001
51.	H	0.0002	0.0012	-0.0033	0.0042	-0.0013	0.0022	-0.0004	0.0007	0.0000
52.	H	0.0001	-0.0005	-0.0005	0.0011	-0.0008	0.0003	0.0003	-0.0002	0.0001
53.	H	0.0007	0.0009	-0.0011	0.0008	0.0033	0.0034	0.0072	0.0000	0.0020
54.	H	0.0009	0.0015	-0.0008	-0.0002	0.0019	0.0015	0.0062	0.0016	-0.0027
55.	H	-0.0050	-0.0048	0.0034	-0.0066	-0.0016	0.0001	0.0012	-0.0005	0.0061
56.	H	-0.0007	-0.0010	0.0005	-0.0014	0.0016	-0.0032	0.0065	0.0003	0.0074
57.	H	0.0048	0.0048	-0.0038	0.0056	0.0082	0.0037	-0.0111	0.0014	0.0103
58.	H	-0.0014	-0.0006	0.0006	-0.0012	-0.0002	0.0014	0.0093	0.0009	-0.0041
59.	H	-0.0020	0.0002	0.0031	0.0157	0.0342	0.0113	0.0206	-0.0129	-0.0279
60.	H	-0.0478	0.0000	-0.0035	-0.0021	-0.0279	0.0499	0.0263	0.0056	0.0151
61.	H	0.1153	0.0064	0.0384	-0.0448	0.0038	-0.0172	-0.0116	0.0054	0.0324
62.	H	0.0042	0.0174	-0.0007	0.0096	-0.0048	-0.0006	0.0007	0.0000	0.0012
63.	H	0.0022	0.0043	-0.0024	0.0063	0.0028	-0.0009	-0.0020	0.0005	0.0004
64.	H	-0.0067	-0.1021	-0.0021	-0.0257	-0.0057	-0.0147	0.0015	-0.0025	-0.0053
65.	H	-0.0029	-0.0031	0.0021	0.0078	-0.0027	0.0005	0.0020	-0.0001	0.0016
66.	H	0.0006	0.0015	-0.0012	-0.0026	0.0010	-0.0001	-0.0005	0.0000	-0.0005
67.	H	0.0007	0.0015	-0.0008	-0.0011	0.0006	0.0004	-0.0002	0.0000	-0.0003
68.	H	-0.0012	-0.0010	0.0006	0.0014	-0.0008	0.0004	0.0007	-0.0001	0.0003
69.	H	-0.0019	-0.0015	0.0016	0.0030	-0.0014	0.0002	0.0010	0.0000	0.0007
70.	H	0.0035	0.0047	-0.0043	-0.0086	0.0031	0.0005	-0.0017	0.0001	-0.0016

Atom	10	11	12	13	14	15	16	17	18
1. O	0.0277	0.0389	-0.0517	-0.0033	0.0058	0.0173	-0.0104	-0.0029	0.0043
2. O	0.0083	-0.0055	0.0101	0.0008	0.0030	0.0167	-0.0054	-0.0008	0.0036
3. C	-0.0026	-0.0054	0.0184	0.0261	-0.0033	-0.0064	0.0058	0.0026	-0.0019
4. C	-0.0370	0.0042	0.0101	-0.0056	0.0028	0.0177	0.0016	-0.0001	0.0018
5. C	0.0610	-0.0417	0.1392	-0.0391	0.0078	0.0024	0.0575	0.0078	0.0046
6. C	-0.1288	-0.1130	0.0015	0.0265	0.0451	0.0082	0.0545	0.0135	-0.0080
7. C	-0.1124	-0.0927	0.0142	0.0373	0.0390	-0.1184	0.1189	-0.0193	-0.0057
8. C	-0.0703	0.0210	-0.0181	-0.0035	0.0099	-0.0282	0.0565	0.0221	0.0016
9. C	-0.0972	-0.0732	-0.0885	0.0150	-0.0051	0.0099	0.8471	0.0205	0.0317
10. C	0.0000	-1.5029	0.1749	0.1651	0.0794	0.0617	-0.0004	-0.0024	0.0002
11. C	-1.5029	0.0000	-0.1647	0.0303	0.1808	0.0265	0.0532	0.0228	-0.0118
12. C	0.1749	-0.1647	0.0000	-0.0410	0.0260	-0.0247	0.0094	0.0182	-0.0049
13. C	0.1651	0.0303	-0.0410	0.0000	0.3391	0.2324	0.1175	-0.0046	0.0046
14. C	0.0794	0.1808	0.0260	0.3391	0.0000	-1.1415	0.1440	0.0271	-0.0625
15. C	0.0617	0.0265	-0.0247	0.2324	-1.1415	0.0000	-0.8420	0.5413	0.0464
16. C	-0.0004	0.0532	0.0094	0.1175	0.1440	-0.8420	0.0000	0.2074	-0.0023
17. C	-0.0024	0.0228	0.0182	-0.0046	0.0271	0.5413	0.2074	0.0000	-0.0141
18. C	0.0002	-0.0118	-0.0049	0.0046	-0.0625	0.0464	-0.0023	-0.0141	0.0000
19. C	0.0000	-0.0145	-0.0038	0.0169	-0.0888	0.0718	0.0344	0.4373	-0.0085
20. C	-0.0323	0.0084	0.0029	0.0025	-0.0004	-0.0124	0.0168	0.0038	-0.0021
21. C	-0.0110	0.0028	-0.0231	0.0152	-0.0086	-0.0264	0.0113	0.0058	-0.0035
22. C	0.0025	-0.0013	0.0027	-0.0038	0.0038	0.0094	-0.0059	0.0000	0.0008
23. C	-0.0003	0.0013	0.0018	-0.0057	-0.0010	0.0029	0.0034	0.0002	0.0014
24. C	-0.0011	0.0010	-0.0016	0.0024	-0.0015	-0.0060	0.0045	0.0023	-0.0010
25. C	-0.0001	-0.0002	-0.0005	-0.0016	-0.0002	0.0005	-0.0007	-0.0002	-0.0001
26. C	-0.0014	0.0003	-0.0026	0.0019	-0.0020	-0.0053	0.0036	0.0009	-0.0006
27. C	-0.0018	0.0043	-0.0023	-0.0029	0.0004	0.0021	0.0014	0.0012	0.0005
28. C	0.0019	0.0003	-0.0007	-0.0007	-0.0001	0.0009	-0.0003	0.0008	-0.0002
29. C	0.0032	-0.0019	0.0023	-0.0004	0.0001	0.0030	-0.0003	-0.0006	0.0005
30. C	-0.0008	-0.0006	-0.0002	0.0026	-0.0007	-0.0034	0.0021	0.0008	-0.0004
31. C	0.0000	0.0002	-0.0004	-0.0003	0.0004	0.0001	-0.0001	0.0002	-0.0001
32. C	0.0003	0.0007	0.0010	-0.0029	0.0011	0.0047	-0.0009	-0.0005	0.0009
33. C	0.0002	-0.0007	-0.0016	0.0014	-0.0012	-0.0025	-0.0003	0.0004	-0.0008
34. C	0.0003	0.0002	-0.0009	-0.0005	-0.0003	0.0000	-0.0002	-0.0001	-0.0001
35. C	0.0003	0.0004	0.0010	-0.0024	0.0012	0.0042	-0.0013	-0.0005	0.0008
36. C	-0.0003	-0.0003	-0.0017	0.0012	-0.0009	-0.0030	0.0011	0.0006	-0.0006
37. H	-0.0207	0.0177	-0.0104	-0.0111	-0.0019	-0.0131	-0.0188	0.0002	-0.0017
38. H	-0.0053	-0.0078	0.0015	-0.0003	-0.0122	0.0122	-0.0411	-0.0041	-0.0006
39. H	-0.0037	0.0008	-0.0031	-0.0025	-0.0049	0.0066	-0.0012	-0.0032	0.0024
40. H	-0.0038	0.0029	-0.0055	0.0002	-0.0032	-0.0038	-0.0217	-0.0027	-0.0046
41. H	0.1584	0.0685	0.0460	1.8668	0.0147	0.1517	0.0143	-0.0135	0.0057
42. H	0.0055	0.1053	0.0143	-0.0330	1.5529	0.0611	0.1977	-0.0274	-0.0058
43. H	-0.0299	0.0016	-0.0107	-0.0233	-0.0801	-0.0761	-0.6932	-0.0278	0.0007
44. H	0.0088	0.0012	-0.0044	0.0022	-0.0289	-0.0634	-0.0841	-0.9850	-0.0400
45. H	0.0004	-0.0013	0.0015	-0.0006	-0.0008	0.0005	0.0001	-0.0003	0.0000
46. H	0.0003	-0.0007	0.0012	-0.0006	-0.0002	0.0006	-0.0002	-0.0002	0.0001
47. H	-0.0003	0.0000	-0.0018	0.0014	-0.0013	-0.0037	0.0021	0.0006	-0.0006
48. H	0.0000	0.0003	0.0006	-0.0019	0.0009	0.0031	-0.0017	-0.0005	0.0004
49. H	0.0004	0.0001	-0.0006	-0.0007	-0.0001	0.0002	-0.0003	0.0002	-0.0001
50. H	0.0001	0.0001	-0.0005	-0.0004	0.0000	0.0001	0.0000	0.0001	0.0000
51. H	0.0002	0.0001	-0.0009	-0.0006	0.0000	0.0002	-0.0003	0.0001	-0.0001
52. H	0.0001	0.0000	-0.0005	-0.0002	-0.0002	-0.0001	-0.0001	-0.0001	-0.0001
53. H	-0.0003	-0.0022	-0.0005	-0.0004	-0.0108	-0.0158	0.0279	-0.0276	0.0012
54. H	0.0002	0.0023	-0.0016	-0.0024	0.0001	-0.0064	0.0120	0.0366	-0.0244
55. H	0.0005	0.0022	-0.0010	-0.0026	0.0003	0.0170	-0.0149	0.0100	0.0101
56. H	0.0006	-0.0020	0.0001	-0.0035	-0.0016	-0.0138	0.0180	-0.0331	1.9080
57. H	-0.0016	0.0045	-0.0032	-0.0013	0.0104	0.0049	0.0045	0.0324	0.2567
58. H	-0.0001	0.0008	-0.0010	0.0001	-0.0055	-0.0045	0.0111	0.0443	0.0128
59. H	0.1604	0.0627	1.9126	0.0207	-0.0008	0.0006	0.0039	0.0027	0.0039
60. H	-0.0546	-0.0043	0.0255	-0.0099	-0.0043	0.0145	0.0200	0.0020	0.0008
61. H	-0.0008	0.0144	0.3082	0.0009	0.0078	-0.0151	-0.0128	0.0030	-0.0085

62.	H	0.0009	0.0002	-0.0019	-0.0007	-0.0008	-0.0005	-0.0001	-0.0001	-0.0001
63.	H	0.0001	0.0001	-0.0004	-0.0003	0.0000	0.0003	-0.0005	-0.0001	0.0000
64.	H	-0.0004	0.0002	-0.0013	-0.0014	-0.0002	0.0006	-0.0011	-0.0010	-0.0001
65.	H	-0.0001	-0.0002	-0.0010	0.0004	-0.0005	-0.0013	0.0004	0.0002	-0.0003
66.	H	0.0001	0.0001	0.0000	-0.0004	0.0001	0.0004	-0.0001	0.0000	0.0001
67.	H	0.0001	0.0000	-0.0004	-0.0003	0.0000	0.0003	-0.0001	-0.0001	0.0000
68.	H	0.0001	-0.0001	-0.0006	0.0000	-0.0002	-0.0002	0.0000	0.0000	-0.0001
69.	H	0.0000	0.0000	-0.0004	0.0002	-0.0002	-0.0005	0.0001	0.0001	-0.0001
70.	H	0.0001	0.0001	-0.0001	-0.0010	0.0003	0.0014	-0.0005	-0.0002	0.0002

Atom		19	20	21	22	23	24	25	26	27
1.	O	0.0015	-0.1407	0.0356	0.0185	-0.1166	-0.0009	0.0102	-0.0169	0.0119
2.	O	0.0021	-0.3692	0.0470	0.0265	0.0294	0.0136	-0.0013	-0.0190	0.0405
3.	C	-0.0014	-0.2241	-0.0079	-0.1257	0.0329	-0.0045	0.0142	0.0482	-0.0058
4.	C	0.0011	-0.3236	0.1528	-0.1171	-0.0936	0.0537	-0.0021	0.0165	-0.0650
5.	C	0.0006	0.0841	-0.0367	0.0342	0.0099	-0.0070	-0.0019	-0.0072	0.0292
6.	C	0.0151	-0.0430	-0.0508	0.0099	-0.0095	-0.0012	-0.0004	-0.0072	-0.0148
7.	C	0.0108	-0.0091	0.0615	-0.0076	-0.0044	0.0046	0.0003	0.0087	0.0012
8.	C	0.0028	-0.0014	-0.0204	0.0026	-0.0042	0.0024	-0.0007	-0.0024	-0.0036
9.	C	0.0074	0.0294	0.0392	-0.0061	-0.0090	0.0081	-0.0020	0.0047	-0.0006
10.	C	0.0000	-0.0323	-0.0110	0.0025	-0.0003	-0.0011	-0.0001	-0.0014	-0.0018
11.	C	-0.0145	0.0084	0.0028	-0.0013	0.0013	0.0010	-0.0002	0.0003	0.0043
12.	C	-0.0038	0.0029	-0.0231	0.0027	0.0018	-0.0016	-0.0005	-0.0026	-0.0023
13.	C	0.0169	0.0025	0.0152	-0.0038	-0.0057	0.0024	-0.0016	0.0019	-0.0029
14.	C	-0.0888	-0.0004	-0.0086	0.0038	-0.0010	-0.0015	-0.0002	-0.0020	0.0004
15.	C	0.0718	-0.0124	-0.0264	0.0094	0.0029	-0.0060	0.0005	-0.0053	0.0021
16.	C	0.0344	0.0168	0.0113	-0.0059	0.0034	0.0045	-0.0007	0.0036	0.0014
17.	C	0.4373	0.0038	0.0058	0.0000	0.0002	0.0023	-0.0002	0.0009	0.0012
18.	C	-0.0085	-0.0021	-0.0035	0.0008	0.0014	-0.0010	-0.0001	-0.0006	0.0005
19.	C	0.0000	-0.0020	-0.0034	0.0017	-0.0008	-0.0006	-0.0001	-0.0008	-0.0001
20.	C	-0.0020	0.0000	-0.2259	0.0467	-0.0605	0.0130	-0.0056	0.0218	-0.0110
21.	C	-0.0034	-0.2259	0.0000	0.5668	0.0058	-0.0026	0.0068	0.0171	0.1838
22.	C	0.0017	0.0467	0.5668	0.0000	-1.2202	-0.0043	-0.0411	-0.1380	-0.1984
23.	C	-0.0008	-0.0605	0.0058	-1.2202	0.0000	0.7006	0.0301	0.1495	-0.1000
24.	C	-0.0006	0.0130	-0.0026	-0.0043	0.7006	0.0000	-0.8844	-1.1356	-0.1090
25.	C	-0.0001	-0.0056	0.0068	-0.0411	0.0301	-0.8844	0.0000	0.0624	-0.0951
26.	C	-0.0008	0.0218	0.0171	-0.1380	0.1495	-1.1356	0.0624	0.0000	-0.2355
27.	C	-0.0001	-0.0110	0.1838	-0.1984	-0.1000	-0.1090	-0.0951	-0.2355	0.0000
28.	C	0.0001	0.0294	0.0731	0.1563	-0.1223	-0.0760	0.0489	-0.0213	-1.4861
29.	C	0.0001	0.0108	-0.0082	0.0787	0.0069	0.0017	-0.0239	-0.0731	-0.0825
30.	C	-0.0003	0.0199	-0.0107	-0.0595	0.0405	0.0336	0.0027	0.0071	-0.0395
31.	C	0.0000	0.0014	0.0120	-0.0037	0.0498	0.0313	-0.0069	-0.0340	0.0686
32.	C	0.0003	-0.0100	0.0300	0.0092	0.0016	-0.1181	-0.0082	0.0768	0.0069
33.	C	-0.0002	0.0171	0.0243	-0.0067	0.0488	-0.1023	0.0362	0.7519	0.1826
34.	C	-0.0001	-0.0017	-0.0045	0.0000	0.0052	-0.0047	0.0085	0.0220	-0.0157
35.	C	0.0004	-0.0143	0.0165	0.0179	-0.0031	-0.0239	-0.0027	0.0063	0.0061
36.	C	-0.0003	0.0119	-0.0049	-0.0111	0.0063	0.0130	-0.0048	-0.0026	0.0068
37.	H	-0.0004	-0.0151	-0.0059	-0.0015	-0.0037	-0.0009	-0.0001	0.0005	-0.0017
38.	H	0.0001	-0.0069	0.0000	-0.0009	-0.0010	0.0001	-0.0001	0.0002	-0.0007
39.	H	-0.0029	-0.0015	-0.0165	0.0003	0.0014	-0.0012	0.0001	-0.0017	0.0011
40.	H	0.0003	0.0021	0.0155	0.0003	-0.0016	0.0003	0.0000	0.0018	0.0000
41.	H	0.0090	-0.0014	0.0007	-0.0003	-0.0022	0.0002	-0.0005	0.0000	-0.0012
42.	H	-0.0099	0.0029	0.0002	-0.0002	-0.0011	0.0001	-0.0002	0.0001	-0.0003
43.	H	0.0102	0.0005	0.0029	-0.0008	-0.0015	0.0003	-0.0003	0.0002	-0.0003
44.	H	-0.0238	0.0010	-0.0010	0.0003	0.0000	-0.0004	0.0001	-0.0001	-0.0003
45.	H	-0.0002	0.0137	-0.0372	0.0054	1.5544	-0.0110	0.0229	0.1422	0.0974
46.	H	0.0000	0.0030	-0.0037	0.0419	-0.0186	0.0525	1.6274	0.1637	-0.0022
47.	H	-0.0005	0.0096	-0.0241	-0.0218	0.0772	0.0601	0.2928	-0.0052	-0.0006
48.	H	0.0003	-0.0117	0.0342	0.0037	-0.0122	0.0279	0.7855	-0.0601	0.0132
49.	H	0.0000	-0.0066	-0.0039	0.0032	-0.0140	-0.0047	-0.0046	-0.0126	-0.0586
50.	H	0.0000	-0.0020	-0.0028	-0.0093	-0.0031	-0.0076	-0.0038	0.0023	0.0060
51.	H	0.0000	-0.0008	0.0056	0.0192	0.0072	0.0226	-0.0470	0.0421	0.1200
52.	H	-0.0001	-0.0007	-0.0027	-0.0002	-0.0016	0.0083	-0.0038	-0.0101	-0.0025
53.	H	1.8887	-0.0009	-0.0026	0.0009	-0.0002	-0.0007	0.0000	-0.0004	0.0000
54.	H	-0.2988	-0.0013	-0.0013	0.0005	0.0000	-0.0005	0.0000	-0.0003	0.0001
55.	H	0.2537	0.0068	0.0101	-0.0034	-0.0018	0.0019	-0.0003	0.0019	-0.0008
56.	H	-0.0122	0.0014	0.0021	-0.0008	0.0000	0.0002	0.0000	0.0004	-0.0002
57.	H	0.0089	-0.0042	-0.0098	0.0030	0.0005	-0.0021	0.0000	-0.0019	0.0007
58.	H	-0.0007	0.0011	0.0015	-0.0006	-0.0006	0.0002	-0.0001	0.0003	-0.0002
59.	H	0.0024	-0.0024	-0.0075	-0.0007	0.0051	0.0006	0.0002	-0.0002	-0.0020
60.	H	-0.0046	0.0143	0.0019	0.0056	0.0009	0.0000	-0.0006	-0.0009	-0.0006
61.	H	-0.0001	0.0132	0.0466	0.0044	0.0150	-0.0021	0.0022	0.0023	0.0072
62.	H	-0.0002	-0.0155	-0.0410	-0.0261	-0.0188	-0.0121	-0.0020	0.0062	-0.0061
63.	H	0.0000	0.0027	-0.0164	-0.0192	-0.0015	-0.0043	0.0059	0.0133	-0.0406
64.	H	-0.0001	-0.0176	0.0055	-0.0090	0.0202	0.0068	-0.0010	-0.0265	-0.0156
65.	H	-0.0002	0.0045	-0.0047	-0.0057	-0.0030	0.0029	0.0008	0.0054	0.0029
66.	H	0.0000	-0.0015	0.0008	0.0014	0.0028	-0.0010	-0.0007	-0.0033	-0.0037
67.	H	0.0000	-0.0008	0.0003	0.0004	-0.0002	-0.0035	-0.0012	-0.0008	0.0003
68.	H	0.0000	0.0013	0.0004	-0.0017	-0.0021	-0.0019	-0.0010	-0.0002	0.0002
69.	H	-0.0001	0.0022	-0.0015	-0.0020	-0.0054	-0.0010	-0.0006	0.0038	-0.0026
70.	H	0.0001	-0.0049	0.0048	0.0031	0.0032	-0.0045	0.0002	0.0021	0.0002

Atom		28	29	30	31	32	33	34	35	36
1.	O	-0.0073	0.0130	-0.0030	-0.0038	0.0083	-0.0099	0.0005	0.0109	-0.0094
2.	O	0.0111	0.0252	0.0093	-0.0056	0.0166	-0.0137	0.0006	0.0159	-0.0104
3.	C	0.0059	0.0007	0.0114	0.0028	-0.0030	0.0030	-0.0026	-0.0087	0.0077

