Supporting Information for **"Thallophilic interactions and Tl-aryl π-interactions are competitive with cation-cation repulsion: $[LTl_2L]^{2+}$ dications as salts of weakly co-ordinating anions"**

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Experimental Details for Synthesis and Characterization of 1 and 2.

Experimental Section

The following compounds were prepared by literature methods: 2-isopropyl-*N*-[(3*E*)-3-(2-isopropylphenyl)imino-2-[*N*-(2-isopropylphenyl)-*C*-methyl-carbonimidoyl]-1-methyl-but-1-enyl]aniline, 2-isopropyl-*N*-[(*E*,3*E*)-3-(2-isopropylphenyl)imino-2-[*N*-(2-isopropylphenyl)-*C*-methyl-carbonimidoyl]-1,4,4-trimethyl-pent-1-enyl]aniline, 2-isopropyl-*N*-[(*E*,3*E*)-2-[*N*-(2-isopropylphenyl)-*C*-methyl-carbonimidoyl]-3-(2-methoxyphenyl)imino-1,4,4-trimethyl-pent-1-enyl]aniline, 2,4,6-trimethyl-*N*-[(3*E*)-1-methyl-2-[*C*-methyl-*N*-(2,4,6-trimethylphenyl)carbonimidoyl]-3-(2,4,6-trimethylphenyl)imino-but-1-enyl]aniline[1] and sodium *tetrakis*(*bis*-trifluoromethylphenyl)borate.[2] Other reagents were purchased from commercial vendors and used as received. Dichloromethane and hexane were used freshly distilled from calcium hydride and sodium-potassium alloy, respectively. Preparation of thallium *tetrakis*(*bis*-trifluoromethylphenyl)borate was done in air. Complex synthesis was conducted via Schlenk techniques under a nitrogen blanket. Once crystallized, complexes were briefly handleable in air. Elemental analyses were obtained from The University of Manchester Microanalytical Laboratory. CAUTION: all thallium reagents, products and wastes must be treated as highly poisonous, and collected for professional disposal.

Preparation of thallium *tetrakis*(*bis*-trifluoromethylphenyl)borate

This preparation was done in air. Na[BArF] (4.20 g, 4.46 mmol) was dissolved in acetone (20 mL). To this stirred solution was added a solution of $TlNO_3$ (1.12 g, 4.46 mmol) in acetone (5 mL) and water (15 mL). Some white solid precipitated. The mixture was slowly concentrated to 40% of its original volume by passage of nitrogen over its surface. The white solid product was Buchner filtered, washed with water and dried in air to yield 2.98 g (61.3%) of white powder Tl[BArF], mp.123-125 ˚C. Powder X-ray diffraction matched the pattern computed from published single crystal data, as did ^{1}H NMR {d 7.75 (s) , 7.60 (s)}.[2]

Complexes **1** and **2** were prepared by identical procedures: Details for **1**: 2-isopropyl-*N*-[(3*E*)-3-(2-isopropylphenyl)imino-2-[*N*-(2-isopropylphenyl)-*C*-methyl-carbonimidoyl]-1-methyl-but-1-enyl]aniline (0.227 g, 0.46 mmol) was placed in a Schlenk tube and dissolved in dichloromethane (20 mL). Solid Tl[BArF] (0.491 g, 0.46 mmol) was added to yield a yellow solution, which was stirred for 3 h prior to being filtered under nitrogen. The volume was then reduced by half *in vacuo*. Layering of the residue with hexane (20 mL) and standing at rt for 3 d gave crystals, isolated by filtration, of $[HC\{MeC{=}N(2\text{-}iPrC_6H_4)\}_3Tl]_2[BArF]_2.C_6H_{14}$, **1** (0.531 g, 72%). m.p. 162-163 ˚C. Elemental anal., calcd. for $C_{69}H_{62}N_3TlF_{24}B$ (%): C, 51.65; H, 3.90; N, 2.62. Found: C, 51.17; H, 3.75; N, 2.56. MS (MALDI) *m/z*: 696-699 $[(L)Tl]^+$, isotope abundances were consistent with gas-phase monomer ions. ^{1}H NMR (400 MHz, 295 K, $CDCl_3$): δ 1.39 (18H, br, apparent s (CH(C*H*$_3$)$_2$), 2.21 (9H, s, C*H*$_3$C=N), 2.82 (3H, br, apparent s, C*H*(CH$_3$)$_2$), 5.32 (1H, br s, α-C*H*), 6.6-7.4 (12H, br, complex m, aryl C*H*), 7.45 (4H, s, BArF *o*-C*H*), 7.62 (8H, s, BArF *p*-C*H*).