4.	C	0.0094	0.0196	0.0218	0.0029	-0.0314	0.0088	-0.0012	-0.0239	0.0178
5.	C	0.0049	-0.0037	-0.0046	0.0001	0.0116	-0.0083	0.0003	0.0092	-0.0064
6.	C	0.0087	0.0122	-0.0006	0.0006	0.0006	0.0019	-0.0002	0.0021	0.0002
7.	C	0.0015	-0.0014	0.0065	-0.0006	-0.0055	0.0071	0.0002	-0.0054	0.0044
8.	C	0.0018	0.0038	-0.0002	0.0005	0.0002	-0.0008	-0.0003	0.0007	0.0000
9.	C	0.0033	0.0025	0.0051	-0.0005	-0.0047	0.0048	-0.0002	-0.0042	0.0034
10.	C	0.0019	0.0032	-0.0008	0.0000	0.0003	0.0002	0.0003	0.0003	-0.0003
11.	C	0.0003	-0.0019	-0.0006	0.0002	0.0007	-0.0007	0.0002	0.0004	-0.0003
12.	C	-0.0007	0.0023	-0.0002	-0.0004	0.0010	-0.0016	-0.0009	0.0010	-0.0017
13.	C	-0.0007	-0.0004	0.0026	-0.0003	-0.0029	0.0014	-0.0005	-0.0024	0.0012
14.	C	-0.0001	0.0001	-0.0007	0.0004	0.0011	-0.0012	-0.0003	0.0012	-0.0009
15.	C	0.0009	0.0030	-0.0034	0.0001	0.0047	-0.0025	0.0000	0.0042	-0.0030
16.	C	-0.0003	-0.0003	0.0021	-0.0001	-0.0009	-0.0003	-0.0002	-0.0013	0.0011
17.	C	0.0008	-0.0006	0.0008	0.0002	-0.0005	0.0004	-0.0001	-0.0005	0.0006
18.	C	-0.0002	0.0005	-0.0004	-0.0001	0.0009	-0.0008	-0.0001	0.0008	-0.0006
19.	C	0.0001	0.0001	-0.0003	0.0000	0.0003	-0.0002	-0.0001	0.0004	-0.0003
20.	C	0.0294	0.0108	0.0199	0.0014	-0.0100	0.0171	-0.0017	-0.0143	0.0119
21.	C	0.0731	-0.0082	-0.0107	0.0120	0.0300	0.0243	-0.0045	0.0165	-0.0049
22.	C	0.1563	0.0787	-0.0595	-0.0037	0.0092	-0.0067	0.0000	0.0179	-0.0111
23.	C	-0.1223	0.0069	0.0405	0.0498	0.0016	0.0488	0.0052	-0.0031	0.0063
24.	C	-0.0760	0.0017	0.0336	0.0313	-0.1181	-0.1023	-0.0047	-0.0239	0.0130
25.	C	0.0489	-0.0239	0.0027	-0.0069	-0.0082	0.0362	0.0085	-0.0027	-0.0048
26.	C	-0.0213	-0.0731	0.0071	-0.0340	0.0768	0.7519	0.0220	0.0063	-0.0026
27.	C	-1.4861	-0.0825	-0.0395	0.0686	0.0069	0.1826	-0.0157	0.0061	0.0068
28.	C	0.0000	-0.1219	0.1181	-0.0371	0.0619	0.0644	-0.0028	0.0089	0.0002
29.	C	-0.1219	0.0000	0.2481	0.0387	-0.0160	0.0204	0.0112	0.0038	-0.0022
30.	C	0.1181	0.2481	0.0000	0.4563	-0.0146	0.1041	0.0025	0.0011	0.0081
31.	C	-0.0371	0.0387	0.4563	0.0000	-1.0927	0.1263	0.2429	0.0380	-0.0069
32.	C	0.0619	-0.0160	-0.0146	-1.0927	0.0000	-0.9020	0.4762	0.0664	0.0680
33.	C	0.0644	0.0204	0.1041	0.1263	-0.9020	0.0000	-0.1051	0.0258	-0.0275
34.	C	-0.0028	0.0112	0.0025	0.2429	0.4762	-0.1051	0.0000	-0.0685	0.3818
35.	C	0.0089	0.0038	0.0011	0.0380	0.0664	0.0258	-0.0685	0.0000	0.0790
36.	C	0.0002	-0.0022	0.0081	-0.0069	0.0680	-0.0275	0.3818	0.0790	0.0000
37.	H	0.0008	-0.0003	0.0006	0.0000	0.0002	0.0000	-0.0002	0.0000	0.0002
38.	H	0.0002	-0.0009	0.0002	0.0001	-0.0001	0.0000	0.0000	-0.0001	0.0002
39.	H	0.0000	0.0008	-0.0013	0.0001	0.0017	-0.0021	0.0001	0.0016	-0.0011
40.	H	0.0002	-0.0007	0.0013	-0.0002	-0.0012	0.0019	0.0000	-0.0012	0.0009
41.	H	0.0001	0.0004	0.0005	-0.0001	-0.0006	0.0004	-0.0001	-0.0004	0.0001
42.	H	-0.0001	0.0000	0.0003	0.0000	-0.0002	0.0000	-0.0001	-0.0002	0.0000
43.	H	0.0004	0.0011	0.0008	-0.0001	-0.0003	0.0004	-0.0001	-0.0002	0.0003
44.	H	-0.0001	0.0003	0.0001	0.0001	0.0001	-0.0001	-0.0001	0.0002	0.0000
45.	H	-0.0280	0.0094	0.0288	0.0111	0.0317	0.0138	-0.0018	0.0036	0.0017
46.	H	0.0314	-0.0079	0.0045	0.0159	0.0039	0.0496	0.0002	0.0020	0.0016
47.	H	0.0061	0.0018	0.0037	-0.0031	0.0046	-0.0283	0.0046	-0.0081	0.0059
48.	H	-0.0053	0.0065	-0.0014	-0.0101	0.0192	-0.0260	0.0109	0.0076	-0.0059
49.	H	-0.0818	-0.0643	-0.9285	-0.0145	-0.0551	-0.0101	0.0059	0.0004	-0.0052
50.	H	-0.0165	-0.0190	0.0771	-0.6010	-0.0707	-0.0716	-0.0262	-0.0030	-0.0095
51.	H	0.0042	0.0249	0.0163	0.1872	0.0679	1.5834	0.0003	-0.0008	-0.0025
52.	H	-0.0036	0.0011	-0.0118	0.1272	0.0325	0.0195	1.8464	0.0634	0.0637
53.	H	0.0000	0.0002	-0.0003	0.0001	0.0003	-0.0002	0.0000	0.0003	-0.0002
54.	H	0.0001	0.0004	-0.0001	0.0000	0.0004	-0.0001	0.0000	0.0003	-0.0002
55.	H	0.0000	-0.0004	0.0014	-0.0001	-0.0016	0.0011	0.0000	-0.0015	0.0010
56.	H	-0.0001	-0.0001	0.0003	0.0000	-0.0003	0.0001	0.0000	-0.0003	0.0002
57.	H	0.0002	0.0009	-0.0011	0.0000	0.0016	-0.0011	0.0000	0.0014	-0.0011
58.	H	0.0001	0.0002	0.0003	0.0000	-0.0002	0.0002	0.0000	-0.0002	0.0002
59.	H	-0.0004	0.0006	-0.0002	0.0000	-0.0003	-0.0002	-0.0001	-0.0001	0.0000
60.	H	-0.0001	0.0007	0.0000	0.0002	0.0004	0.0000	-0.0002	0.0003	-0.0003
61.	H	-0.0003	0.0008	0.0017	0.0005	0.0010	0.0006	0.0000	0.0004	-0.0002
62.	H	-0.0258	0.8308	0.0586	0.0012	-0.0129	-0.0126	-0.0021	-0.0091	0.0075
63.	H	-0.0807	-0.9246	-0.0772	0.0200	0.0061	-0.0024	-0.0001	-0.0015	0.0021
64.	H	-0.0172	0.5164	0.0359	-0.0172	0.0112	0.0130	-0.0019	0.0137	-0.0084
65.	H	-0.0011	0.0009	0.0059	-0.0028	0.0492	-0.0110	-0.0183	0.6363	-0.0305
66.	H	0.0010	0.0026	0.0048	0.0027	-0.0230	-0.0102	0.0388	-0.9704	-0.0048
67.	H	0.0005	0.0006	-0.0033	-0.0076	-0.0198	-0.0048	-0.0375	0.8704	0.0613
68.	H	-0.0006	0.0004	-0.0007	-0.0121	-0.0224	-0.0015	-0.0202	0.0859	1.1905
69.	H	0.0018	0.0037	0.0032	0.0064	-0.0250	-0.0214	0.0512	-0.0109	-0.9505
70.	H	-0.0005	0.0007	0.0073	0.0113	0.0474	0.0071	-0.0200	-0.0409	0.6445

Atom	37	38	39	40	41	42	43	44	45
1.	O	-0.0043	0.0001	-0.0039	0.0030	-0.0047	-0.0020	-0.0027	-0.0004	0.0165
2.	O	-0.0303	0.0015	-0.0013	0.0004	0.0019	-0.0007	0.0015	0.0008	0.0045
3.	C	0.0000	0.0011	-0.0034	-0.0018	0.0094	0.0014	0.0035	-0.0001	0.0196
4.	C	0.0094	-0.0030	0.0297	-0.0167	0.0062	0.0036	0.0141	0.0004	0.0111
5.	C	-0.0131	-0.0240	-0.0041	-0.0010	-0.0139	0.0188	-0.0303	0.0064	0.0012
6.	C	-0.5078	-0.0246	-0.0235	0.0563	0.0246	0.0061	0.0127	0.0041	0.0080
7.	C	0.0676	-0.0686	-0.0609	-0.0900	0.0210	0.0306	-0.0967	-0.0075	0.0009
8.	C	-0.0342	-0.6381	0.6062	0.0268	0.0010	0.0090	0.0622	-0.0034	0.0004
9.	C	-0.0595	-0.0499	-0.0098	0.0244	0.0043	-0.0046	-0.0579	0.0287	0.0004
10.	C	-0.0207	-0.0053	-0.0037	-0.0038	0.1584	0.0055	-0.0299	0.0088	0.0004
11.	C	0.0177	-0.0078	0.0008	0.0029	0.0685	0.1053	0.0016	0.0012	-0.0013
12.	C	-0.0104	0.0015	-0.0031	-0.0055	0.0460	0.0143	-0.0107	-0.0044	0.0015
13.	C	-0.0111	-0.0003	-0.0025	0.0002	1.8668	-0.0330	-0.0233	0.0022	-0.0006
14.	C	-0.0019	-0.0122	-0.0049	-0.0032	0.0147	1.5529	-0.0801	-0.0289	-0.0008
15.	C	-0.0131	0.0122	0.0066	-0.0038	0.1517	0.0611	-0.0761	-0.0634	0.0005
16.	C	-0.0188	-0.0411	-0.0012	-0.0217	0.0143	0.1977	-0.6932	-0.0841	0.0001
17.	C	0.0002	-0.0041	-0.0032	-0.0027	-0.0135	-0.0274	-0.0278	-0.9850	-0.0003
18.	C	-0.0017	-0.0006	0.0024	-0.0046	0.0057	-0.0058	0.0007	-0.0400	0.0000

19.	C	-0.0004	0.0001	-0.0029	0.0003	0.0090	-0.0099	0.0102	-0.0238	-0.0002
20.	C	-0.0151	-0.0069	-0.0015	0.0021	-0.0014	0.0029	0.0005	0.0010	0.0137
21.	C	-0.0059	0.0000	-0.0165	0.0155	0.0007	0.0002	0.0029	-0.0010	-0.0372
22.	C	-0.0015	-0.0009	0.0003	0.0003	-0.0003	-0.0002	-0.0008	0.0003	0.0054
23.	C	-0.0037	-0.0010	0.0014	-0.0016	-0.0022	-0.0011	-0.0015	0.0000	1.5544
24.	C	-0.0009	0.0001	-0.0012	0.0003	0.0002	0.0001	0.0003	-0.0004	-0.0110
25.	C	-0.0001	-0.0001	0.0001	0.0000	-0.0005	-0.0002	-0.0003	0.0001	0.0229
26.	C	0.0005	0.0002	-0.0017	0.0018	0.0000	0.0001	0.0002	-0.0001	0.1422
27.	C	-0.0017	-0.0007	0.0011	0.0000	-0.0012	-0.0003	-0.0003	-0.0003	0.0974
28.	C	0.0008	0.0002	0.0000	0.0002	0.0001	-0.0001	0.0004	-0.0001	-0.0280
29.	C	-0.0003	-0.0009	0.0008	-0.0007	0.0004	0.0000	0.0011	0.0003	0.0094
30.	C	0.0006	0.0002	-0.0013	0.0013	0.0005	0.0003	0.0008	0.0001	0.0288
31.	C	0.0000	0.0001	0.0001	-0.0002	-0.0001	0.0000	-0.0001	0.0001	0.0111
32.	C	0.0002	-0.0001	0.0017	-0.0012	-0.0006	-0.0002	-0.0003	0.0001	0.0317
33.	C	0.0000	0.0000	-0.0021	0.0019	0.0004	0.0000	0.0004	-0.0001	0.0138
34.	C	-0.0002	0.0000	0.0001	0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0018
35.	C	0.0000	-0.0001	0.0016	-0.0012	-0.0004	-0.0002	-0.0002	0.0002	0.0036
36.	C	0.0002	0.0002	-0.0011	0.0009	0.0001	0.0000	0.0003	0.0000	0.0017
37.	H	0.0000	-0.0020	0.0064	0.0046	-0.0058	0.0020	-0.0072	-0.0027	0.0007
38.	H	-0.0020	0.0000	0.0313	0.0327	0.0008	-0.0045	0.0018	0.0011	0.0001
39.	H	0.0064	0.0313	0.0000	0.0204	0.0004	-0.0001	0.0073	-0.0016	0.0001
40.	H	0.0046	0.0327	0.0204	0.0000	-0.0009	0.0000	0.0098	-0.0036	-0.0002
41.	H	-0.0058	0.0008	0.0004	-0.0009	0.0000	-0.0499	0.0052	0.0105	0.0000
42.	H	0.0020	-0.0045	-0.0001	0.0000	-0.0499	0.0000	-0.0177	0.0164	-0.0002
43.	H	-0.0072	0.0018	0.0073	0.0098	0.0052	-0.0177	0.0000	0.0139	0.0001
44.	H	-0.0027	0.0011	-0.0016	-0.0036	0.0105	0.0164	0.0139	0.0000	0.0000
45.	H	0.0007	0.0001	0.0001	-0.0002	0.0000	-0.0002	0.0001	0.0000	0.0000
46.	H	0.0001	0.0000	0.0003	-0.0003	-0.0001	-0.0001	0.0000	0.0000	0.0116
47.	H	0.0001	0.0002	-0.0008	0.0005	0.0001	0.0001	0.0003	-0.0001	0.0001
48.	H	-0.0001	-0.0002	0.0006	-0.0003	-0.0004	-0.0002	-0.0005	0.0001	-0.0027
49.	H	-0.0001	-0.0001	0.0000	-0.0001	-0.0001	-0.0001	-0.0001	-0.0001	-0.0066
50.	H	-0.0001	0.0000	0.0001	-0.0001	-0.0001	-0.0001	0.0000	0.0000	0.0016
51.	H	-0.0002	-0.0001	0.0000	-0.0002	-0.0001	-0.0001	-0.0001	0.0000	-0.0047
52.	H	-0.0001	0.0000	-0.0001	0.0000	0.0000	-0.0001	-0.0001	0.0000	-0.0029
53.	H	0.0006	0.0000	-0.0007	-0.0003	0.0012	0.0134	-0.0004	0.0688	0.0000
54.	H	0.0004	0.0005	-0.0004	-0.0008	-0.0008	-0.0062	-0.0041	-0.0422	0.0001
55.	H	-0.0012	-0.0012	-0.0018	0.0030	-0.0035	-0.0093	-0.0087	-0.0414	-0.0002
56.	H	0.0006	-0.0001	0.0002	-0.0010	0.0010	0.0164	-0.0018	0.0715	0.0000
57.	H	-0.0018	-0.0010	0.0031	-0.0019	-0.0052	-0.0105	-0.0091	-0.0392	0.0000
58.	H	0.0005	0.0004	-0.0005	-0.0003	-0.0005	-0.0076	-0.0063	-0.0421	0.0000
59.	H	-0.0004	0.0019	0.0006	-0.0015	0.0293	-0.0064	-0.0032	-0.0008	0.0016
60.	H	-0.0003	-0.0001	-0.0062	0.0056	-0.0002	0.0042	0.0014	0.0004	-0.0004
61.	H	0.0006	0.0005	0.0055	-0.0047	-0.0019	0.0061	0.0037	-0.0004	0.0032
62.	H	-0.0011	0.0001	-0.0001	-0.0001	-0.0001	-0.0003	0.0000	0.0000	0.0021
63.	H	-0.0002	0.0003	0.0002	-0.0004	-0.0001	0.0000	0.0000	0.0000	0.0009
64.	H	0.0026	0.0009	0.0000	0.0004	-0.0004	0.0000	-0.0007	0.0001	0.0032
65.	H	0.0000	0.0001	-0.0005	0.0004	0.0001	0.0000	0.0002	0.0000	-0.0014
66.	H	0.0000	0.0000	0.0002	-0.0001	-0.0001	0.0000	-0.0001	0.0000	0.0004
67.	H	0.0001	0.0000	0.0001	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0004
68.	H	0.0001	0.0000	-0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0003
69.	H	0.0000	0.0000	-0.0002	0.0002	0.0000	0.0000	0.0000	0.0000	-0.0001
70.	H	0.0000	0.0000	0.0005	-0.0005	-0.0002	-0.0001	-0.0001	0.0001	-0.0006

Atom	46	47	48	49	50	51	52	53	54
1.	O	-0.0032	-0.0028	0.0045	-0.0023	0.0001	0.0002	0.0001	0.0007	0.0009
2.	O	0.0003	-0.0009	0.0025	0.0026	0.0015	0.0012	-0.0005	0.0009	0.0015
3.	C	0.0054	0.0105	-0.0029	-0.0014	-0.0013	-0.0033	-0.0005	-0.0011	-0.0008
4.	C	-0.0007	0.0296	-0.0281	0.0014	0.0000	0.0042	0.0011	0.0008	-0.0002
5.	C	0.0017	-0.0063	0.0043	-0.0011	0.0002	-0.0013	-0.0008	0.0033	0.0019
6.	C	0.0020	-0.0003	-0.0009	0.0021	0.0005	0.0022	0.0003	0.0034	0.0015
7.	C	-0.0006	0.0044	-0.0029	0.0000	0.0000	-0.0004	0.0003	0.0072	0.0062
8.	C	0.0001	0.0001	-0.0006	0.0006	0.0002	0.0007	-0.0002	0.0000	0.0016
9.	C	-0.0004	0.0043	-0.0044	0.0002	-0.0001	0.0000	0.0001	0.0020	-0.0027
10.	C	0.0003	-0.0003	0.0000	0.0004	0.0001	0.0002	0.0001	-0.0003	0.0002
11.	C	-0.0007	0.0000	0.0003	0.0001	0.0001	0.0001	0.0000	-0.0022	0.0023
12.	C	0.0012	-0.0018	0.0006	-0.0006	-0.0005	-0.0009	-0.0005	-0.0005	-0.0016
13.	C	-0.0006	0.0014	-0.0019	-0.0007	-0.0004	-0.0006	-0.0002	-0.0004	-0.0024
14.	C	-0.0002	-0.0013	0.0009	-0.0001	0.0000	0.0000	-0.0002	-0.0108	0.0001
15.	C	0.0006	-0.0037	0.0031	0.0002	0.0001	0.0002	-0.0001	-0.0158	-0.0064
16.	C	-0.0002	0.0021	-0.0017	-0.0003	0.0000	-0.0003	-0.0001	0.0279	0.0120
17.	C	-0.0002	0.0006	-0.0005	0.0002	0.0001	0.0001	-0.0001	-0.0276	0.0366
18.	C	0.0001	-0.0006	0.0004	-0.0001	0.0000	-0.0001	-0.0001	0.0012	-0.0244
19.	C	0.0000	-0.0005	0.0003	0.0000	0.0000	0.0000	-0.0001	1.8887	-0.2988
20.	C	0.0030	0.0096	-0.0117	-0.0066	-0.0020	-0.0008	-0.0007	-0.0009	-0.0013
21.	C	-0.0037	-0.0241	0.0342	-0.0039	-0.0028	0.0056	-0.0027	-0.0026	-0.0013
22.	C	0.0419	-0.0218	0.0037	0.0032	-0.0093	0.0192	-0.0002	0.0009	0.0005
23.	C	-0.0186	0.0772	-0.0122	-0.0140	-0.0031	0.0072	-0.0016	-0.0002	0.0000
24.	C	0.0525	0.0601	0.0279	-0.0047	-0.0076	0.0226	0.0083	-0.0007	-0.0005
25.	C	1.6274	0.2928	0.7855	-0.0046	-0.0038	-0.0470	-0.0038	0.0000	0.0000
26.	C	0.1637	-0.0052	-0.0601	-0.0126	0.0023	0.0421	-0.0101	-0.0004	-0.0003
27.	C	-0.0022	-0.0006	0.0132	-0.0586	0.0060	0.1200	-0.0025	0.0000	0.0001
28.	C	0.0314	0.0061	-0.0053	-0.0818	-0.0165	0.0042	-0.0036	0.0000	0.0001
29.	C	-0.0079	0.0018	0.0065	-0.0643	-0.0190	0.0249	0.0011	0.0002	0.0004
30.	C	0.0045	0.0037	-0.0014	-0.9285	0.0771	0.0163	-0.0118	-0.0003	-0.0001
31.	C	0.0159	-0.0031	-0.0101	-0.0145	-0.6010	0.1872	0.1272	0.0001	0.0000
32.	C	0.0039	0.0046	0.0192	-0.0551	-0.0707	0.0679	0.0325	0.0003	0.0004
33.	C	0.0496	-0.0283	-0.0260	-0.0101	-0.0716	1.5834	0.0195	-0.0002	-0.0001

34.	C	0.0002	0.0046	0.0109	0.0059	-0.0262	0.0003	1.8464	0.0000	0.0000
35.	C	0.0020	-0.0081	0.0076	0.0004	-0.0030	-0.0008	0.0634	0.0003	0.0003
36.	C	0.0016	0.0059	-0.0059	-0.0052	-0.0095	-0.0025	0.0637	-0.0002	-0.0002
37.	H	0.0001	0.0001	-0.0001	-0.0001	-0.0001	-0.0002	-0.0001	0.0006	0.0004
38.	H	0.0000	0.0002	-0.0002	-0.0001	0.0000	-0.0001	0.0000	0.0000	0.0005
39.	H	0.0003	-0.0008	0.0006	0.0000	0.0001	0.0000	-0.0001	-0.0007	-0.0004
40.	H	-0.0003	0.0005	-0.0003	-0.0001	-0.0001	-0.0002	0.0000	-0.0003	-0.0008
41.	H	-0.0001	0.0001	-0.0004	-0.0001	-0.0001	-0.0001	0.0000	0.0012	-0.0008
42.	H	-0.0001	0.0001	-0.0002	-0.0001	-0.0001	-0.0001	-0.0001	0.0134	-0.0062
43.	H	0.0000	0.0003	-0.0005	-0.0001	0.0000	-0.0001	-0.0001	-0.0004	-0.0041
44.	H	0.0000	-0.0001	0.0001	-0.0001	0.0000	0.0000	0.0000	0.0688	-0.0422
45.	H	0.0116	0.0001	-0.0027	-0.0066	0.0016	-0.0047	-0.0029	0.0000	0.0001
46.	H	0.0000	0.0218	0.0229	0.0003	-0.0033	-0.0090	-0.0004	0.0000	0.0001
47.	H	0.0218	0.0000	0.0095	-0.0004	0.0020	0.0020	-0.0009	-0.0003	-0.0002
48.	H	0.0229	0.0095	0.0000	-0.0012	0.0026	0.0093	0.0000	0.0002	0.0002
49.	H	0.0003	-0.0004	-0.0012	0.0000	-0.0741	0.0087	0.0097	0.0000	0.0000
50.	H	-0.0033	0.0020	0.0026	-0.0741	0.0000	-0.0138	0.0072	0.0000	0.0000
51.	H	-0.0090	0.0020	0.0093	0.0087	-0.0138	0.0000	0.0251	0.0000	-0.0001
52.	H	-0.0004	-0.0009	0.0000	0.0097	0.0072	0.0251	0.0000	0.0000	0.0000
53.	H	0.0000	-0.0003	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0156
54.	H	0.0001	-0.0002	0.0002	0.0000	0.0000	-0.0001	0.0000	0.0156	0.0000
55.	H	-0.0002	0.0013	-0.0011	-0.0001	0.0000	-0.0002	0.0000	0.0255	0.0209
56.	H	0.0000	0.0002	-0.0002	-0.0001	0.0000	-0.0001	0.0000	0.0054	0.0026
57.	H	0.0002	-0.0013	0.0010	0.0000	0.0000	-0.0001	-0.0001	-0.0051	0.0144
58.	H	0.0000	0.0002	-0.0002	0.0000	0.0000	-0.0001	0.0000	0.0012	-0.0229
59.	H	0.0007	0.0001	-0.0005	0.0000	0.0000	0.0001	-0.0001	0.0006	-0.0002
60.	H	0.0003	-0.0006	0.0003	-0.0002	-0.0002	-0.0004	-0.0001	-0.0011	0.0003
61.	H	0.0014	-0.0009	0.0009	-0.0005	0.0001	-0.0008	-0.0001	0.0006	-0.0001
62.	H	0.0003	-0.0025	0.0025	0.0126	0.0034	0.0007	0.0013	-0.0001	-0.0001
63.	H	0.0024	0.0008	-0.0010	0.0041	-0.0039	-0.0032	-0.0021	0.0000	0.0000
64.	H	0.0002	0.0044	-0.0032	0.0059	0.0064	0.0036	0.0000	0.0002	0.0002
65.	H	-0.0009	0.0010	-0.0009	-0.0030	-0.0034	-0.0087	-0.0256	-0.0001	-0.0001
66.	H	0.0003	-0.0005	-0.0002	0.0002	0.0051	0.0034	0.0640	0.0000	0.0000
67.	H	0.0011	0.0009	-0.0003	-0.0001	-0.0041	-0.0021	-0.0270	0.0000	0.0000
68.	H	0.0008	-0.0001	0.0008	-0.0003	-0.0039	-0.0007	-0.0246	0.0000	0.0000
69.	H	0.0004	-0.0001	-0.0008	0.0017	0.0026	0.0024	0.0616	0.0000	0.0000
70.	H	-0.0012	-0.0009	0.0010	-0.0024	-0.0041	-0.0085	-0.0282	0.0001	0.0001

Atom	55	56	57	58	59	60	61	62	63
1.	O	-0.0050	-0.0007	0.0048	-0.0014	-0.0020	-0.0478	0.1153	0.0042	0.0022
2.	O	-0.0048	-0.0010	0.0048	-0.0006	0.0002	0.0000	0.0064	0.0174	0.0043
3.	C	0.0034	0.0005	-0.0038	0.0006	0.0031	-0.0035	0.0384	-0.0007	-0.0024
4.	C	-0.0066	-0.0014	0.0056	-0.0012	0.0157	-0.0021	-0.0448	0.0096	0.0063
5.	C	-0.0016	0.0016	0.0082	-0.0002	0.0342	-0.0279	0.0038	-0.0048	0.0028
6.	C	0.0001	-0.0032	0.0037	0.0014	0.0113	0.0499	-0.0172	-0.0006	-0.0009
7.	C	0.0012	0.0065	-0.0111	0.0093	0.0206	0.0263	-0.0116	0.0007	-0.0020
8.	C	-0.0005	0.0003	0.0014	0.0009	-0.0129	0.0056	0.0054	0.0000	0.0005
9.	C	0.0061	0.0074	0.0103	-0.0041	-0.0279	0.0151	0.0324	0.0012	0.0004
10.	C	0.0005	0.0006	-0.0016	-0.0001	0.1604	-0.0546	-0.0008	0.0009	0.0001
11.	C	0.0022	-0.0020	0.0045	0.0008	0.0627	-0.0043	0.0144	0.0002	0.0001
12.	C	-0.0010	0.0001	-0.0032	-0.0010	1.9126	0.0255	0.3082	-0.0019	-0.0004
13.	C	-0.0026	-0.0035	-0.0013	0.0001	0.0207	-0.0099	0.0009	-0.0007	-0.0003
14.	C	0.0003	-0.0016	0.0104	-0.0055	-0.0008	-0.0043	0.0078	-0.0008	0.0000
15.	C	0.0170	-0.0138	0.0049	-0.0045	0.0006	0.0145	-0.0151	-0.0005	0.0003
16.	C	-0.0149	0.0180	0.0045	0.0111	0.0039	0.0200	-0.0128	-0.0001	-0.0005
17.	C	0.0100	-0.0331	0.0324	0.0443	0.0027	0.0020	0.0030	-0.0001	-0.0001
18.	C	0.0101	1.9080	0.2567	0.0128	0.0039	0.0008	-0.0085	-0.0001	0.0000
19.	C	0.2537	-0.0122	0.0089	-0.0007	0.0024	-0.0046	-0.0001	-0.0002	0.0000
20.	C	0.0068	0.0014	-0.0042	0.0011	-0.0024	0.0143	0.0132	-0.0155	0.0027
21.	C	0.0101	0.0021	-0.0098	0.0015	-0.0075	0.0019	0.0466	-0.0410	-0.0164
22.	C	-0.0034	-0.0008	0.0030	-0.0006	-0.0007	0.0056	0.0044	-0.0261	-0.0192
23.	C	-0.0018	0.0000	0.0005	-0.0006	0.0051	0.0009	0.0150	-0.0188	-0.0015
24.	C	0.0019	0.0002	-0.0021	0.0002	0.0006	0.0000	-0.0021	-0.0121	-0.0043
25.	C	-0.0003	0.0000	0.0000	-0.0001	0.0002	-0.0006	0.0022	-0.0020	0.0059
26.	C	0.0019	0.0004	-0.0019	0.0003	-0.0002	-0.0009	0.0023	0.0062	0.0133
27.	C	-0.0008	-0.0002	0.0007	-0.0002	-0.0020	-0.0006	0.0072	-0.0061	-0.0406
28.	C	0.0000	-0.0001	0.0002	0.0001	-0.0004	-0.0001	-0.0003	-0.0258	-0.0807
29.	C	-0.0004	-0.0001	0.0009	0.0002	0.0006	0.0007	0.0008	0.8308	-0.9246
30.	C	0.0014	0.0003	-0.0011	0.0003	-0.0002	0.0000	0.0017	0.0586	-0.0772
31.	C	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0002	0.0005	0.0012	0.0200
32.	C	-0.0016	-0.0003	0.0016	-0.0002	-0.0003	0.0004	0.0010	-0.0129	0.0061
33.	C	0.0011	0.0001	-0.0011	0.0002	-0.0002	0.0000	0.0006	-0.0126	-0.0024
34.	C	0.0000	0.0000	0.0000	0.0000	-0.0001	-0.0002	0.0000	-0.0021	-0.0001
35.	C	-0.0015	-0.0003	0.0014	-0.0002	-0.0001	0.0003	0.0004	-0.0091	-0.0015
36.	C	0.0010	0.0002	-0.0011	0.0002	0.0000	-0.0003	-0.0002	0.0075	0.0021
37.	H	-0.0012	0.0006	-0.0018	0.0005	-0.0004	-0.0003	0.0006	-0.0011	-0.0002
38.	H	-0.0012	-0.0001	-0.0010	0.0004	0.0019	-0.0001	0.0005	0.0001	0.0003
39.	H	-0.0018	0.0002	0.0031	-0.0005	0.0006	-0.0062	0.0055	-0.0001	0.0002
40.	H	0.0030	-0.0010	-0.0019	-0.0003	-0.0015	0.0056	-0.0047	-0.0001	-0.0004
41.	H	-0.0035	0.0010	-0.0052	-0.0005	0.0293	-0.0002	-0.0019	-0.0001	-0.0001
42.	H	-0.0093	0.0164	-0.0105	-0.0076	-0.0064	0.0042	0.0061	-0.0003	0.0000
43.	H	-0.0087	-0.0018	-0.0091	-0.0063	-0.0032	0.0014	0.0037	0.0000	0.0000
44.	H	-0.0414	0.0715	-0.0392	-0.0421	-0.0008	0.0004	-0.0004	0.0000	0.0000
45.	H	-0.0002	0.0000	0.0000	0.0000	0.0016	-0.0004	0.0032	0.0021	0.0009
46.	H	-0.0002	0.0000	0.0002	0.0000	0.0007	0.0003	0.0014	0.0003	0.0024
47.	H	0.0013	0.0002	-0.0013	0.0002	0.0001	-0.0006	-0.0009	-0.0025	0.0008
48.	H	-0.0011	-0.0002	0.0010	-0.0002	-0.0005	0.0003	0.0009	0.0025	-0.0010

49.	H	-0.0001	-0.0001	0.0000	0.0000	0.0000	-0.0002	-0.0005	0.0126	0.0041
50.	H	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0001	0.0034	-0.0039
51.	H	-0.0002	-0.0001	-0.0001	-0.0001	0.0001	-0.0004	-0.0008	0.0007	-0.0032
52.	H	0.0000	0.0000	-0.0001	0.0000	-0.0001	-0.0001	-0.0001	0.0013	-0.0021
53.	H	0.0255	0.0054	-0.0051	0.0012	0.0006	-0.0011	0.0006	-0.0001	0.0000
54.	H	0.0209	0.0026	0.0144	-0.0229	-0.0002	0.0003	-0.0001	-0.0001	0.0000
55.	H	0.0000	-0.0056	-0.0008	0.0139	-0.0013	-0.0027	0.0040	0.0001	-0.0002
56.	H	-0.0056	0.0000	0.0245	0.0110	0.0010	0.0002	-0.0012	0.0001	-0.0001
57.	H	-0.0008	0.0245	0.0000	0.0225	-0.0003	0.0023	-0.0035	-0.0004	0.0001
58.	H	0.0139	0.0110	0.0225	0.0000	-0.0003	-0.0010	0.0015	0.0000	0.0000
59.	H	-0.0013	0.0010	-0.0003	-0.0003	0.0000	0.0183	0.0249	0.0002	0.0002
60.	H	-0.0027	0.0002	0.0023	-0.0010	0.0183	0.0000	0.0328	-0.0010	-0.0005
61.	H	0.0040	-0.0012	-0.0035	0.0015	0.0249	0.0328	0.0000	-0.0002	-0.0012
62.	H	0.0001	0.0001	-0.0004	0.0000	0.0002	-0.0010	-0.0002	0.0000	0.0296
63.	H	-0.0002	-0.0001	0.0001	0.0000	0.0002	-0.0005	-0.0012	0.0296	0.0000
64.	H	-0.0002	0.0000	0.0002	0.0001	-0.0009	0.0009	0.0025	0.0302	0.0523
65.	H	0.0004	0.0001	-0.0005	0.0001	0.0000	-0.0002	-0.0001	0.0017	0.0002
66.	H	-0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0007	-0.0001
67.	H	-0.0001	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	-0.0003	0.0000
68.	H	0.0001	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0001	0.0004	-0.0002
69.	H	0.0002	0.0000	-0.0002	0.0000	0.0000	-0.0001	-0.0001	-0.0007	-0.0004
70.	H	-0.0005	-0.0001	0.0004	-0.0001	-0.0001	0.0001	0.0002	-0.0016	-0.0007

Atom		64	65	66	67	68	69	70
1.	O	-0.0067	-0.0029	0.0006	0.0007	-0.0012	-0.0019	0.0035
2.	O	-0.1021	-0.0031	0.0015	0.0015	-0.0010	-0.0015	0.0047
3.	C	-0.0021	0.0021	-0.0012	-0.0008	0.0006	0.0016	-0.0043
4.	C	-0.0257	0.0078	-0.0026	-0.0011	0.0014	0.0030	-0.0086
5.	C	-0.0057	-0.0027	0.0010	0.0006	-0.0008	-0.0014	0.0031
6.	C	-0.0147	0.0005	-0.0001	0.0004	0.0004	0.0002	0.0005
7.	C	0.0015	0.0020	-0.0005	-0.0002	0.0007	0.0010	-0.0017
8.	C	-0.0025	-0.0001	0.0000	0.0000	-0.0001	0.0000	0.0001
9.	C	-0.0053	0.0016	-0.0005	-0.0003	0.0003	0.0007	-0.0016
10.	C	-0.0004	-0.0001	0.0001	0.0001	0.0001	0.0000	0.0001
11.	C	0.0002	-0.0002	0.0001	0.0000	-0.0001	0.0000	0.0001
12.	C	-0.0013	-0.0010	0.0000	-0.0004	-0.0006	-0.0004	-0.0001
13.	C	-0.0014	0.0004	-0.0004	-0.0003	0.0000	0.0002	-0.0010
14.	C	-0.0002	-0.0005	0.0001	0.0000	-0.0002	-0.0002	0.0003
15.	C	0.0006	-0.0013	0.0004	0.0003	-0.0002	-0.0005	0.0014
16.	C	-0.0011	0.0004	-0.0001	-0.0001	0.0000	0.0001	-0.0005
17.	C	-0.0010	0.0002	0.0000	-0.0001	0.0000	0.0001	-0.0002
18.	C	-0.0001	-0.0003	0.0001	0.0000	-0.0001	-0.0001	0.0002
19.	C	-0.0001	-0.0002	0.0000	0.0000	0.0000	-0.0001	0.0001
20.	C	-0.0176	0.0045	-0.0015	-0.0008	0.0013	0.0022	-0.0049
21.	C	0.0055	-0.0047	0.0008	0.0003	0.0004	-0.0015	0.0048
22.	C	-0.0090	-0.0057	0.0014	0.0004	-0.0017	-0.0020	0.0031
23.	C	0.0202	-0.0030	0.0028	-0.0002	-0.0021	-0.0054	0.0032
24.	C	0.0068	0.0029	-0.0010	-0.0035	-0.0019	-0.0010	-0.0045
25.	C	-0.0010	0.0008	-0.0007	-0.0012	-0.0010	-0.0006	0.0002
26.	C	-0.0265	0.0054	-0.0033	-0.0008	-0.0002	0.0038	0.0021
27.	C	-0.0156	0.0029	-0.0037	0.0003	0.0002	-0.0026	0.0002
28.	C	-0.0172	-0.0011	0.0010	0.0005	-0.0006	0.0018	-0.0005
29.	C	0.5164	0.0009	0.0026	0.0006	0.0004	0.0037	0.0007
30.	C	0.0359	0.0059	0.0048	-0.0033	-0.0007	0.0032	0.0073
31.	C	-0.0172	-0.0028	0.0027	-0.0076	-0.0121	0.0064	0.0113
32.	C	0.0112	0.0492	-0.0230	-0.0198	-0.0224	-0.0250	0.0474
33.	C	0.0130	-0.0110	-0.0102	-0.0048	-0.0015	-0.0214	0.0071
34.	C	-0.0019	-0.0183	0.0388	-0.0375	-0.0202	0.0512	-0.0200
35.	C	0.0137	0.6363	-0.9704	0.8704	0.0859	-0.0109	-0.0409
36.	C	-0.0084	-0.0305	-0.0048	0.0613	1.1905	-0.9505	0.6445
37.	H	0.0026	0.0000	0.0000	0.0001	0.0001	0.0000	0.0000
38.	H	0.0009	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
39.	H	0.0000	-0.0005	0.0002	0.0001	-0.0001	-0.0002	0.0005
40.	H	0.0004	0.0004	-0.0001	-0.0001	0.0001	0.0002	-0.0005
41.	H	-0.0004	0.0001	-0.0001	0.0000	0.0000	0.0000	-0.0002
42.	H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001
43.	H	-0.0007	0.0002	-0.0001	0.0000	0.0000	0.0000	-0.0001
44.	H	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
45.	H	0.0032	-0.0014	0.0004	0.0004	0.0003	-0.0001	-0.0006
46.	H	0.0002	-0.0009	0.0003	0.0011	0.0008	0.0004	-0.0012
47.	H	0.0044	0.0010	-0.0005	0.0009	-0.0001	-0.0001	-0.0009
48.	H	-0.0032	-0.0009	-0.0002	-0.0003	0.0008	-0.0008	0.0010
49.	H	0.0059	-0.0030	0.0002	-0.0001	-0.0003	0.0017	-0.0024
50.	H	0.0064	-0.0034	0.0051	-0.0041	-0.0039	0.0026	-0.0041
51.	H	0.0036	-0.0087	0.0034	-0.0021	-0.0007	0.0024	-0.0085
52.	H	0.0000	-0.0256	0.0640	-0.0270	-0.0246	0.0616	-0.0282
53.	H	0.0002	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
54.	H	0.0002	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0001
55.	H	-0.0002	0.0004	-0.0001	-0.0001	0.0001	0.0002	-0.0005
56.	H	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001
57.	H	0.0002	-0.0005	0.0001	0.0001	-0.0001	-0.0002	0.0004
58.	H	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0001
59.	H	-0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001
60.	H	0.0009	-0.0002	0.0000	0.0000	0.0000	-0.0001	0.0001
61.	H	0.0025	-0.0001	0.0000	0.0001	0.0001	-0.0001	0.0002
62.	H	0.0302	0.0017	0.0007	-0.0003	0.0004	-0.0007	-0.0016
63.	H	0.0523	0.0002	-0.0001	0.0000	-0.0002	-0.0004	-0.0007

64.	H	0.0000	-0.0016	-0.0007	0.0010	0.0003	0.0002	0.0028
65.	H	-0.0016	0.0000	0.0268	0.0217	0.0062	-0.0090	-0.0065
66.	H	-0.0007	0.0268	0.0000	0.0235	0.0141	-0.0101	-0.0094
67.	H	0.0010	0.0217	0.0235	0.0000	-0.0145	0.0146	0.0079
68.	H	0.0003	0.0062	0.0141	-0.0145	0.0000	0.0266	0.0173
69.	H	0.0002	-0.0090	-0.0101	0.0146	0.0266	0.0000	0.0279
70.	H	0.0028	-0.0065	-0.0094	0.0079	0.0173	0.0279	0.0000

MO atomic valencies:

Atom		1
1.	O	0.2785
2.	O	-0.0444
3.	C	-0.2082
4.	C	0.8791
5.	C	-0.5744
6.	C	-1.0285
7.	C	-1.9227
8.	C	-0.7776
9.	C	-0.5081
10.	C	-1.2004
11.	C	-1.3653
12.	C	2.2608
13.	C	2.7145
14.	C	1.0274
15.	C	-1.0820
16.	C	0.3008
17.	C	0.2971
18.	C	2.0901
19.	C	2.2972
20.	C	-1.1851
21.	C	0.8096
22.	C	-0.9729
23.	C	0.9707
24.	C	-1.4747
25.	C	1.8060
26.	C	-0.2415
27.	C	-1.8134
28.	C	-1.4799
29.	C	0.5584
30.	C	0.1904
31.	C	-0.4045
32.	C	-1.3218
33.	C	1.7331
34.	C	2.7720
35.	C	0.7972
36.	C	1.4799
37.	H	-0.6634
38.	H	-0.8095
39.	H	0.5632
40.	H	0.0393
41.	H	2.3450
42.	H	1.8692
43.	H	-1.0349
44.	H	-1.1794
45.	H	1.9264
46.	H	2.0199
47.	H	0.4455
48.	H	0.7871
49.	H	-1.3006
50.	H	-0.8404
51.	H	2.0542
52.	H	2.1797
53.	H	1.9988
54.	H	-0.2974
55.	H	0.2708
56.	H	1.9980
57.	H	0.3151
58.	H	0.0336
59.	H	2.2675
60.	H	0.0741
61.	H	0.5913
62.	H	0.8215
63.	H	-1.0313
64.	H	0.4507
65.	H	0.6305
66.	H	-0.8479
67.	H	0.8773
68.	H	1.2362
69.	H	-0.8314
70.	H	0.6500

NATURAL BOND ORBITAL ANALYSIS:

Occupancies	Lewis Structure	Low	High

Cycle	Occ. Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	occ (L)	occ (NL)	Dev
1(1)	1.90	240.44372	13.55628	36	77	0	14	15	14	0.49
2(2)	1.90	240.44372	13.55628	36	77	0	14	15	14	0.49
3(1)	1.80	240.88103	13.11897	36	76	0	15	11	13	0.49
4(2)	1.80	240.88103	13.11897	36	76	0	15	11	13	0.49
5(1)	1.70	240.88103	13.11897	36	76	0	15	11	13	0.49
6(2)	1.70	240.88103	13.11897	36	76	0	15	11	13	0.49
7(1)	1.60	244.77109	9.22891	36	82	0	9	5	13	0.38
8(2)	1.60	244.77109	9.22891	36	82	0	9	5	13	0.38
9(1)	1.50	246.00549	7.99451	36	84	0	7	1	13	0.59
10(2)	1.50	246.00549	7.99451	36	84	0	7	1	13	0.59

Strongly delocalized structure accepted

1 low occupancy (<1.9990e) core orbital found on C10
1 low occupancy (<1.9990e) core orbital found on C27

Core	71.97219	(99.961% of 72)
Valence Lewis	174.03329	(95.623% of 182)
Total Lewis	246.00549	(96.853% of 254)
Valence non-Lewis	7.56415	(2.978% of 254)
Rydberg non-Lewis	0.43036	(0.169% of 254)
Total non-Lewis	7.99451	(3.147% of 254)

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99584) BD (1) O 1- C 3
(64.15%) 0.8009* O 1 s(38.75%)p 1.57(60.68%)d 0.01(0.54%)
f 0.00(0.03%)
0.0000 -0.6223 -0.0152 -0.0013 0.0004
0.6562 -0.0283 -0.0027 0.0973 -0.0047
-0.0002 0.4069 -0.0177 -0.0014 -0.0129
-0.0567 -0.0094 -0.0436 0.0077 -0.0078
0.0034 0.0008 0.0117 0.0042 0.0068
0.0033
(35.85%) 0.5988* C 3 s(35.70%)p 1.80(64.24%)d 0.00(0.04%)
f 0.00(0.02%)
0.0000 -0.5939 -0.0653 0.0055 -0.0002
-0.6628 0.0310 -0.0126 -0.1184 0.0013
-0.0022 -0.4329 0.0205 -0.0080 -0.0023
-0.0174 -0.0050 -0.0089 0.0047 0.0051
-0.0027 -0.0005 -0.0088 -0.0030 -0.0053
-0.0030

2. (1.99585) BD (1) O 2- C 20
(64.15%) 0.8009* O 2 s(38.75%)p 1.57(60.68%)d 0.01(0.54%)
f 0.00(0.03%)
0.0000 0.6223 0.0152 0.0013 -0.0004
0.6563 -0.0283 -0.0027 0.0972 -0.0047
-0.0002 0.4067 -0.0177 -0.0014 0.0129
0.0567 0.0094 0.0436 -0.0077 -0.0078
0.0033 0.0008 0.0117 0.0042 0.0068
0.0033
(35.85%) 0.5988* C 20 s(35.70%)p 1.80(64.24%)d 0.00(0.04%)
f 0.00(0.02%)
0.0000 0.5939 0.0654 -0.0055 0.0002
-0.6627 0.0310 -0.0126 -0.1190 0.0014
-0.0022 -0.4329 0.0205 -0.0080 0.0023
0.0174 0.0050 0.0089 -0.0048 0.0051
-0.0027 -0.0005 -0.0088 -0.0030 -0.0053
-0.0030

3. (1.96951) BD (1) C 3- C 4
(47.76%) 0.6911* C 3 s(32.29%)p 2.09(67.64%)d 0.00(0.06%)
f 0.00(0.01%)
-0.0001 0.5678 -0.0241 0.0009 -0.0001
-0.7004 -0.0117 0.0019 -0.2358 -0.0022
0.0011 0.3606 -0.0034 0.0039 0.0108
-0.0112 -0.0021 0.0158 -0.0119 -0.0011
0.0024 0.0010 0.0008 0.0012 -0.0047
-0.0051
(52.24%) 0.7228* C 4 s(31.53%)p 2.17(68.41%)d 0.00(0.06%)
f 0.00(0.01%)
-0.0004 0.5615 -0.0036 -0.0009 -0.0001
0.7792 0.0053 -0.0011 0.2692 0.0078
-0.0018 0.0644 -0.0093 0.0069 0.0109
-0.0048 -0.0015 0.0176 -0.0103 0.0014
-0.0028 -0.0004 -0.0025 -0.0026 0.0039
0.0065

4. (1.95784) BD (1) C 3- C 21
(48.38%) 0.6956* C 3 s(32.34%)p 2.09(67.59%)d 0.00(0.07%)

```
                                        f 0.00(  0.01%)
                                   -0.0001  0.5681 -0.0248  0.0013 -0.0001
                                   -0.0018 -0.0072  0.0046  0.1349  0.0001
                                    0.0017 -0.8109 -0.0105  0.0005 -0.0018
                                    0.0089 -0.0048 -0.0017  0.0239 -0.0051
                                   -0.0042  0.0017 -0.0029 -0.0004 -0.0014
                                   -0.0006
            ( 51.62%)   0.7185* C 21 s( 28.03%)p 2.57( 71.90%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                   -0.0005  0.5294 -0.0038 -0.0010 -0.0002
                                    0.3157 -0.0050  0.0043  0.0010  0.0028
                                    0.0010  0.7869  0.0057 -0.0027  0.0017
                                    0.0106 -0.0030  0.0038  0.0240  0.0066
                                    0.0010 -0.0031  0.0021  0.0010 -0.0002
                                    0.0004
5. (1.98477) BD ( 1) C  4- C  5
            ( 49.43%)   0.7030* C  4 s( 40.39%)p 1.47( 59.55%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                    0.0000  0.6352  0.0208  0.0014  0.0002
                                   -0.4305  0.0021  0.0006 -0.2228  0.0026
                                    0.0005  0.6004 -0.0072  0.0013  0.0072
                                   -0.0178 -0.0101  0.0017  0.0058 -0.0006
                                   -0.0073 -0.0042  0.0037  0.0066 -0.0003
                                   -0.0031
            ( 50.57%)   0.7111* C  5 s( 36.07%)p 1.77( 63.86%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                   -0.0001  0.6005  0.0089  0.0000  0.0000
                                    0.4927 -0.0026  0.0007  0.3619 -0.0009
                                    0.0005 -0.5147 -0.0019  0.0014  0.0088
                                   -0.0173 -0.0099  0.0045  0.0050  0.0017
                                    0.0051  0.0034 -0.0029 -0.0071 -0.0009
                                    0.0038
6. (1.56777) BD ( 2) C  4- C  5
            ( 45.52%)   0.6747* C  4 s(  0.01%)p99.99( 99.96%)d 0.68(  0.01%)
                                        f 1.85(  0.02%)
                                   -0.0002 -0.0089 -0.0048 -0.0003  0.0000
                                   -0.3273  0.0072 -0.0010  0.9366 -0.0123
                                    0.0051  0.1225  0.0043  0.0004 -0.0043
                                   -0.0018  0.0011  0.0069 -0.0001  0.0025
                                   -0.0033  0.0061  0.0068 -0.0030 -0.0083
                                    0.0034
            ( 54.48%)   0.7381* C  5 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.01%)
                                        f 0.00(  0.02%)
                                    0.0002 -0.0054 -0.0039  0.0003  0.0001
                                   -0.4884  0.0079 -0.0033  0.8623 -0.0058
                                    0.0038  0.1325 -0.0022 -0.0007  0.0031
                                    0.0024 -0.0069 -0.0018 -0.0021  0.0020
                                   -0.0047  0.0063  0.0033  0.0008 -0.0086
                                   -0.0004
7. (1.95783) BD ( 1) C  4- C 20
            ( 51.62%)   0.7185* C  4 s( 28.03%)p 2.57( 71.90%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                   -0.0005  0.5294 -0.0038 -0.0010 -0.0002
                                   -0.3155  0.0050 -0.0043 -0.0023 -0.0028
                                   -0.0010 -0.7870 -0.0057  0.0027  0.0017
                                    0.0106 -0.0029  0.0038  0.0240 -0.0066
                                   -0.0009  0.0031 -0.0021 -0.0010  0.0002
                                   -0.0004
            ( 48.38%)   0.6955* C 20 s( 32.34%)p 2.09( 67.59%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                   -0.0001  0.5681 -0.0248  0.0013 -0.0001
                                    0.0019  0.0072 -0.0046 -0.1347 -0.0001
                                   -0.0017  0.8109  0.0105 -0.0005 -0.0018
                                    0.0089 -0.0047 -0.0017  0.0239  0.0051
                                    0.0042 -0.0016  0.0029  0.0004  0.0014
                                    0.0006
8. (1.96197) BD ( 1) C  5- C  6
            ( 50.91%)   0.7135* C  5 s( 30.25%)p 2.30( 69.69%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                   -0.0002  0.5500 -0.0014 -0.0011  0.0001
                                   -0.7034  0.0011  0.0013 -0.3521 -0.0031
                                    0.0022 -0.2794  0.0112 -0.0021  0.0182
                                    0.0088  0.0051  0.0090 -0.0055  0.0008
                                    0.0011  0.0009 -0.0019 -0.0021  0.0001
                                   -0.0074
            ( 49.09%)   0.7006* C  6 s( 32.54%)p 2.07( 67.37%)d 0.00(  0.08%)
                                        f 0.00(  0.01%)
                                    0.0001  0.5704 -0.0006  0.0026 -0.0001
                                    0.6715 -0.0062  0.0001  0.4410 -0.0071
                                    0.0012  0.1676  0.0127 -0.0036  0.0214
                                    0.0132  0.0060  0.0111 -0.0068 -0.0009
                                   -0.0017 -0.0022  0.0022  0.0034 -0.0009
                                    0.0074
9. (1.96898) BD ( 1) C  5- C 10
            ( 50.02%)   0.7073* C  5 s( 33.61%)p 1.97( 66.33%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                    0.0000  0.5797 -0.0061  0.0005 -0.0001
                                    0.1523 -0.0077  0.0035 -0.0328 -0.0032
```

```
                                    0.0028  0.7993  0.0070 -0.0028  0.0014
                                    0.0037 -0.0040  0.0009  0.0215  0.0089
                                    0.0014 -0.0021  0.0006  0.0016  0.0008
                                   -0.0002
              ( 49.98%)   0.7069* C 10 s( 32.56%)p 2.07( 67.38%)d 0.00(  0.05%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.5706 -0.0020 -0.0002 -0.0001
                                    0.0125  0.0062  0.0027  0.1339  0.0028
                                    0.0013 -0.8097  0.0067  0.0017  0.0025
                                    0.0026 -0.0056 -0.0002  0.0224 -0.0081
                                   -0.0016  0.0014 -0.0004 -0.0019 -0.0006
                                   -0.0007
 10. (1.97753) BD ( 1) C  6- C  7
              ( 49.46%)   0.7033* C  6 s( 35.82%)p 1.79( 64.08%)d 0.00(  0.09%)
                                             f 0.00(  0.01%)
                                   -0.0001 -0.5985 -0.0065 -0.0036  0.0000
                                    0.4033 -0.0205  0.0047  0.3792 -0.0143
                                    0.0022 -0.5776 -0.0086  0.0026 -0.0118
                                    0.0149  0.0183 -0.0001 -0.0142 -0.0005
                                    0.0040  0.0054 -0.0003 -0.0070 -0.0019
                                    0.0016
              ( 50.54%)   0.7109* C  7 s( 34.41%)p 1.90( 65.52%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0000 -0.5866 -0.0028  0.0004  0.0001
                                   -0.2654 -0.0091  0.0052 -0.3618 -0.0035
                                    0.0029  0.6735 -0.0155  0.0024 -0.0101
                                    0.0130  0.0152  0.0004 -0.0097  0.0013
                                   -0.0041 -0.0056 -0.0009  0.0055  0.0021
                                   -0.0025
 11. (1.69127) BD ( 2) C  6- C  7
              ( 46.79%)   0.6840* C  6 s(  0.01%)p 1.00( 99.91%)d 0.00(  0.07%)
                                             f 0.00(  0.01%)
                                    0.0001 -0.0088 -0.0011 -0.0002  0.0000
                                   -0.5631 -0.0066 -0.0056  0.8121  0.0083
                                    0.0077  0.1491  0.0037  0.0026  0.0027
                                   -0.0157  0.0191  0.0072  0.0069  0.0033
                                   -0.0042  0.0060  0.0016  0.0031 -0.0076
                                   -0.0021
              ( 53.21%)   0.7295* C  7 s(  0.00%)p 1.00( 99.93%)d 0.00(  0.05%)
                                             f 0.00(  0.01%)
                                    0.0000 -0.0068 -0.0020 -0.0001  0.0000
                                   -0.5841 -0.0098 -0.0056  0.7890  0.0133
                                    0.0077  0.1878  0.0038  0.0022  0.0046
                                    0.0083 -0.0051 -0.0195 -0.0025  0.0024
                                   -0.0030  0.0038  0.0016  0.0034 -0.0094
                                   -0.0033
 12. (1.98216) BD ( 1) C  6- H 37
              ( 62.66%)   0.7916* C  6 s( 31.53%)p 2.17( 68.40%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0002 -0.5615  0.0031  0.0049 -0.0001
                                    0.2609 -0.0009 -0.0009  0.0309  0.0027
                                    0.0016  0.7842  0.0004 -0.0098  0.0008
                                   -0.0116 -0.0024 -0.0013 -0.0203  0.0082
                                    0.0066 -0.0005  0.0025  0.0018  0.0002
                                    0.0009
              ( 37.34%)   0.6111* H 37 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                   -0.9995 -0.0016 -0.0020 -0.0068  0.0039
                                   -0.0294  0.0002 -0.0044 -0.0012 -0.0010
                                   -0.0061
 13. (1.98475) BD ( 1) C  7- C  8
              ( 49.46%)   0.7033* C  7 s( 33.22%)p 2.01( 66.74%)d 0.00(  0.03%)
                                             f 0.00(  0.01%)
                                    0.0000  0.5764  0.0068  0.0001  0.0003
                                   -0.6605  0.0058  0.0065 -0.4803  0.0012
                                    0.0047 -0.0159  0.0107  0.0004  0.0143
                                    0.0006  0.0006  0.0043 -0.0087 -0.0001
                                    0.0036  0.0027 -0.0005  0.0001  0.0025
                                   -0.0074
              ( 50.54%)   0.7109* C  8 s( 29.60%)p 2.38( 70.33%)d 0.00(  0.07%)
                                             f 0.00(  0.00%)
                                    0.0003  0.5439  0.0103  0.0015 -0.0001
                                    0.6785 -0.0008 -0.0016  0.4913  0.0013
                                   -0.0009  0.0384 -0.0063 -0.0009  0.0214
                                    0.0018  0.0012  0.0071 -0.0130 -0.0023
                                   -0.0038 -0.0007 -0.0003 -0.0012 -0.0018
                                    0.0042
 14. (1.96706) BD ( 1) C  7- C  9
              ( 49.13%)   0.7009* C  7 s( 32.29%)p 2.10( 67.64%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0001  0.5681 -0.0084  0.0001 -0.0003
                                    0.3891  0.0052 -0.0038  0.1230  0.0040
                                   -0.0031  0.7140 -0.0036  0.0007  0.0073
                                    0.0186  0.0062  0.0062  0.0123  0.0025
                                    0.0060  0.0013  0.0033  0.0031  0.0001
                                    0.0029
              ( 50.87%)   0.7133* C  9 s( 31.82%)p 2.14( 68.12%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.5640 -0.0038 -0.0001 -0.0002
```

```
                                    -0.4787 -0.0029 -0.0014 -0.2044 -0.0037
                                    -0.0010 -0.6403  0.0136  0.0023  0.0084
                                     0.0179  0.0060  0.0055  0.0111 -0.0027
                                    -0.0061 -0.0009 -0.0033 -0.0035 -0.0002
                                    -0.0023
15. (1.98643) BD ( 1) C  8- H 38
              ( 61.41%)   0.7837* C  8 s( 23.79%)p 3.20( 76.10%)d 0.00(  0.10%)
                                              f 0.00(  0.01%)
                                     0.0001 -0.4878 -0.0006  0.0012 -0.0001
                                     0.3202  0.0017  0.0044  0.0339  0.0030
                                     0.0030  0.8107 -0.0077  0.0005 -0.0002
                                    -0.0170 -0.0008 -0.0030 -0.0257  0.0041
                                     0.0051  0.0001  0.0012  0.0019  0.0016
                                    -0.0027
              ( 38.59%)   0.6212* H 38 s( 99.96%)p 0.00(  0.03%)d 0.00(  0.01%)
                                    -0.9998 -0.0005 -0.0005 -0.0059  0.0000
                                    -0.0168 -0.0002 -0.0051 -0.0009 -0.0010
                                    -0.0062
16. (1.97891) BD ( 1) C  8- H 39
              ( 61.03%)   0.7812* C  8 s( 23.32%)p 3.28( 76.58%)d 0.00(  0.10%)
                                              f 0.00(  0.00%)
                                     0.0001 -0.4828  0.0048  0.0001  0.0000
                                     0.6318  0.0063  0.0021 -0.2974  0.0023
                                    -0.0009 -0.5273  0.0034  0.0028  0.0133
                                     0.0236 -0.0124 -0.0099 -0.0031  0.0033
                                     0.0036 -0.0006 -0.0013  0.0025  0.0023
                                    -0.0035
              ( 38.97%)   0.6243* H 39 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    -0.9998 -0.0022 -0.0007 -0.0148  0.0095
                                     0.0101  0.0035  0.0059 -0.0024 -0.0034
                                    -0.0005
17. (1.97836) BD ( 1) C  8- H 40
              ( 60.98%)   0.7809* C  8 s( 23.28%)p 3.29( 76.62%)d 0.00(  0.10%)
                                              f 0.00(  0.00%)
                                     0.0001 -0.4825  0.0050  0.0001  0.0000
                                    -0.1912  0.0049  0.0005  0.8171  0.0046
                                     0.0012 -0.2487  0.0037  0.0036  0.0123
                                    -0.0047  0.0155  0.0214  0.0112  0.0033
                                     0.0027 -0.0011  0.0017  0.0018  0.0018
                                    -0.0045
              ( 39.02%)   0.6247* H 40 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    -0.9998 -0.0023 -0.0007  0.0061 -0.0194
                                     0.0028  0.0024 -0.0009  0.0034  0.0063
                                     0.0026
18. (1.96526) BD ( 1) C  9- C 10
              ( 50.17%)   0.7083* C  9 s( 31.95%)p 2.13( 67.99%)d 0.00(  0.05%)
                                              f 0.00(  0.01%)
                                    -0.0001  0.5652 -0.0075 -0.0007  0.0000
                                     0.6321 -0.0045 -0.0016  0.5112 -0.0060
                                    -0.0024 -0.1377  0.0046  0.0033  0.0192
                                    -0.0061 -0.0063  0.0037 -0.0078  0.0018
                                    -0.0018 -0.0008  0.0001 -0.0043 -0.0037
                                     0.0063
              ( 49.83%)   0.7059* C 10 s( 30.43%)p 2.28( 69.51%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                    -0.0002  0.5516 -0.0039 -0.0009 -0.0001
                                    -0.5598  0.0082  0.0028 -0.5455  0.0054
                                     0.0015  0.2899  0.0028  0.0011  0.0198
                                    -0.0082 -0.0071  0.0044 -0.0062 -0.0014
                                     0.0012  0.0012 -0.0003  0.0029  0.0040
                                    -0.0059
19. (1.98194) BD ( 1) C  9- C 16
              ( 50.10%)   0.7078* C  9 s( 36.17%)p 1.76( 63.77%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                     0.0000  0.6012  0.0145  0.0005  0.0001
                                    -0.1529 -0.0042 -0.0002 -0.2783 -0.0041
                                     0.0000  0.7327 -0.0013  0.0001  0.0027
                                    -0.0077 -0.0139 -0.0022  0.0170  0.0055
                                    -0.0034 -0.0075 -0.0020  0.0032  0.0008
                                    -0.0003
              ( 49.90%)   0.7064* C 16 s( 36.65%)p 1.73( 63.26%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0000  0.6054  0.0079  0.0019 -0.0001
                                     0.1839  0.0039 -0.0001  0.3574  0.0026
                                     0.0002 -0.6863  0.0077 -0.0004  0.0063
                                    -0.0100 -0.0177 -0.0027  0.0167 -0.0051
                                     0.0037  0.0081  0.0023 -0.0033 -0.0012
                                     0.0003
20. (1.58177) BD ( 2) C  9- C 16
              ( 50.60%)   0.7114* C  9 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.01%)
                                              f 0.00(  0.02%)
                                     0.0000  0.0080  0.0010 -0.0002  0.0000
                                     0.5893  0.0086  0.0026 -0.7867 -0.0101
                                    -0.0043 -0.1824 -0.0011 -0.0014  0.0000
                                     0.0073 -0.0057 -0.0066 -0.0033 -0.0038
                                     0.0046 -0.0052 -0.0029 -0.0039  0.0075
                                     0.0036
              ( 49.40%)   0.7028* C 16 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.02%)
```

```
                                        f 0.00(  0.02%)
                                  0.0001  0.0088  0.0009 -0.0003  0.0000
                                  0.6149 -0.0010  0.0048 -0.7565  0.0008
                                 -0.0060 -0.2214  0.0006 -0.0012 -0.0001
                                 -0.0072  0.0057  0.0105  0.0031 -0.0052
                                  0.0054 -0.0066 -0.0011 -0.0048  0.0057
                                  0.0029
21. (1.97947) BD ( 1) C 10- C 11
             ( 50.32%)   0.7094* C 10 s( 36.94%)p 1.71( 62.99%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                  0.0000  0.6077  0.0102  0.0010  0.0001
                                  0.4829 -0.0007  0.0012  0.3841  0.0002
                                  0.0006  0.4992 -0.0060 -0.0007  0.0119
                                  0.0151  0.0148  0.0005  0.0027 -0.0028
                                  0.0039  0.0034  0.0016  0.0079 -0.0022
                                  0.0036
             ( 49.68%)   0.7048* C 11 s( 35.58%)p 1.81( 64.34%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                  0.0000  0.5965 -0.0013  0.0004 -0.0002
                                 -0.4368  0.0033  0.0001 -0.4436  0.0003
                                 -0.0004 -0.5058  0.0018 -0.0011  0.0134
                                  0.0155  0.0145  0.0006  0.0016  0.0022
                                 -0.0039 -0.0033 -0.0008 -0.0073  0.0027
                                 -0.0029
22. (1.56509) BD ( 2) C 10- C 11
             ( 53.76%)   0.7332* C 10 s(  0.01%)p99.99( 99.96%)d 0.88(  0.01%)
                                        f 1.04(  0.02%)
                                  0.0004  0.0121  0.0004  0.0000  0.0002
                                  0.6728  0.0095  0.0029 -0.7323 -0.0108
                                 -0.0035 -0.1022 -0.0030  0.0008  0.0020
                                  0.0063 -0.0058  0.0071 -0.0015 -0.0015
                                  0.0044 -0.0059  0.0026 -0.0022  0.0075
                                  0.0055
             ( 46.24%)   0.6800* C 11 s(  0.02%)p99.99( 99.94%)d 2.05(  0.03%)
                                        f 0.88(  0.01%)
                                 -0.0004 -0.0123 -0.0023 -0.0002  0.0000
                                  0.7625  0.0052  0.0042 -0.6362 -0.0056
                                 -0.0023 -0.1149  0.0017 -0.0009 -0.0013
                                 -0.0021  0.0042 -0.0172 -0.0003 -0.0026
                                  0.0052 -0.0046  0.0028 -0.0026  0.0046
                                  0.0069
23. (1.97536) BD ( 1) C 11- C 12
             ( 50.55%)   0.7110* C 11 s( 30.54%)p 2.27( 69.42%)d 0.00(  0.03%)
                                        f 0.00(  0.01%)
                                 -0.0002  0.5526 -0.0010 -0.0003  0.0002
                                  0.4766 -0.0033 -0.0028  0.6145 -0.0015
                                 -0.0035 -0.2988  0.0110  0.0005  0.0142
                                 -0.0048 -0.0077 -0.0049 -0.0055  0.0016
                                 -0.0007 -0.0004  0.0018 -0.0034 -0.0056
                                  0.0023
             ( 49.45%)   0.7032* C 12 s( 28.73%)p 2.48( 71.19%)d 0.00(  0.08%)
                                        f 0.00(  0.00%)
                                  0.0003  0.5359  0.0099  0.0028 -0.0001
                                 -0.4604  0.0005 -0.0005 -0.6447 -0.0019
                                 -0.0012  0.2902 -0.0104 -0.0005  0.0204
                                 -0.0089 -0.0130 -0.0067 -0.0084 -0.0004
                                  0.0016  0.0020 -0.0018  0.0054  0.0031
                                 -0.0007
24. (1.98007) BD ( 1) C 11- C 13
             ( 50.14%)   0.7081* C 11 s( 33.81%)p 1.96( 66.13%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                  0.0000  0.5814  0.0035 -0.0004  0.0000
                                  0.0114  0.0082  0.0010 -0.1422  0.0065
                                  0.0013  0.8005 -0.0032  0.0006 -0.0001
                                  0.0007 -0.0082 -0.0005  0.0221  0.0084
                                  0.0018 -0.0033 -0.0005  0.0006  0.0004
                                 -0.0003
             ( 49.86%)   0.7061* C 13 s( 36.69%)p 1.72( 63.23%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                  0.0001  0.6057  0.0015  0.0030 -0.0003
                                 -0.0986 -0.0087 -0.0006  0.1098 -0.0096
                                 -0.0010 -0.7812  0.0068  0.0025 -0.0006
                                  0.0052 -0.0055  0.0002  0.0255 -0.0095
                                 -0.0018  0.0044  0.0004 -0.0002  0.0001
                                 -0.0004
25. (1.98624) BD ( 1) C 12- H 59
             ( 60.49%)   0.7777* C 12 s( 23.92%)p 3.18( 75.98%)d 0.00(  0.10%)
                                        f 0.00(  0.01%)
                                 -0.0001  0.4891  0.0039 -0.0015  0.0001
                                  0.3403 -0.0029  0.0025  0.4592 -0.0049
                                  0.0053  0.6580  0.0080 -0.0033  0.0096
                                  0.0152  0.0203 -0.0031  0.0150  0.0004
                                  0.0026  0.0030 -0.0020  0.0064  0.0005
                                 -0.0001
             ( 39.51%)   0.6286* H 59 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                  0.9998  0.0005  0.0005 -0.0102 -0.0143
                                 -0.0104  0.0033  0.0043  0.0052 -0.0013
                                  0.0027
```

```
26. (1.96928) BD ( 1) C 12- H 60
             ( 61.61%)   0.7850* C 12 s( 23.01%)p 3.34( 76.89%)d 0.00(  0.09%)
                                      f 0.00(  0.00%)
                                    -0.0002  0.4797 -0.0054 -0.0008 -0.0001
                                    -0.4998 -0.0068  0.0001  0.5412 -0.0074
                                     0.0019 -0.4754  0.0027  0.0052 -0.0178
                                     0.0178 -0.0164  0.0024 -0.0024  0.0017
                                     0.0002  0.0022 -0.0007  0.0061  0.0021
                                    -0.0004
             ( 38.39%)   0.6196* H 60 s( 99.93%)p 0.00(  0.06%)d 0.00(  0.01%)
                                     0.9996  0.0012  0.0009  0.0116 -0.0159
                                     0.0157 -0.0049  0.0047 -0.0052 -0.0011
                                    -0.0007
27. (1.95592) BD ( 1) C 12- H 61
             ( 64.12%)   0.8008* C 12 s( 24.32%)p 3.11( 75.60%)d 0.00(  0.08%)
                                      f 0.00(  0.00%)
                                     0.0000  0.4931 -0.0067 -0.0004  0.0000
                                     0.6489 -0.0012  0.0042 -0.2815 -0.0118
                                     0.0010 -0.5054 -0.0009  0.0052 -0.0131
                                    -0.0206  0.0117  0.0076  0.0003  0.0015
                                     0.0026  0.0009 -0.0031  0.0050  0.0022
                                    -0.0004
             ( 35.88%)   0.5990* H 61 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                     0.9995  0.0036  0.0015 -0.0223  0.0043
                                     0.0191 -0.0032 -0.0064  0.0029  0.0039
                                     0.0004
28. (1.98382) BD ( 1) C 13- C 14
             ( 49.90%)   0.7064* C 13 s( 37.35%)p 1.68( 62.57%)d 0.00(  0.07%)
                                      f 0.00(  0.01%)
                                     0.0001  0.6109  0.0172  0.0007  0.0001
                                    -0.3691 -0.0056  0.0007 -0.5396  0.0014
                                     0.0011  0.4444 -0.0264 -0.0013  0.0150
                                    -0.0121 -0.0174 -0.0053 -0.0006 -0.0033
                                    -0.0025 -0.0039 -0.0029  0.0072  0.0046
                                    -0.0014
             ( 50.10%)   0.7078* C 14 s( 37.20%)p 1.69( 62.71%)d 0.00(  0.07%)
                                      f 0.00(  0.01%)
                                     0.0000  0.6097  0.0163  0.0012  0.0000
                                     0.3479 -0.0183  0.0002  0.4892 -0.0158
                                    -0.0004 -0.5158 -0.0121  0.0007  0.0130
                                    -0.0119 -0.0191 -0.0051  0.0044  0.0034
                                     0.0022  0.0038  0.0026 -0.0079 -0.0045
                                     0.0015
29. (1.65429) BD ( 2) C 13- C 14
             ( 51.58%)   0.7182* C 13 s(  0.01%)p99.99( 99.96%)d 1.32(  0.01%)
                                      f 1.34(  0.02%)
                                     0.0000 -0.0106  0.0000  0.0000  0.0000
                                     0.7217  0.0050  0.0077 -0.6644 -0.0033
                                    -0.0058 -0.1928 -0.0015 -0.0015 -0.0016
                                     0.0029 -0.0005 -0.0117 -0.0011 -0.0035
                                     0.0064 -0.0041 -0.0031 -0.0044  0.0039
                                     0.0062
             ( 48.42%)   0.6958* C 14 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.02%)
                                      f 0.00(  0.01%)
                                     0.0000 -0.0002  0.0003  0.0000  0.0001
                                     0.6917  0.0044  0.0061 -0.6955 -0.0042
                                    -0.0064 -0.1932 -0.0014 -0.0023  0.0033
                                    -0.0086  0.0067  0.0074  0.0043 -0.0020
                                     0.0025 -0.0020 -0.0018 -0.0041  0.0073
                                     0.0079
30. (1.97168) BD ( 1) C 13- H 41
             ( 60.63%)   0.7786* C 13 s( 25.91%)p 2.86( 74.00%)d 0.00(  0.08%)
                                      f 0.00(  0.01%)
                                    -0.0005  0.5088 -0.0163 -0.0040  0.0001
                                     0.5763  0.0049 -0.0039  0.5040  0.0057
                                    -0.0040  0.3922 -0.0006 -0.0018  0.0194
                                     0.0143  0.0130  0.0016 -0.0040 -0.0011
                                     0.0016  0.0000  0.0012  0.0052 -0.0049
                                     0.0053
             ( 39.37%)   0.6275* H 41 s( 99.93%)p 0.00(  0.07%)d 0.00(  0.01%)
                                     0.9996  0.0014  0.0017 -0.0174 -0.0148
                                    -0.0127  0.0056  0.0042  0.0037  0.0004
                                    -0.0014
31. (1.98005) BD ( 1) C 14- C 15
             ( 50.22%)   0.7087* C 14 s( 36.81%)p 1.71( 63.10%)d 0.00(  0.07%)
                                      f 0.00(  0.01%)
                                     0.0001  0.6067  0.0017  0.0027 -0.0002
                                    -0.5733  0.0025  0.0003 -0.5241  0.0038
                                     0.0002 -0.1665 -0.0051 -0.0008  0.0225
                                     0.0079  0.0064  0.0034 -0.0113  0.0021
                                     0.0037  0.0038 -0.0006 -0.0034  0.0053
                                    -0.0072
             ( 49.78%)   0.7055* C 15 s( 34.35%)p 1.91( 65.58%)d 0.00(  0.06%)
                                      f 0.00(  0.01%)
                                     0.0000  0.5861  0.0056 -0.0002  0.0000
                                     0.6133  0.0036  0.0019  0.5126  0.0025
                                     0.0006  0.1299  0.0021  0.0031  0.0208
                                     0.0040  0.0035  0.0022 -0.0113 -0.0023
```

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                                    -0.0029 -0.0027  0.0010  0.0033 -0.0042
                                     0.0066
32. (1.97095) BD ( 1) C 14- H 42
            ( 60.57%)   0.7783* C 14 s( 25.94%)p 2.85( 73.98%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                    -0.0005  0.5090 -0.0156 -0.0041  0.0001
                                     0.2664 -0.0025 -0.0005  0.0380 -0.0039
                                     0.0013  0.8168  0.0091 -0.0062  0.0015
                                     0.0135  0.0015  0.0020  0.0236  0.0061
                                     0.0056 -0.0014  0.0015  0.0036 -0.0003
                                     0.0014
            ( 39.43%)   0.6279* H 42 s( 99.92%)p 0.00(  0.07%)d 0.00(  0.01%)
                                     0.9996  0.0015  0.0019 -0.0112 -0.0031
                                    -0.0247  0.0003  0.0043  0.0005  0.0007
                                     0.0070
33. (1.97954) BD ( 1) C 15- C 16
            ( 49.67%)   0.7048* C 15 s( 35.24%)p 1.84( 64.70%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                     0.0000  0.5936  0.0076  0.0005 -0.0001
                                    -0.3363 -0.0085 -0.0017 -0.0924 -0.0066
                                    -0.0016 -0.7247 -0.0024 -0.0004  0.0019
                                     0.0155  0.0030  0.0034  0.0175 -0.0043
                                    -0.0077 -0.0017 -0.0029 -0.0025 -0.0004
                                    -0.0010
            ( 50.33%)   0.7094* C 16 s( 37.41%)p 1.67( 62.51%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0001  0.6116  0.0093  0.0015  0.0000
                                     0.3678  0.0072  0.0007  0.1036  0.0084
                                     0.0005  0.6920 -0.0075  0.0007  0.0041
                                     0.0189  0.0055  0.0050  0.0169  0.0053
                                     0.0087  0.0019  0.0034  0.0019  0.0004
                                     0.0011
34. (1.96538) BD ( 1) C 15- C 17
            ( 50.13%)   0.7080* C 15 s( 30.36%)p 2.29( 69.60%)d 0.00(  0.04%)
                                              f 0.00(  0.01%)
                                    -0.0001  0.5509 -0.0098 -0.0007  0.0001
                                    -0.2838  0.0032  0.0009 -0.4525  0.0073
                                     0.0021  0.6405 -0.0180 -0.0049  0.0076
                                    -0.0079 -0.0133 -0.0024  0.0080  0.0009
                                    -0.0017 -0.0047 -0.0022  0.0043  0.0024
                                    -0.0012
            ( 49.87%)   0.7062* C 17 s( 27.19%)p 2.68( 72.76%)d 0.00(  0.05%)
                                              f 0.00(  0.00%)
                                     0.0003  0.5215 -0.0001  0.0008 -0.0001
                                     0.3037  0.0084  0.0015  0.4724  0.0080
                                     0.0012 -0.6419  0.0028  0.0005  0.0073
                                    -0.0105 -0.0157 -0.0035  0.0069 -0.0001
                                     0.0008  0.0034  0.0002 -0.0050  0.0002
                                    -0.0023
35. (1.96909) BD ( 1) C 16- H 43
            ( 60.59%)   0.7784* C 16 s( 25.89%)p 2.86( 74.04%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0005 -0.5085  0.0156  0.0036 -0.0001
                                     0.6721  0.0028 -0.0060  0.5371  0.0030
                                    -0.0050  0.0115  0.0000 -0.0002 -0.0232
                                    -0.0008 -0.0002 -0.0042  0.0120  0.0000
                                    -0.0015 -0.0015  0.0016 -0.0001 -0.0040
                                     0.0077
            ( 39.41%)   0.6278* H 43 s( 99.91%)p 0.00(  0.08%)d 0.00(  0.01%)
                                    -0.9995 -0.0024 -0.0015 -0.0224 -0.0181
                                    -0.0011 -0.0069  0.0000  0.0001 -0.0013
                                     0.0039
36. (1.97282) BD ( 1) C 17- C 18
            ( 50.25%)   0.7089* C 17 s( 25.81%)p 2.87( 74.15%)d 0.00(  0.04%)
                                              f 0.00(  0.00%)
                                     0.0002  0.5079  0.0089  0.0005  0.0001
                                    -0.3409  0.0189 -0.0011  0.4953  0.0092
                                     0.0022  0.6161 -0.0048 -0.0018 -0.0074
                                    -0.0083  0.0138 -0.0044  0.0051  0.0001
                                    -0.0007  0.0027  0.0003 -0.0047  0.0003
                                    -0.0016
            ( 49.75%)   0.7054* C 18 s( 28.45%)p 2.51( 71.49%)d 0.00(  0.06%)
                                              f 0.00(  0.00%)
                                     0.0004  0.5333  0.0079  0.0030  0.0000
                                     0.3441 -0.0071 -0.0021 -0.4787 -0.0040
                                     0.0017 -0.6059  0.0050  0.0004 -0.0102
                                    -0.0129  0.0171 -0.0030  0.0058  0.0004
                                     0.0009 -0.0031  0.0002  0.0054 -0.0005
                                     0.0013
37. (1.97302) BD ( 1) C 17- C 19
            ( 50.31%)   0.7093* C 17 s( 25.84%)p 2.87( 74.12%)d 0.00(  0.04%)
                                              f 0.00(  0.00%)
                                     0.0002  0.5083  0.0089  0.0005  0.0001
                                     0.6117  0.0093  0.0014 -0.5089  0.0194
                                    -0.0004  0.3280 -0.0015 -0.0027 -0.0136
                                     0.0087 -0.0070  0.0044 -0.0050 -0.0005
                                     0.0002  0.0022 -0.0005 -0.0048 -0.0005
                                    -0.0021
```

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            ( 49.69%)   0.7049* C 19 s( 28.43%)p 2.52( 71.51%)d 0.00(  0.06%)
                                          f 0.00(  0.00%)
                                     0.0004  0.5331  0.0079  0.0030  0.0000
                                    -0.5931 -0.0033  0.0015  0.5094 -0.0082
                                    -0.0021 -0.3221  0.0038 -0.0007 -0.0183
                                     0.0107 -0.0096  0.0023 -0.0077  0.0009
                                     0.0003 -0.0024  0.0001  0.0052  0.0010
                                     0.0026
38. (1.96868) BD ( 1) C 17- H 44
            ( 60.77%)   0.7795* C 17 s( 21.14%)p 3.73( 78.79%)d 0.00(  0.06%)
                                          f 0.00(  0.00%)
                                     0.0002 -0.4596  0.0155  0.0019  0.0001
                                     0.6451  0.0103  0.0008  0.5212  0.0084
                                     0.0030  0.3160  0.0036 -0.0066 -0.0178
                                    -0.0127 -0.0101 -0.0043  0.0068 -0.0001
                                    -0.0002 -0.0025  0.0001  0.0045 -0.0004
                                     0.0023
            ( 39.23%)   0.6264* H 44 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                    -0.9995 -0.0036 -0.0016 -0.0212 -0.0186
                                    -0.0080 -0.0076 -0.0046 -0.0035 -0.0016
                                     0.0029
39. (1.98930) BD ( 1) C 18- H 56
            ( 60.36%)   0.7769* C 18 s( 23.92%)p 3.18( 75.97%)d 0.00(  0.10%)
                                          f 0.00(  0.01%)
                                     0.0000  0.4891 -0.0052 -0.0010  0.0000
                                     0.5998 -0.0043 -0.0025  0.5199  0.0083
                                    -0.0008  0.3600  0.0077  0.0012  0.0225
                                     0.0146  0.0130  0.0053 -0.0082 -0.0013
                                    -0.0001 -0.0022 -0.0001  0.0061 -0.0010
                                     0.0029
            ( 39.64%)   0.6296* H 56 s( 99.94%)p 0.00(  0.05%)d 0.00(  0.01%)
                                     0.9997  0.0021  0.0005 -0.0121 -0.0160
                                    -0.0098  0.0058  0.0040  0.0040  0.0010
                                    -0.0020
40. (1.98581) BD ( 1) C 18- H 57
            ( 60.64%)   0.7787* C 18 s( 23.50%)p 3.25( 76.38%)d 0.00(  0.11%)
                                          f 0.00(  0.01%)
                                     0.0001 -0.4848  0.0000  0.0010  0.0000
                                     0.3385  0.0020  0.0029  0.5017 -0.0074
                                     0.0001 -0.6304 -0.0005 -0.0038 -0.0127
                                     0.0149  0.0239  0.0068 -0.0088  0.0004
                                     0.0011  0.0042  0.0010 -0.0066 -0.0007
                                    -0.0016
            ( 39.36%)   0.6274* H 57 s( 99.97%)p 0.00(  0.02%)d 0.00(  0.01%)
                                    -0.9999 -0.0008 -0.0006 -0.0065 -0.0075
                                     0.0113 -0.0032  0.0038  0.0056  0.0010
                                    -0.0025
41. (1.98906) BD ( 1) C 18- H 58
            ( 61.00%)   0.7810* C 18 s( 24.09%)p 3.15( 75.80%)d 0.00(  0.10%)
                                          f 0.00(  0.01%)
                                     0.0000 -0.4908  0.0008  0.0008  0.0000
                                     0.6372  0.0008  0.0001 -0.4975 -0.0021
                                     0.0000  0.3232 -0.0067 -0.0017  0.0225
                                    -0.0158  0.0118 -0.0054  0.0083 -0.0012
                                    -0.0006  0.0025  0.0005 -0.0060 -0.0009
                                    -0.0034
            ( 39.00%)   0.6245* H 58 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    -0.9998 -0.0004 -0.0008 -0.0135  0.0126
                                    -0.0074  0.0061 -0.0040  0.0028 -0.0014
                                     0.0028
42. (1.98929) BD ( 1) C 19- H 53
            ( 60.37%)   0.7770* C 19 s( 23.93%)p 3.17( 75.97%)d 0.00(  0.10%)
                                          f 0.00(  0.01%)
                                     0.0000  0.4892 -0.0052 -0.0010  0.0000
                                     0.6504  0.0097 -0.0007  0.4650 -0.0065
                                    -0.0027  0.3468  0.0034  0.0007  0.0220
                                     0.0161  0.0116  0.0051 -0.0089 -0.0013
                                    -0.0003 -0.0024  0.0010  0.0058 -0.0001
                                     0.0032
            ( 39.63%)   0.6295* H 53 s( 99.94%)p 0.00(  0.05%)d 0.00(  0.01%)
                                     0.9997  0.0021  0.0005 -0.0193 -0.0085
                                    -0.0075  0.0055  0.0047  0.0030  0.0019
                                    -0.0024
43. (1.98899) BD ( 1) C 19- H 54
            ( 61.08%)   0.7815* C 19 s( 24.13%)p 3.14( 75.77%)d 0.00(  0.10%)
                                          f 0.00(  0.01%)
                                     0.0000  0.4912 -0.0009 -0.0008  0.0000
                                     0.3302  0.0038  0.0004 -0.5188 -0.0027
                                    -0.0005 -0.6160  0.0054  0.0015 -0.0119
                                    -0.0143  0.0231 -0.0052  0.0091  0.0006
                                     0.0010 -0.0037  0.0010  0.0062 -0.0008
                                     0.0014
            ( 38.92%)   0.6238* H 54 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                     0.9998  0.0004  0.0008 -0.0089  0.0109
                                     0.0143 -0.0034 -0.0039  0.0063 -0.0014
                                     0.0017
44. (1.98558) BD ( 1) C 19- H 55
            ( 60.63%)   0.7787* C 19 s( 23.48%)p 3.25( 76.40%)d 0.00(  0.11%)
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                                        f 0.00(  0.01%)
                                   0.0001 -0.4846 -0.0001  0.0010  0.0000
                                   0.3390 -0.0071 -0.0007  0.5039  0.0022
                                   0.0038 -0.6286  0.0022 -0.0027 -0.0130
                                   0.0167  0.0230  0.0033 -0.0093  0.0004
                                   0.0013  0.0042  0.0006 -0.0065 -0.0011
                                  -0.0017
            ( 39.37%)   0.6274* H 55 s( 99.97%)p 0.00(  0.02%)d 0.00(  0.01%)
                                  -0.9999 -0.0008 -0.0006 -0.0046 -0.0096
                                   0.0106 -0.0032  0.0036  0.0057  0.0014
                                  -0.0023
45. (1.96952) BD ( 1) C 20- C 21
            ( 47.76%)   0.6911* C 20 s( 32.29%)p 2.09( 67.64%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                  -0.0001  0.5678 -0.0241  0.0009 -0.0001
                                   0.7003  0.0118 -0.0019  0.2361  0.0022
                                  -0.0011 -0.3606  0.0034 -0.0039  0.0108
                                  -0.0112 -0.0021  0.0158 -0.0119  0.0011
                                  -0.0024 -0.0009 -0.0008 -0.0012  0.0046
                                   0.0051
            ( 52.24%)   0.7228* C 21 s( 31.53%)p 2.17( 68.41%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                  -0.0004  0.5615 -0.0036 -0.0009 -0.0001
                                  -0.7791 -0.0054  0.0011 -0.2697 -0.0078
                                   0.0018 -0.0647  0.0093 -0.0069  0.0109
                                  -0.0047 -0.0015  0.0176 -0.0103 -0.0014
                                   0.0028  0.0003  0.0025  0.0026 -0.0038
                                  -0.0065
46. (1.98477) BD ( 1) C 21- C 22
            ( 49.43%)   0.7030* C 21 s( 40.39%)p 1.47( 59.55%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                   0.0000  0.6352  0.0208  0.0014  0.0002
                                   0.4303 -0.0021 -0.0006  0.2238 -0.0026
                                  -0.0005 -0.6001  0.0072 -0.0013  0.0072
                                  -0.0177 -0.0101  0.0017  0.0058  0.0007
                                   0.0073  0.0043 -0.0037 -0.0066  0.0003
                                   0.0031
            ( 50.57%)   0.7112* C 22 s( 36.08%)p 1.77( 63.86%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                  -0.0001  0.6006  0.0089  0.0000  0.0000
                                  -0.4924  0.0026 -0.0007 -0.3633  0.0009
                                  -0.0005  0.5140  0.0019 -0.0014  0.0088
                                  -0.0173 -0.0100  0.0045  0.0050 -0.0018
                                  -0.0051 -0.0034  0.0029  0.0071  0.0009
                                  -0.0038
47. (1.56794) BD ( 2) C 21- C 22
            ( 45.52%)   0.6747* C 21 s(  0.01%)p99.99( 99.96%)d 0.64(  0.01%)
                                        f 1.75(  0.02%)
                                   0.0002  0.0093  0.0048  0.0003  0.0000
                                  -0.3278  0.0072 -0.0010  0.9362 -0.0123
                                   0.0051  0.1241  0.0042  0.0003  0.0043
                                   0.0018 -0.0010 -0.0069  0.0001  0.0025
                                  -0.0033  0.0061  0.0069 -0.0030 -0.0083
                                   0.0034
            ( 54.48%)   0.7381* C 22 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.01%)
                                        f 0.00(  0.02%)
                                  -0.0002  0.0053  0.0039 -0.0003 -0.0001
                                  -0.4888  0.0079 -0.0033  0.8617 -0.0058
                                   0.0038  0.1347 -0.0022 -0.0007 -0.0031
                                  -0.0024  0.0070  0.0019  0.0022  0.0021
                                  -0.0047  0.0063  0.0033  0.0009 -0.0086
                                  -0.0004
48. (1.96197) BD ( 1) C 22- C 23
            ( 50.91%)   0.7135* C 22 s( 30.24%)p 2.30( 69.70%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                  -0.0002  0.5499 -0.0014 -0.0011  0.0001
                                   0.7033 -0.0011 -0.0013  0.3518  0.0032
                                  -0.0022  0.2800 -0.0111  0.0021  0.0182
                                   0.0088  0.0051  0.0090 -0.0055 -0.0008
                                  -0.0011 -0.0009  0.0019  0.0021 -0.0001
                                   0.0074
            ( 49.09%)   0.7006* C 23 s( 32.53%)p 2.07( 67.37%)d 0.00(  0.08%)
                                        f 0.00(  0.01%)
                                   0.0001  0.5704 -0.0006  0.0026 -0.0001
                                  -0.6713  0.0062 -0.0001 -0.4410  0.0071
                                  -0.0012 -0.1686 -0.0126  0.0036  0.0213
                                   0.0132  0.0060  0.0111 -0.0068  0.0009
                                   0.0017  0.0022 -0.0022 -0.0034  0.0009
                                  -0.0074
49. (1.96899) BD ( 1) C 22- C 27
            ( 50.02%)   0.7073* C 22 s( 33.61%)p 1.97( 66.33%)d 0.00(  0.05%)
                                        f 0.00(  0.01%)
                                   0.0000  0.5797 -0.0061  0.0005 -0.0001
                                  -0.1526  0.0077 -0.0035  0.0347  0.0032
                                  -0.0028 -0.7992 -0.0070  0.0027  0.0014
                                   0.0038 -0.0041  0.0009  0.0215 -0.0089
                                  -0.0014  0.0022 -0.0006 -0.0016 -0.0008
                                   0.0002
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            ( 49.98%)   0.7069* C 27 s( 32.55%)p 2.07( 67.39%)d 0.00(  0.05%)
                                              f 0.00(  0.01%)
                                     -0.0001  0.5705 -0.0021 -0.0002 -0.0001
                                     -0.0120 -0.0062 -0.0027 -0.1362 -0.0027
                                     -0.0013  0.8094 -0.0067 -0.0017  0.0024
                                      0.0026 -0.0057 -0.0002  0.0224  0.0081
                                      0.0016 -0.0015  0.0004  0.0019  0.0006
                                      0.0007
50. (1.97754) BD ( 1) C 23- C 24
            ( 49.46%)   0.7033* C 23 s( 35.83%)p 1.79( 64.07%)d 0.00(  0.09%)
                                              f 0.00(  0.01%)
                                      0.0001  0.5985  0.0065  0.0036  0.0000
                                      0.4028 -0.0204  0.0047  0.3809 -0.0143
                                      0.0022 -0.5767 -0.0086  0.0026  0.0118
                                     -0.0148 -0.0184  0.0000  0.0141 -0.0005
                                      0.0039  0.0054 -0.0003 -0.0070 -0.0019
                                      0.0015
            ( 50.54%)   0.7109* C 24 s( 34.41%)p 1.90( 65.52%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                      0.0000  0.5866  0.0028 -0.0004 -0.0001
                                     -0.2646 -0.0091  0.0052 -0.3641 -0.0035
                                      0.0029  0.6725 -0.0155  0.0024  0.0102
                                     -0.0130 -0.0152 -0.0005  0.0096  0.0013
                                     -0.0041 -0.0056 -0.0010  0.0055  0.0022
                                     -0.0025
51. (1.69132) BD ( 2) C 23- C 24
            ( 46.79%)   0.6840* C 23 s(  0.01%)p 1.00( 99.91%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     -0.0001  0.0089  0.0011  0.0002 -0.0001
                                     -0.5636 -0.0066 -0.0056  0.8113  0.0083
                                      0.0077  0.1514  0.0037  0.0026 -0.0028
                                      0.0157 -0.0191 -0.0072 -0.0070  0.0034
                                     -0.0042  0.0059  0.0016  0.0032 -0.0076
                                     -0.0021
            ( 53.21%)   0.7295* C 24 s(  0.01%)p 1.00( 99.93%)d 0.00(  0.05%)
                                              f 0.00(  0.01%)
                                      0.0000  0.0068  0.0020  0.0001  0.0000
                                     -0.5849 -0.0098 -0.0056  0.7877  0.0133
                                      0.0077  0.1905  0.0038  0.0022 -0.0045
                                     -0.0084  0.0050  0.0196  0.0025  0.0024
                                     -0.0030  0.0037  0.0016  0.0035 -0.0094
                                     -0.0033
52. (1.98215) BD ( 1) C 23- H 45
            ( 62.66%)   0.7916* C 23 s( 31.53%)p 2.17( 68.40%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                     -0.0002  0.5615 -0.0031 -0.0049  0.0001
                                      0.2612 -0.0009 -0.0009  0.0289  0.0027
                                      0.0016  0.7841  0.0004 -0.0098 -0.0008
                                      0.0116  0.0023  0.0013  0.0203  0.0082
                                      0.0066 -0.0006  0.0025  0.0018  0.0002
                                      0.0008
            ( 37.34%)   0.6110* H 45 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                      0.9995  0.0016  0.0020 -0.0068  0.0039
                                     -0.0294 -0.0002  0.0044  0.0012  0.0010
                                      0.0061
53. (1.98475) BD ( 1) C 24- C 25
            ( 49.46%)   0.7033* C 24 s( 33.23%)p 2.01( 66.74%)d 0.00(  0.03%)
                                              f 0.00(  0.01%)
                                      0.0000  0.5764  0.0069  0.0001  0.0003
                                      0.6600 -0.0058 -0.0065  0.4809 -0.0012
                                     -0.0047  0.0170 -0.0107 -0.0004  0.0143
                                      0.0006  0.0006  0.0042 -0.0087  0.0000
                                     -0.0036 -0.0027  0.0005  0.0000 -0.0025
                                      0.0074
            ( 50.54%)   0.7109* C 25 s( 29.60%)p 2.38( 70.33%)d 0.00(  0.07%)
                                              f 0.00(  0.00%)
                                      0.0003  0.5440  0.0103  0.0015 -0.0001
                                     -0.6779  0.0008  0.0016 -0.4921 -0.0014
                                      0.0009 -0.0396  0.0063  0.0009  0.0214
                                      0.0018  0.0012  0.0071 -0.0130  0.0023
                                      0.0038  0.0006  0.0003  0.0012  0.0019
                                     -0.0042
54. (1.96706) BD ( 1) C 24- C 26
            ( 49.13%)   0.7009* C 24 s( 32.28%)p 2.10( 67.65%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                      0.0001  0.5681 -0.0084  0.0001 -0.0003
                                     -0.3894 -0.0052  0.0038 -0.1213 -0.0040
                                      0.0031 -0.7142  0.0036 -0.0007  0.0073
                                      0.0186  0.0061  0.0062  0.0123 -0.0025
                                     -0.0060 -0.0013 -0.0033 -0.0031 -0.0001
                                     -0.0029
            ( 50.87%)   0.7133* C 26 s( 31.81%)p 2.14( 68.12%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                     -0.0001  0.5640 -0.0038 -0.0001 -0.0002
                                      0.4791  0.0029  0.0014  0.2028  0.0038
                                      0.0010  0.6405 -0.0136 -0.0023  0.0084
                                      0.0180  0.0059  0.0055  0.0111  0.0027
                                      0.0061  0.0009  0.0034  0.0034  0.0002
```

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                                    0.0023
55. (1.98643) BD ( 1) C 25- H 46
             ( 61.42%)   0.7837* C 25 s( 23.79%)p 3.20( 76.11%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.4878  0.0006 -0.0012  0.0001
                                    0.3208  0.0017  0.0044  0.0315  0.0030
                                    0.0030  0.8106 -0.0076  0.0005  0.0002
                                    0.0171  0.0006  0.0030  0.0257  0.0040
                                    0.0052  0.0001  0.0012  0.0019  0.0016
                                   -0.0027
             ( 38.58%)   0.6212* H 46 s( 99.96%)p 0.00(  0.03%)d 0.00(  0.01%)
                                    0.9998  0.0005  0.0005 -0.0059  0.0000
                                   -0.0168  0.0002  0.0051  0.0009  0.0010
                                    0.0061
56. (1.97892) BD ( 1) C 25- H 47
             ( 61.03%)   0.7812* C 25 s( 23.31%)p 3.28( 76.58%)d 0.00(  0.10%)
                                             f 0.00(  0.00%)
                                   -0.0001  0.4828 -0.0048 -0.0001  0.0000
                                    0.6318  0.0062  0.0021 -0.2947  0.0023
                                   -0.0009 -0.5289  0.0034  0.0028 -0.0132
                                   -0.0237  0.0123  0.0100  0.0032  0.0033
                                    0.0036 -0.0006 -0.0014  0.0025  0.0023
                                   -0.0035
             ( 38.97%)   0.6243* H 47 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    0.9998  0.0022  0.0007 -0.0148  0.0094
                                    0.0102 -0.0035 -0.0059  0.0024  0.0034
                                    0.0005
57. (1.97834) BD ( 1) C 25- H 48
             ( 60.98%)   0.7809* C 25 s( 23.28%)p 3.29( 76.62%)d 0.00(  0.10%)
                                             f 0.00(  0.00%)
                                   -0.0001  0.4825 -0.0050 -0.0001  0.0000
                                   -0.1925  0.0049  0.0005  0.8177  0.0046
                                    0.0012 -0.2456  0.0037  0.0036 -0.0124
                                    0.0047 -0.0153 -0.0214 -0.0113  0.0033
                                    0.0027 -0.0012  0.0016  0.0018  0.0018
                                   -0.0045
             ( 39.02%)   0.6247* H 48 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    0.9998  0.0023  0.0007  0.0061 -0.0194
                                    0.0028 -0.0025  0.0009 -0.0034 -0.0063
                                   -0.0027
58. (1.96526) BD ( 1) C 26- C 27
             ( 50.16%)   0.7083* C 26 s( 31.95%)p 2.13( 67.99%)d 0.00(  0.05%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.5652 -0.0075 -0.0007  0.0000
                                   -0.6313  0.0045  0.0016 -0.5124  0.0060
                                    0.0024  0.1366 -0.0046 -0.0033  0.0192
                                   -0.0061 -0.0063  0.0036 -0.0078 -0.0018
                                    0.0018  0.0008 -0.0002  0.0043  0.0037
                                   -0.0063
             ( 49.84%)   0.7059* C 27 s( 30.43%)p 2.28( 69.51%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                   -0.0002  0.5516 -0.0039 -0.0009 -0.0001
                                    0.5594 -0.0082 -0.0028  0.5466 -0.0054
                                   -0.0015 -0.2887 -0.0028 -0.0011  0.0198
                                   -0.0082 -0.0071  0.0044 -0.0062  0.0014
                                   -0.0012 -0.0012  0.0003 -0.0029 -0.0041
                                    0.0059
59. (1.98194) BD ( 1) C 26- C 33
             ( 50.10%)   0.7078* C 26 s( 36.17%)p 1.76( 63.77%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0000  0.6012  0.0145  0.0005  0.0001
                                    0.1518  0.0042  0.0002  0.2810  0.0041
                                    0.0000 -0.7319  0.0013 -0.0001  0.0027
                                   -0.0076 -0.0140 -0.0022  0.0169 -0.0055
                                    0.0033  0.0076  0.0020 -0.0032 -0.0009
                                    0.0003
             ( 49.90%)   0.7064* C 33 s( 36.65%)p 1.73( 63.26%)d 0.00(  0.07%)
                                             f 0.00(  0.01%)
                                    0.0000  0.6054  0.0079  0.0019 -0.0001
                                   -0.1819 -0.0039  0.0001 -0.3607 -0.0026
                                   -0.0002  0.6850 -0.0077  0.0004  0.0063
                                   -0.0099 -0.0179 -0.0029  0.0166  0.0050
                                   -0.0036 -0.0082 -0.0024  0.0033  0.0012
                                   -0.0003
60. (1.58180) BD ( 2) C 26- C 33
             ( 50.60%)   0.7114* C 26 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.01%)
                                             f 0.00(  0.02%)
                                    0.0000 -0.0080 -0.0010  0.0002  0.0000
                                    0.5901  0.0086  0.0026 -0.7853 -0.0101
                                   -0.0043 -0.1857 -0.0011 -0.0014  0.0001
                                   -0.0073  0.0057  0.0066  0.0034 -0.0039
                                    0.0046 -0.0051 -0.0029 -0.0040  0.0074
                                    0.0036
             ( 49.40%)   0.7028* C 33 s(  0.01%)p 1.00( 99.95%)d 0.00(  0.02%)
                                             f 0.00(  0.02%)
                                   -0.0001 -0.0090 -0.0010  0.0003  0.0000
                                    0.6161 -0.0010  0.0048 -0.7543  0.0008
                                   -0.0060 -0.2256  0.0006 -0.0013  0.0000
```

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                                    0.0072 -0.0057 -0.0105 -0.0032 -0.0053
                                    0.0053 -0.0065 -0.0011 -0.0049  0.0056
                                    0.0029
61. (1.97947) BD ( 1) C 27- C 28
             ( 50.32%)   0.7094* C 27 s( 36.94%)p 1.71( 62.99%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0000  0.6077  0.0102  0.0010  0.0001
                                   -0.4830  0.0007 -0.0012 -0.3829 -0.0002
                                   -0.0006 -0.4999  0.0060  0.0007  0.0119
                                    0.0151  0.0148  0.0005  0.0028  0.0028
                                   -0.0039 -0.0034 -0.0016 -0.0079  0.0022
                                   -0.0036
             ( 49.68%)   0.7048* C 28 s( 35.58%)p 1.81( 64.34%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0000  0.5965 -0.0013  0.0004 -0.0002
                                    0.4368 -0.0033  0.0000  0.4426 -0.0003
                                    0.0004  0.5067 -0.0018  0.0011  0.0133
                                    0.0155  0.0145  0.0006  0.0016 -0.0022
                                    0.0039  0.0033  0.0008  0.0073 -0.0027
                                    0.0029
62. (1.56511) BD ( 2) C 27- C 28
             ( 53.76%)   0.7332* C 27 s(  0.01%)p99.99( 99.96%)d 0.89(  0.01%)
                                             f 1.06(  0.02%)
                                   -0.0004 -0.0121 -0.0003  0.0000 -0.0002
                                    0.6730  0.0095  0.0029 -0.7317 -0.0108
                                   -0.0035 -0.1046 -0.0030  0.0008 -0.0020
                                   -0.0063  0.0058 -0.0071  0.0015 -0.0016
                                    0.0044 -0.0059  0.0026 -0.0023  0.0075
                                    0.0055
             ( 46.24%)   0.6800* C 28 s(  0.02%)p99.99( 99.94%)d 2.03(  0.03%)
                                             f 0.88(  0.01%)
                                    0.0004  0.0124  0.0023  0.0002  0.0000
                                    0.7627  0.0052  0.0042 -0.6356 -0.0056
                                   -0.0023 -0.1167  0.0016 -0.0010  0.0013
                                    0.0021 -0.0043  0.0172  0.0002 -0.0026
                                    0.0052 -0.0046  0.0028 -0.0026  0.0046
                                    0.0069
63. (1.97535) BD ( 1) C 28- C 29
             ( 50.55%)   0.7110* C 28 s( 30.54%)p 2.27( 69.42%)d 0.00(  0.03%)
                                             f 0.00(  0.01%)
                                   -0.0002  0.5526 -0.0010 -0.0003  0.0002
                                   -0.4762  0.0033  0.0028 -0.6154  0.0015
                                    0.0035  0.2976 -0.0110 -0.0005  0.0142
                                   -0.0047 -0.0077 -0.0050 -0.0055 -0.0016
                                    0.0007  0.0005 -0.0018  0.0034  0.0056
                                   -0.0023
             ( 49.45%)   0.7032* C 29 s( 28.73%)p 2.48( 71.19%)d 0.00(  0.08%)
                                             f 0.00(  0.00%)
                                    0.0003  0.5359  0.0099  0.0028 -0.0001
                                    0.4603 -0.0005  0.0005  0.6453  0.0019
                                    0.0012 -0.2889  0.0105  0.0005  0.0204
                                   -0.0088 -0.0130 -0.0068 -0.0085  0.0004
                                   -0.0016 -0.0020  0.0019 -0.0054 -0.0031
                                    0.0007
64. (1.98007) BD ( 1) C 28- C 30
             ( 50.14%)   0.7081* C 28 s( 33.81%)p 1.96( 66.13%)d 0.00(  0.06%)
                                             f 0.00(  0.01%)
                                    0.0000  0.5814  0.0035 -0.0004  0.0000
                                   -0.0118 -0.0082 -0.0010  0.1441 -0.0065
                                   -0.0013 -0.8002  0.0032 -0.0006 -0.0001
                                    0.0007 -0.0083 -0.0005  0.0221 -0.0084
                                   -0.0018  0.0034  0.0005 -0.0006 -0.0004
                                    0.0003
             ( 49.86%)   0.7061* C 30 s( 36.69%)p 1.72( 63.23%)d 0.00(  0.07%)
                                             f 0.00(  0.01%)
                                    0.0001  0.6057  0.0015  0.0030 -0.0003
                                    0.0989  0.0087  0.0006 -0.1115  0.0096
                                    0.0010  0.7809 -0.0067 -0.0025 -0.0007
                                    0.0052 -0.0056  0.0002  0.0255  0.0095
                                    0.0018 -0.0045 -0.0004  0.0001 -0.0001
                                    0.0004
65. (1.96933) BD ( 1) C 29- H 62
             ( 61.61%)   0.7849* C 29 s( 23.01%)p 3.34( 76.89%)d 0.00(  0.09%)
                                             f 0.00(  0.00%)
                                    0.0002 -0.4797  0.0054  0.0008  0.0001
                                   -0.4998 -0.0068  0.0001  0.5417 -0.0074
                                    0.0019 -0.4749  0.0027  0.0053  0.0178
                                   -0.0178  0.0164 -0.0023  0.0024  0.0017
                                    0.0002  0.0022 -0.0007  0.0060  0.0021
                                   -0.0004
             ( 38.39%)   0.6196* H 62 s( 99.93%)p 0.00(  0.06%)d 0.00(  0.01%)
                                   -0.9996 -0.0012 -0.0009  0.0116 -0.0159
                                    0.0157  0.0049 -0.0047  0.0052  0.0011
                                    0.0007
66. (1.98623) BD ( 1) C 29- H 63
             ( 60.49%)   0.7777* C 29 s( 23.92%)p 3.18( 75.97%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                    0.0001 -0.4891 -0.0039  0.0015 -0.0001
```

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                                     0.3398 -0.0029  0.0025  0.4583 -0.0049
                                     0.0053  0.6588  0.0080 -0.0033 -0.0096
                                    -0.0152 -0.0203  0.0031 -0.0150  0.0004
                                     0.0026  0.0030 -0.0020  0.0064  0.0005
                                    -0.0001
              ( 39.51%)   0.6286* H 63 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    -0.9998 -0.0005 -0.0005 -0.0102 -0.0143
                                    -0.0105 -0.0033 -0.0043 -0.0052  0.0013
                                    -0.0027
 67. (1.95588) BD ( 1) C 29- H 64
              ( 64.12%)   0.8008* C 29 s( 24.31%)p 3.11( 75.60%)d 0.00(  0.08%)
                                              f 0.00(  0.00%)
                                     0.0000 -0.4930  0.0067  0.0004  0.0000
                                     0.6493 -0.0012  0.0042 -0.2806 -0.0118
                                     0.0009 -0.5055 -0.0009  0.0052  0.0131
                                     0.0207 -0.0117 -0.0076 -0.0004  0.0015
                                     0.0026  0.0009 -0.0031  0.0049  0.0022
                                    -0.0004
              ( 35.88%)   0.5990* H 64 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                    -0.9995 -0.0036 -0.0015 -0.0223  0.0042
                                     0.0191  0.0032  0.0064 -0.0029 -0.0039
                                    -0.0004
 68. (1.98382) BD ( 1) C 30- C 31
              ( 49.90%)   0.7064* C 30 s( 37.35%)p 1.68( 62.57%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0001  0.6109  0.0172  0.0007  0.0001
                                     0.3682  0.0056 -0.0007  0.5414 -0.0015
                                    -0.0011 -0.4430  0.0263  0.0013  0.0150
                                    -0.0121 -0.0174 -0.0054 -0.0007  0.0034
                                     0.0024  0.0039  0.0029 -0.0072 -0.0047
                                     0.0014
              ( 50.10%)   0.7078* C 31 s( 37.20%)p 1.69( 62.71%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0000  0.6097  0.0163  0.0012  0.0000
                                    -0.3462  0.0182 -0.0002 -0.4919  0.0158
                                     0.0004  0.5143  0.0121 -0.0007  0.0130
                                    -0.0118 -0.0192 -0.0052  0.0043 -0.0034
                                    -0.0021 -0.0038 -0.0027  0.0079  0.0045
                                    -0.0015
 69. (1.65424) BD ( 2) C 30- C 31
              ( 51.58%)   0.7182* C 30 s(  0.01%)p99.99( 99.96%)d 1.37(  0.01%)
                                              f 1.40(  0.02%)
                                     0.0000  0.0104  0.0000  0.0000  0.0000
                                     0.7230  0.0050  0.0077 -0.6626 -0.0033
                                    -0.0058 -0.1943 -0.0015 -0.0015  0.0016
                                    -0.0029  0.0004  0.0117  0.0011 -0.0035
                                     0.0064 -0.0041 -0.0030 -0.0045  0.0038
                                     0.0063
              ( 48.42%)   0.6958* C 31 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.02%)
                                              f 0.00(  0.01%)
                                    -0.0001  0.0000 -0.0003  0.0000 -0.0001
                                     0.6938  0.0044  0.0062 -0.6928 -0.0042
                                    -0.0064 -0.1956 -0.0015 -0.0023 -0.0034
                                     0.0086 -0.0066 -0.0074 -0.0043 -0.0020
                                     0.0025 -0.0019 -0.0018 -0.0042  0.0072
                                     0.0079
 70. (1.97170) BD ( 1) C 30- H 49
              ( 60.63%)   0.7786* C 30 s( 25.92%)p 2.86( 74.00%)d 0.00(  0.08%)
                                              f 0.00(  0.01%)
                                     0.0005 -0.5088  0.0163  0.0040 -0.0001
                                     0.5752  0.0049 -0.0039  0.5042  0.0057
                                    -0.0040  0.3935 -0.0006 -0.0018 -0.0193
                                    -0.0144 -0.0130 -0.0016  0.0040 -0.0011
                                     0.0016  0.0000  0.0012  0.0052 -0.0049
                                     0.0052
              ( 39.37%)   0.6275* H 49 s( 99.93%)p 0.00(  0.07%)d 0.00(  0.01%)
                                    -0.9996 -0.0014 -0.0017 -0.0174 -0.0148
                                    -0.0128 -0.0056 -0.0042 -0.0037 -0.0003
                                     0.0014
 71. (1.98005) BD ( 1) C 31- C 32
              ( 50.22%)   0.7087* C 31 s( 36.81%)p 1.71( 63.10%)d 0.00(  0.07%)
                                              f 0.00(  0.01%)
                                     0.0001  0.6067  0.0017  0.0027 -0.0002
                                     0.5718 -0.0025 -0.0003  0.5251 -0.0038
                                    -0.0002  0.1679  0.0050  0.0008  0.0225
                                     0.0079  0.0065  0.0033 -0.0112 -0.0021
                                    -0.0037 -0.0037  0.0006  0.0034 -0.0054
                                     0.0071
              ( 49.78%)   0.7055* C 32 s( 34.35%)p 1.91( 65.58%)d 0.00(  0.06%)
                                              f 0.00(  0.01%)
                                     0.0000  0.5861  0.0056 -0.0002  0.0000
                                    -0.6120 -0.0036 -0.0019 -0.5138 -0.0025
                                    -0.0006 -0.1312 -0.0021 -0.0031  0.0208
                                     0.0041  0.0036  0.0021 -0.0113  0.0023
                                     0.0029  0.0027 -0.0010 -0.0033  0.0042
                                    -0.0066
 72. (1.97094) BD ( 1) C 31- H 50
              ( 60.57%)   0.7783* C 31 s( 25.94%)p 2.85( 73.98%)d 0.00(  0.07%)
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```
                                        f 0.00(  0.01%)
                                 0.0005 -0.5090  0.0156  0.0041 -0.0001
                                 0.2665 -0.0025 -0.0005  0.0363 -0.0040
                                 0.0013  0.8169  0.0091 -0.0061 -0.0015
                                -0.0135 -0.0014 -0.0020 -0.0236  0.0060
                                 0.0056 -0.0014  0.0015  0.0036 -0.0003
                                 0.0014
            ( 39.43%)   0.6279* H 50 s( 99.92%)p 0.00(  0.07%)d 0.00(  0.01%)
                                -0.9996 -0.0015 -0.0019 -0.0112 -0.0030
                                -0.0247 -0.0003 -0.0043 -0.0005 -0.0007
                                -0.0070
73. (1.97954) BD ( 1) C 32- C 33
            ( 49.67%)   0.7048* C 32 s( 35.24%)p 1.84( 64.70%)d 0.00(  0.06%)
                                        f 0.00(  0.01%)
                                 0.0000  0.5936  0.0076  0.0005 -0.0001
                                 0.3371  0.0085  0.0017  0.0903  0.0066
                                 0.0016  0.7246  0.0024  0.0004  0.0018
                                 0.0156  0.0029  0.0034  0.0175  0.0043
                                 0.0077  0.0017  0.0029  0.0025  0.0004
                                 0.0010
            ( 50.33%)   0.7094* C 33 s( 37.41%)p 1.67( 62.51%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                 0.0001  0.6115  0.0093  0.0015  0.0000
                                -0.3687 -0.0072 -0.0007 -0.1014 -0.0085
                                -0.0005 -0.6919  0.0075 -0.0007  0.0041
                                 0.0189  0.0054  0.0050  0.0169 -0.0053
                                -0.0087 -0.0018 -0.0034 -0.0018 -0.0004
                                -0.0011
74. (1.96538) BD ( 1) C 32- C 34
            ( 50.13%)   0.7080* C 32 s( 30.36%)p 2.29( 69.60%)d 0.00(  0.04%)
                                        f 0.00(  0.01%)
                                -0.0001  0.5509 -0.0098 -0.0007  0.0001
                                 0.2816 -0.0033 -0.0009  0.4561 -0.0073
                                -0.0022 -0.6390  0.0180  0.0049  0.0076
                                -0.0078 -0.0133 -0.0025  0.0080 -0.0009
                                 0.0017  0.0047  0.0022 -0.0043 -0.0024
                                 0.0012
            ( 49.87%)   0.7062* C 34 s( 27.19%)p 2.68( 72.76%)d 0.00(  0.05%)
                                        f 0.00(  0.00%)
                                 0.0003  0.5214 -0.0001  0.0008 -0.0001
                                -0.3015 -0.0084 -0.0015 -0.4759 -0.0081
                                -0.0012  0.6404 -0.0028 -0.0005  0.0073
                                -0.0104 -0.0158 -0.0036  0.0068  0.0000
                                -0.0007 -0.0034 -0.0003  0.0050 -0.0003
                                 0.0023
75. (1.96908) BD ( 1) C 33- H 51
            ( 60.59%)   0.7784* C 33 s( 25.89%)p 2.86( 74.03%)d 0.00(  0.07%)
                                        f 0.00(  0.01%)
                                -0.0005  0.5085 -0.0156 -0.0036  0.0001
                                 0.6711  0.0028 -0.0060  0.5382  0.0030
                                -0.0050  0.0126  0.0000 -0.0002  0.0232
                                 0.0008  0.0002  0.0041 -0.0120  0.0000
                                -0.0015 -0.0015  0.0016  0.0000 -0.0041
                                 0.0077
            ( 39.41%)   0.6278* H 51 s( 99.91%)p 0.00(  0.08%)d 0.00(  0.01%)
                                 0.9995  0.0024  0.0015 -0.0224 -0.0181
                                -0.0012  0.0069  0.0000 -0.0001  0.0013
                                -0.0039
76. (1.97272) BD ( 1) C 34- C 35
            ( 50.25%)   0.7089* C 34 s( 25.79%)p 2.88( 74.17%)d 0.00(  0.04%)
                                        f 0.00(  0.00%)
                                -0.0002 -0.5078 -0.0088 -0.0005 -0.0001
                                -0.3463  0.0188 -0.0011  0.4917  0.0094
                                 0.0023  0.6160 -0.0048 -0.0017  0.0075
                                 0.0084 -0.0137  0.0043 -0.0051  0.0001
                                -0.0007  0.0027  0.0003 -0.0047  0.0004
                                -0.0016
            ( 49.75%)   0.7053* C 35 s( 28.44%)p 2.51( 71.49%)d 0.00(  0.06%)
                                        f 0.00(  0.00%)
                                -0.0004 -0.5332 -0.0079 -0.0030  0.0000
                                 0.3491 -0.0070 -0.0021 -0.4753 -0.0041
                                 0.0017 -0.6059  0.0050  0.0004  0.0103
                                 0.0130 -0.0169  0.0028 -0.0058  0.0004
                                 0.0009 -0.0030  0.0001  0.0054 -0.0006
                                 0.0013
77. (1.97312) BD ( 1) C 34- C 36
            ( 50.30%)   0.7093* C 34 s( 25.85%)p 2.87( 74.11%)d 0.00(  0.04%)
                                        f 0.00(  0.00%)
                                 0.0002  0.5084  0.0089  0.0005  0.0001
                                -0.6148 -0.0092 -0.0013  0.5046 -0.0196
                                 0.0004 -0.3287  0.0014  0.0027 -0.0136
                                 0.0088 -0.0070  0.0046 -0.0050  0.0005
                                -0.0002 -0.0022  0.0004  0.0048  0.0004
                                 0.0021
            ( 49.70%)   0.7050* C 36 s( 28.43%)p 2.51( 71.50%)d 0.00(  0.06%)
                                        f 0.00(  0.00%)
                                 0.0004  0.5332  0.0079  0.0030  0.0000
                                 0.5960  0.0033 -0.0016 -0.5053  0.0083
```

```
                                    0.0021  0.3230 -0.0038  0.0007 -0.0183
                                    0.0108 -0.0095  0.0025 -0.0077 -0.0008
                                   -0.0003  0.0023  0.0000 -0.0052 -0.0010
                                   -0.0026
78. (1.96868) BD ( 1) C 34- H 52
             ( 60.77%)   0.7795* C 34 s( 21.14%)p 3.73( 78.79%)d 0.00(  0.06%)
                                             f 0.00(  0.00%)
                                   -0.0002  0.4596 -0.0155 -0.0019 -0.0001
                                    0.6403  0.0103  0.0007  0.5256  0.0085
                                    0.0030  0.3184  0.0036 -0.0066  0.0179
                                    0.0127  0.0102  0.0040 -0.0067 -0.0001
                                   -0.0002 -0.0025  0.0001  0.0045 -0.0004
                                    0.0023
             ( 39.23%)   0.6263* H 52 s( 99.90%)p 0.00(  0.09%)d 0.00(  0.01%)
                                    0.9995  0.0036  0.0016 -0.0210 -0.0188
                                   -0.0081  0.0076  0.0046  0.0036  0.0015
                                   -0.0029
79. (1.98581) BD ( 1) C 35- H 65
             ( 60.64%)   0.7787* C 35 s( 23.51%)p 3.25( 76.38%)d 0.00(  0.11%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.4848  0.0000 -0.0010  0.0000
                                    0.3344  0.0021  0.0028  0.5051 -0.0074
                                    0.0001 -0.6299 -0.0005 -0.0038  0.0126
                                   -0.0147 -0.0240 -0.0070  0.0087  0.0004
                                    0.0011  0.0042  0.0012 -0.0066 -0.0007
                                   -0.0016
             ( 39.36%)   0.6274* H 65 s( 99.97%)p 0.00(  0.02%)d 0.00(  0.01%)
                                    0.9999  0.0008  0.0006 -0.0065 -0.0076
                                    0.0113  0.0032 -0.0038 -0.0057 -0.0011
                                    0.0025
80. (1.98930) BD ( 1) C 35- H 66
             ( 60.37%)   0.7770* C 35 s( 23.93%)p 3.18( 75.97%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                    0.0000 -0.4891  0.0052  0.0010  0.0000
                                    0.5946 -0.0044 -0.0025  0.5252  0.0082
                                   -0.0009  0.3607  0.0077  0.0012 -0.0226
                                   -0.0145 -0.0131 -0.0048  0.0082 -0.0013
                                   -0.0001 -0.0022 -0.0002  0.0061 -0.0011
                                    0.0029
             ( 39.63%)   0.6295* H 66 s( 99.94%)p 0.00(  0.05%)d 0.00(  0.01%)
                                   -0.9997 -0.0021 -0.0005 -0.0120 -0.0161
                                   -0.0098 -0.0058 -0.0040 -0.0040 -0.0009
                                    0.0020
81. (1.98906) BD ( 1) C 35- H 67
             ( 61.00%)   0.7810* C 35 s( 24.09%)p 3.15( 75.80%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                    0.0000  0.4908 -0.0008 -0.0008  0.0000
                                    0.6415  0.0009  0.0001 -0.4917 -0.0021
                                    0.0000  0.3236 -0.0067 -0.0017 -0.0224
                                    0.0159 -0.0117  0.0058 -0.0083 -0.0012
                                   -0.0006  0.0025  0.0007 -0.0060 -0.0009
                                   -0.0034
             ( 39.00%)   0.6245* H 67 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                    0.9998  0.0004  0.0008 -0.0135  0.0125
                                   -0.0073 -0.0061  0.0040 -0.0028  0.0015
                                   -0.0028
82. (1.98900) BD ( 1) C 36- H 68
             ( 61.08%)   0.7816* C 36 s( 24.13%)p 3.14( 75.77%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                    0.0000 -0.4912  0.0009  0.0008  0.0000
                                    0.3365  0.0038  0.0004 -0.5148 -0.0027
                                   -0.0005 -0.6160  0.0055  0.0015  0.0121
                                    0.0146 -0.0230  0.0049 -0.0091  0.0006
                                    0.0011 -0.0037  0.0009  0.0062 -0.0008
                                    0.0013
             ( 38.92%)   0.6238* H 68 s( 99.95%)p 0.00(  0.04%)d 0.00(  0.01%)
                                   -0.9998 -0.0004 -0.0008 -0.0091  0.0108
                                    0.0142  0.0034  0.0039 -0.0063  0.0013
                                   -0.0017
83. (1.98929) BD ( 1) C 36- H 69
             ( 60.37%)   0.7770* C 36 s( 23.93%)p 3.17( 75.97%)d 0.00(  0.10%)
                                             f 0.00(  0.01%)
                                    0.0000 -0.4891  0.0052  0.0010  0.0000
                                    0.6455  0.0098 -0.0007  0.4694 -0.0065
                                   -0.0027  0.3501  0.0034  0.0007 -0.0220
                                   -0.0162 -0.0118 -0.0047  0.0087 -0.0013
                                   -0.0003 -0.0024  0.0009  0.0059 -0.0002
                                    0.0032
             ( 39.63%)   0.6295* H 69 s( 99.94%)p 0.00(  0.05%)d 0.00(  0.01%)
                                   -0.9997 -0.0021 -0.0005 -0.0192 -0.0086
                                   -0.0077 -0.0055 -0.0047 -0.0031 -0.0018
                                    0.0023
84. (1.98558) BD ( 1) C 36- H 70
             ( 60.64%)   0.7787* C 36 s( 23.48%)p 3.25( 76.41%)d 0.00(  0.11%)
                                             f 0.00(  0.01%)
                                   -0.0001  0.4845  0.0001 -0.0010  0.0000
                                    0.3371 -0.0071 -0.0007  0.5080  0.0022
                                    0.0038 -0.6263  0.0022 -0.0027  0.0131
```

```
                          -0.0165 -0.0232 -0.0035  0.0091  0.0005
                           0.0013  0.0042  0.0006 -0.0065 -0.0010
                          -0.0017
( 39.36%)   0.6274* H 70 s( 99.97%)p 0.00(  0.02%)d 0.00(  0.01%)
                           0.9999  0.0008  0.0006 -0.0046 -0.0097
                           0.0106  0.0032 -0.0036 -0.0058 -0.0015
                           0.0023
```

b) Computed IR Spectrum.

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
3.957159	0.000000	0.000000
24.518731	86.008353	0.528587
27.620198	10.559199	0.073103
31.896488	123.035941	0.983678
40.648074	14.323709	0.145940
45.557350	18.965284	0.216569
60.571308	0.299504	0.004547
61.530259	49.028868	0.756169
77.388191	0.054692	0.001061
103.136191	0.008157	0.000211
114.459918	68.166143	1.955691
124.394109	15.778622	0.491979
126.457614	0.180354	0.005717
131.530530	0.092325	0.003044
133.425841	19.952820	0.667302
147.402521	57.317554	2.117730
151.736235	4.864319	0.185008
152.774680	58.308362	2.232854
158.311259	0.334534	0.013275
186.041320	0.014256	0.000665
198.154184	41.261372	2.049392
208.139488	0.291773	0.015222
209.338531	83.889446	4.401843
218.410187	0.102910	0.005634
225.942984	43.284048	2.451347
229.663784	8.356290	0.481043
230.475571	89.226045	5.154596
231.369488	47.141986	2.733959
232.537234	93.982741	5.477958
246.052706	0.165153	0.010186
248.085941	18.213580	1.132597
262.299255	26.320032	1.730460
265.236552	21.449795	1.426049
265.496290	151.559344	10.086006
287.240482	0.017875	0.001287
306.062310	2.811993	0.215726
307.189893	62.726112	4.829847
321.974328	84.655666	6.832118
353.425162	0.009573	0.000848
365.184165	11.184019	1.023736
375.334607	0.121688	0.011448
376.714486	48.989632	4.625882
382.007158	0.747584	0.071583
383.031181	86.417818	8.296893
390.374113	0.025433	0.002489
401.481626	108.304532	10.899093
408.982950	13.720035	1.406496
430.236346	0.008895	0.000959
471.997565	0.005142	0.000608
479.000947	4.877678	0.585636
486.040500	0.002288	0.000279
525.962504	36.428176	4.802532
534.804902	0.004227	0.000567
541.903619	60.961477	8.280482
568.562966	0.028700	0.004090
591.177321	422.407707	62.593274
594.279928	0.555193	0.082702
604.105215	564.210921	85.434276
626.712111	1.792959	0.281654
631.364400	0.000366	0.000058
636.932597	0.002375	0.000379
649.784231	0.011341	0.001847
650.955695	160.019186	26.109681
657.851113	0.001416	0.000234
663.655770	28.579550	4.754188
671.421616	0.000976	0.000164
702.070691	0.356735	0.062778
702.270946	11.419175	2.010099
748.047857	33.485826	6.278682
748.804694	0.276822	0.051957
797.649742	105.903802	21.173949
801.259324	0.094766	0.019033
808.000339	74.689206	15.126814

809.762902	0.012985	0.002636
828.693665	0.019688	0.004089
833.431464	262.010198	54.735130
849.106992	0.008926	0.001900
888.574543	80.163889	17.854624
889.189373	8.667381	1.931791
897.718682	653.546111	147.060002
898.914909	9.561766	2.154442
899.855517	77.858903	17.561400
901.607111	6.451088	1.457902
913.910720	35.614930	8.158568
915.183591	0.842370	0.193236
917.087399	123.945758	28.491838
932.410740	0.827353	0.193364
932.548746	0.512641	0.119829
954.960477	9.375779	2.244248
956.145161	550.612258	131.961662
964.805976	0.209305	0.050617
965.794353	53.123919	12.860351
972.074331	0.091718	0.022348
978.629782	41.627583	10.211221
996.911864	0.086812	0.021693
1014.830139	136.860489	34.813646
1015.798675	1.833661	0.466879
1017.340752	2164.462350	551.943404
1023.225539	33.837807	8.678640
1023.417016	5.293755	1.357984
1029.302278	66.842465	17.245408
1034.317006	0.388742	0.100784
1042.380137	165.070461	43.129414
1043.078598	2.741142	0.716682
1084.946061	12.182403	3.312983
1084.969702	0.652321	0.177401
1088.597342	228.994288	62.484168
1089.223817	10.298457	2.811689
1113.672698	0.002360	0.000659
1129.016224	2.756228	0.779998
1132.364239	0.022260	0.006318
1137.870990	177.208771	50.542452
1174.406740	0.026442	0.007784
1175.332831	111.456479	32.835547
1197.659563	46.290406	13.896404
1197.842109	17.047030	5.118307
1216.072642	0.008795	0.002681
1219.537285	30.025295	9.178262
1248.218506	931.593625	291.470895
1248.532613	105.949277	33.157056
1287.650391	165.852455	53.530086
1287.808490	3.093206	0.998477
1297.510393	11.095499	3.608575
1297.516490	9.076021	2.951797
1305.245518	6.411582	2.097662
1305.690795	0.056169	0.018383
1341.441115	776.562061	261.111412
1341.518711	1179.126983	396.492871
1347.177080	2652.379406	895.650150
1347.929144	11.382631	3.845810
1348.198223	9.592623	3.241673
1356.167677	1.575842	0.535678
1368.036344	74.370877	25.502256
1368.360825	60.546291	20.766640
1368.480718	2.857088	0.980032
1368.864289	3.032240	1.040404
1372.825769	664.704949	228.729618
1373.418072	4.634440	1.595431
1393.256171	2129.058293	743.526750
1404.574579	0.002178	0.000767
1419.993348	26.453245	9.415499
1420.190095	0.632459	0.225142
1432.781907	1070.299756	384.382481
1434.500292	31.756098	11.418415
1437.489289	2030.058657	731.461166
1438.308011	2.137721	0.770692
1438.454985	5.132559	1.850582
1440.609495	7.187040	2.595221
1440.783055	6.140637	2.217635
1442.961368	18.209435	6.586114
1443.145950	26.541113	9.600801
1452.664107	3.221822	1.173126
1453.531455	153.417866	55.895705
1453.871476	24.749069	9.019095
1456.104674	310.521678	113.334619
1460.002188	370.470048	135.576581
1461.219752	6.815203	2.496160
1461.451223	85.496337	31.319146
1463.377400	1.048875	0.384732
1506.298554	0.012804	0.004834
1508.069939	59.865495	22.629561

1518.337588	0.009546	0.003633
1521.781565	0.352746	0.134553
1530.210644	0.013613	0.005221
1543.943085	601.770021	232.884136
1545.998023	0.058526	0.022680
1590.313613	68.979660	27.496784
1591.126679	0.636764	0.253958
1613.871257	1356.833226	548.874971
1720.957476	0.005070	0.002187
2895.843896	261.470666	189.791252
2897.172132	7.548230	5.481475
2950.280493	68.573578	50.710535
2950.602659	51.200010	37.866821
2951.372573	25.872227	19.139735
2951.717462	25.658629	18.983938
2953.577881	129.243572	95.683147
2953.794356	40.026005	29.634703
2956.792914	40.824767	30.256779
2957.013777	38.403841	28.464665
2994.985175	14.858904	11.154742
2995.358326	15.553179	11.677397
2999.545461	25.075946	18.853450
2999.696766	6.135884	4.613521
3015.368036	0.672878	0.508574
3015.678023	1.352423	1.022294
3020.503206	179.843879	136.161094
3020.885171	108.834053	82.409464
3029.576344	21.380721	16.236122
3029.645255	18.228580	13.842760
3031.119341	40.300577	30.619097
3032.198130	34.699197	26.372729
3046.321196	9.675777	7.388217
3046.764128	8.737854	6.673009
3051.829133	40.085551	30.663812
3051.913506	12.329564	9.431875
3056.939224	5.476059	4.195976
3056.967724	0.934868	0.716340
3057.972522	92.962388	71.255587
3058.010198	7.211122	5.527387
3080.566853	45.127697	34.845915
3080.643111	9.282411	7.167707
3154.836906	0.019333	0.015288
3154.911185	48.484068	38.341073

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

       5357.3849      49125.7366      53086.7972
-----------------------------------------------
         -0.3240         -0.7705          0.5490
         -0.3288         -0.4525         -0.8290
          0.8871         -0.4491         -0.1068


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	44.358	37.877	129.813	212.048
	Internal Energy (Kcal/mole):	0.889	0.889	374.641	376.418
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	130.259	136.221

```
****************************************************************************************************


================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
================================================================
```

Figure 1. Plot of the computed IR spectrum of **SQ1** in vacuum following the BP/TZ2P scheme.

c) Experimental IR spectrum of SQ1

Figure 2. ATR/TF-IR of neat crystalline SQ1 , full spectrum.

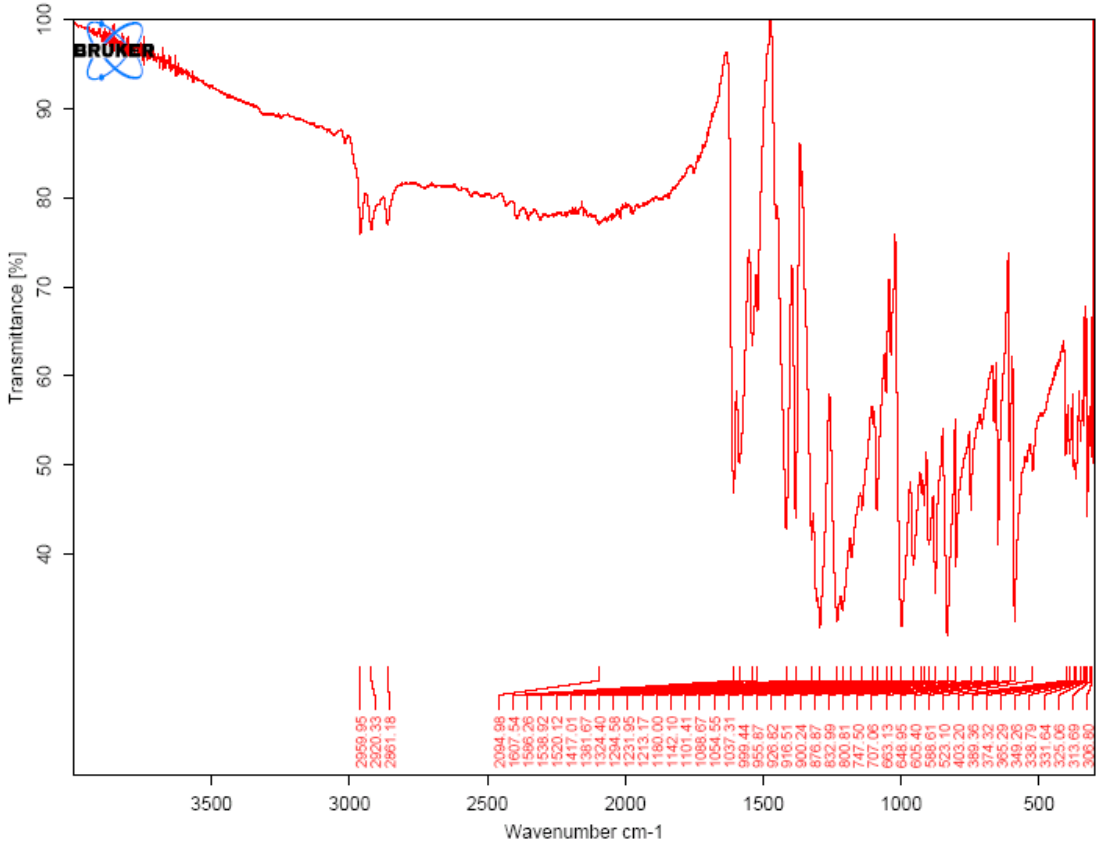
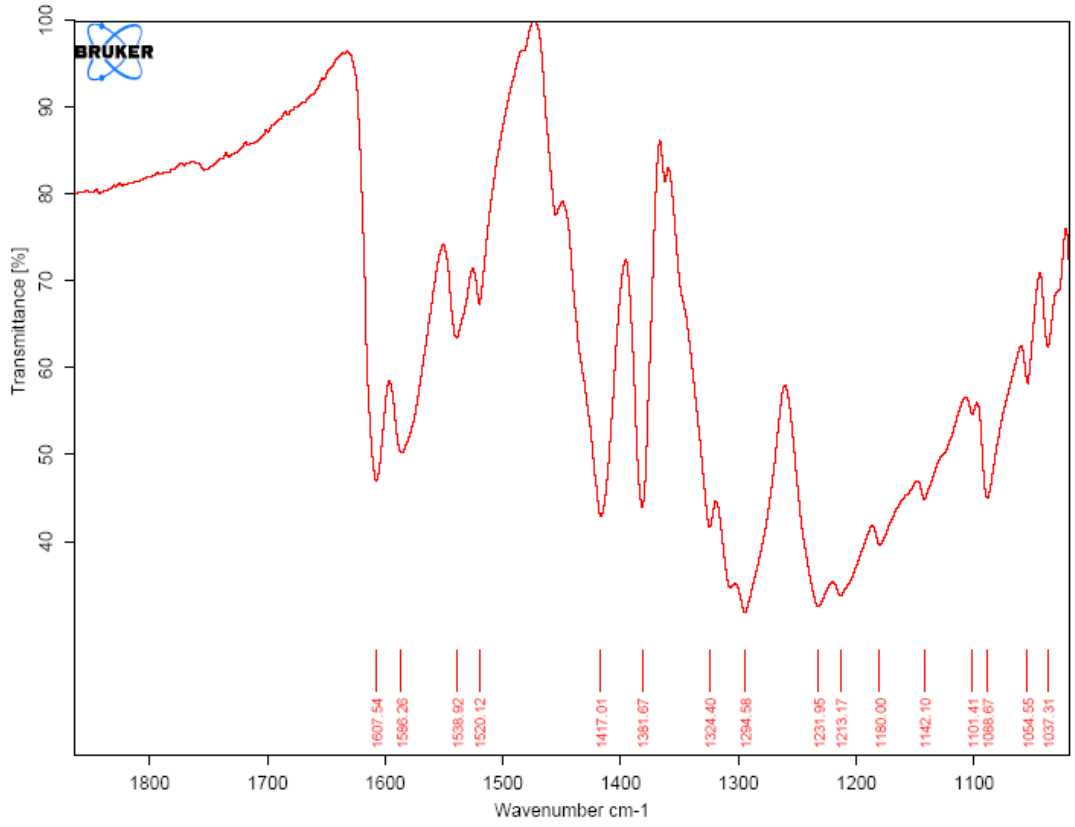


Figure 3. ATR/TF-IR of neat crystalline SQ1 , enlargement.



d) **SQ1**, COSMO CH_2Cl_2**,** Becke-Perdew/TZ2P level.

```
*****************************************************************************
 *                                                                           *
 *  ------------------------------------                                     *
 *   Amsterdam Density Functional  (ADF)         2008.01   September 22, 2008  *
 *  ------------------------------------                                     *
 *                                          Build 200901172115               *
 *                                                                           *
 *                                                                           *
 *                             =================                             *
 *                             |               |                             *
 *                             |     A D F     |                             *
 *                             |               |                             *
 *                             =================                             *
 *                                                                           *
 *                                                                           *
 *   Online information and documentation:  http://www.scm.com               *
 *   E-mail:  support@scm.com   info@scm.com                                 *
 *                                                                           *
 *   Scientific publications using ADF results must be properly referenced   *
 *   See the User Manuals (or the web site) for recommended citations        *
 *   The terms and conditions of the End User License Agreement apply to     *
 *   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
 *                                                                           *
 ************************  pentium64_linux / hpmpi  ***************************

 ADF 2008.01  RunTime: Apr14-2009 12:40:20

 Temporary files are created in /tmp/kid_0.P6nB3a

 squarain-iso1true_



 ============================
 A T T A C H E D   F I L E S
 ============================




 ==============================
 M O D E L   P A R A M E T E R S
 ==============================

 DENSITY FUNCTIONAL POTENTIAL (scf)
    LDA:                              VWN
    Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

 SPIN  (restricted / unrestr.)
    Molecule:                         Restricted
    Fragments:                        Restricted

 OTHER ASPECTS
    Relativistic Corrections:         ---
    Core Treatment:                   Frozen Orbital(s)

    Electric Field:                   ---

    Hyperfine or Zeeman Interaction:  ---

 SOLVATION
-------------------------------------------

  The Solvent-Excluding surface is calculated

       Division Level for Surface Triangles (NDIV)                3
       Final Division Level for Triangles (NFDIV)                 1
       Radius of the Solvent (RSOL)                         2.94000 angstr
       Minimum Radius for new sphere (RMINSOLV)             0.50000 angstr
       Overlapping Factor (OFAC)                            0.80000
       New spheres will be assigned to the initials using ASSG1

  Dielectric Constant (EPSL)                                8.90000

       COSMO equation is solved iteratively-              conjugate-gradient

       Maximun of Iterations for Charges (NCIX)                300
       Criterion for Charge convergence (CCNV)              1.0E-06

  Geometry-dependent empirical factor                       0.00000

  COSMO charges included variationally in SCF

       COSMO included at every SCF cycle
```

C-Matrix calculated in cspmtx

In cspmtx, C-Matrix calculated using fitted potential

Geometry CYCLE 13

==========

Energy gradients wrt nuclear displacements

==========

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000065	0.000164	0.000174
2	C	0.000429	-0.000572	-0.000164
3	C	0.000156	-0.000112	0.000299
4	C	-0.000079	0.000137	0.000034
5	C	-0.000065	-0.000219	0.000042
6	H	0.000056	-0.000005	-0.000007
7	C	-0.000065	0.000256	0.000007
8	C	-0.000111	0.000127	0.000079
9	H	0.000003	-0.000032	-0.000015
10	H	-0.000010	0.000014	0.000040
11	H	0.000038	-0.000088	-0.000062
12	C	0.000093	-0.000043	-0.000161
13	C	0.000187	0.000104	0.000107
14	C	-0.000099	0.000068	-0.000107
15	C	-0.000130	-0.000148	0.000141
16	C	-0.000227	0.000007	-0.000158
17	H	0.000051	0.000023	-0.000114
18	C	-0.000065	-0.000124	0.000074
19	H	-0.000182	-0.000191	0.000010
20	C	0.000101	-0.000025	0.000020
21	C	0.000166	-0.000114	-0.000037
22	H	0.000023	-0.000046	-0.000001
23	C	-0.000085	0.000115	0.000039
24	H	-0.000046	-0.000016	0.000029
25	C	0.000003	-0.000097	-0.000014
26	C	-0.000006	-0.000062	-0.000018
27	O	0.000312	-0.000427	-0.000204
28	C	-0.000583	0.000784	-0.000308
29	C	-0.000064	-0.000132	0.000108
30	C	0.000128	-0.000175	-0.000037
31	C	0.000044	0.000274	0.000126
32	H	-0.000046	0.000023	0.000030
33	C	-0.000231	-0.000043	-0.000201
34	C	-0.000074	-0.000148	-0.000051
35	H	0.000080	0.000001	0.000042
36	H	0.000066	0.000069	-0.000014
37	H	0.000016	0.000078	0.000008
38	C	0.000566	0.000152	-0.000082
39	C	-0.000525	-0.000023	-0.000134
40	C	0.000054	0.000254	0.000184
41	C	-0.000102	0.000021	-0.000040
42	C	0.000119	0.000012	-0.000005
43	H	0.000013	-0.000027	-0.000045
44	C	0.000000	0.000193	0.000112
45	H	0.000023	-0.000075	-0.000038
46	C	-0.000120	0.000063	-0.000017
47	C	0.000085	-0.000356	-0.000072
48	H	0.000013	0.000048	0.000041
49	C	-0.000131	0.000030	0.000010
50	H	-0.000004	0.000107	0.000030
51	C	-0.000042	-0.000004	0.000140
52	C	0.000063	-0.000031	-0.000088
53	H	0.000021	0.000027	0.000047
54	H	0.000044	0.000025	-0.000028
55	H	-0.000006	0.000018	0.000068
56	H	0.000001	0.000055	0.000015
57	H	0.000002	-0.000002	0.000050
58	H	0.000047	0.000051	0.000036
59	H	0.000138	0.000082	0.000064
60	H	-0.000036	0.000041	-0.000073
61	H	0.000074	0.000110	-0.000116
62	H	-0.000014	-0.000051	0.000063
63	H	-0.000038	0.000009	0.000068
64	H	0.000037	-0.000078	0.000157
65	H	0.000056	0.000040	-0.000037
66	H	-0.000110	-0.000094	0.000015
67	H	0.000026	-0.000065	0.000002
68	H	0.000043	0.000020	0.000022
69	H	-0.000007	0.000014	-0.000038
70	H	-0.000006	0.000006	-0.000048

```
-------------------------------------
Geometry Convergence after Step  13
-------------------------------------
current energy                              -16.05187912 Hartree
abs of energy change               0.00004282     0.00100000    T
constrained gradient max           0.00078119     0.00100000    T
constrained gradient rms           0.00014352     0.00066667    T
gradient max                       0.00078388
gradient rms                       0.00014354
cart. step max                     0.00729693     0.01000000    T
cart. step rms                     0.00228725     0.00666667    T


 About initial set of coordinates
 --------------------------------
 Number of spheres               =      70
 Number of TOTAL coord.          =      70

 about final set of coordinates
 ------------------------------
 ncor,nptsaf,npsurf=     225      60    2487


 ----------------------------------------
  COSMO surface
  Area             =         1876.190
  Volume           =         4136.226
  Number of Points =         2487
 ----------------------------------------

 Number of elements of the density matrix on this node (used, total):    138300   1107816



 ==================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ==================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   46896
    Points in the Atomic Polyhedra                389302
    Points in the Outer Region                     54465
    ------------------------------------------------------
    Total                                         490663

    Sum of Weights                                110649.827322

 Total nr. of points:     490663
 Nr. of blocks:             3834
 Block length:               128
 Nr. of dummy points:         89


 Test of Precision of the Numerical Integration Grid
 ==================================================

 Integral of the Total Core Density:                   0.00000000000000


============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.
```

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.100391796121301	4465.3989	102974.56	430845.52
Delta V^Pauli Coulomb:	-77.402381157060077	-2106.2260	-48570.73	-203219.92
Delta V^Pauli LDA-XC:	-21.617973468361093	-588.2550	-13565.48	-56757.98
Delta V^Pauli GGA-Exchange:	1.142407114108789	31.0865	716.87	2999.39
Delta V^Pauli GGA-Correlation:	-0.279786514489516	-7.6134	-175.57	-734.58
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	65.942657770319414	1794.3910	41379.65	173132.42
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	65.942657770319414	1794.3910	41379.65	173132.42
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-13.018089896992173	-354.2402	-8168.98	-34178.99
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	52.924567873327241	1440.1508	33210.67	138953.43
Orbital Interactions				
A:	-68.921378079200039	-1875.4461	-43248.82	-180953.05
Total Orbital Interactions:	-68.946231551451120	-1876.1224	-43264.42	-181018.31
Alternative Decomposition Orb.Int.				
Kinetic:	-148.985335915011206	-4054.0973	-93489.72	-391160.94
Coulomb:	73.994478078181501	2013.4922	46432.24	194272.47
XC:	6.044626285378516	164.4827	3793.06	15870.16
Total Orbital Interactions:	-68.946231551451191	-1876.1224	-43264.42	-181018.31
Residu (E=Steric+OrbInt+Res):	0.000067476699952	0.0018	0.04	0.18
Solvation Energy (el):	-0.037178458752535	-1.0117	-23.33	-97.61
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.006895534090559	0.1876	4.33	18.10
Total Bonding Energy:	-16.051879126085900	-436.7939	-10072.71	-42144.20

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.018089896992173	-354.2402	-8168.98	-34178.99
Kinetic Energy:	15.115055881110095	411.3016	9484.84	39684.57
Coulomb (Steric+OrbInt) Energy:	-3.407835602178622	-92.7319	-2138.45	-8947.27
XC Energy:	-14.710726583363304	-400.2992	-9231.12	-38623.01
Solvation:	-0.030282924661976	-0.8240	-19.00	-79.51
Total Bonding Energy:	-16.051879126085979	-436.7939	-10072.71	-42144.20

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): 0.0071025615
2. Electrostatic (Fit correction): 0.0000000000