Compound **2** was prepared and characterized analogously. **2**: from 2-isopropyl-*N*-[(*E*,*3E*)-3-(2-isopropylphenyl)imino-2-[*N*-(2-isopropylphenyl)-*C*-methyl-carbonimidoyl]-1,4,4-trimethyl-pent-1-enyl]aniline (0.220 g, 0.41 mmol), yielded 0.38 g (57.7%) of $[HC\{MeC{=}N(2\text{-}iPrC_6H_4)\}_2tBuC{=}N(2\text{-}iPrC_6H_4)Tl]_2[BArF]_2$, **2**. m.p. = 168-170 ˚C. Elemental analysis, calcd. for $C_{69}H_{61}N_3TlF_{24}B$ (%): C, 51.59; H, 3.83; N, 2.61. Found: C, 50.48; H, 3.65; N, 2.48; Tl, 11.93. ^{1}H NMR (400 MHz, 295 K, $CDCl_3$): δ): δ 1.12-1.18 (9H, 3 overlapping d, CH(C*H*$_3$)$_2$), 1.20 (3H, d, CH(C*H*$_3$)$_2$), 1.23 (9H, s, C(C*H*$_3$)$_3$), 1.25-1.31 (6H, 2 overlapping d, CH(C*H*$_3$)$_2$), 2.33 (3H, s, C*H*$_3$C=N), 2.41 (3H, s, C*H*$_3$C=N), 2.48 (1H, septet, C*H*(CH$_3$)$_2$), 2.54 (1H, septet, C*H*(CH$_3$)$_2$), 2.63 (1H, septet, C*H*(CH$_3$)$_2$), 5.74 (1H, s, α-C*H*), 6.53 (1H, d, *o*-C*H*), 6.56 (1H, *o*-C*H*), 6.60 (1H, d, *o*-C*H*), 7.23-7.54 (9H, non-first-order m, other aromatic C*H*), 7.54 (4H, s, BArF$_4$ *p*-C*H*), 7.71 (8H, s, BArF$_4$ *o*-C*H*). ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.20 (s, BAr^F_4 C*F*$_3$).

Crystals were mounted in perfluoropolyether oil onto the goniometer of an Oxford Diffraction X-Calibur 2 diffractometer fitted with an Oxford Diffraction Cryostream 700. Reflections were collected using graphite-monochromated Mo-K_α radiation. Data were collected and processed by the programs CrysAlis PRO and CrysAlis RED,[3] and solved and refined using SHELXS and SHELXL.[4]

X-Ray Data Collection Summary Tabulated overleaf.

Table 1. X-ray data collection and refinement details

Compound	**1**	**2**
Formula	$C_{34}H_{43}N_3Tl$ $C_{32}H_{12}BF_{24}$ $(C_6H_{14})_{0.5}$	$C_{37}H_{49}N_3TlC$ $C_{32}H_{12}BF_{24}$
M_w	1604.41	1603.40
Crystal system	Triclinic	Triclinic
a/Å	12.8319(4)	14.8168(4)
b/Å	16.0697(5)	16.3174(7)
c/Å	17.3854(6)	16.4832(6)
α/°	98.692(3)	73.129(4)
β/°	105.005(3)	79.390(3)
γ/°	90.030(2)	63.442(3)
Space group	P-1	P-1
Z	2	2
Temp. (K)	120(2)	120(2)
μ/mm^{-1}	2.470	2.481
Reflns. measd.	24638	38437
Reflns. Obsd[a] (R_{int})	10498 (0.037)	15407 (0.036)
R_1(observed)	0.0346	0.0345
wR_2(all data)[b]	0.0611	0.0642

[a] $I = I > 2\sigma(I)$. [b] $wR_2 = \{\sigma[w(F_0^2 - F_c^2)^2]/\sigma[w(F_0^2)^2]\}^{1/2}$.

Discussion of Energetics of dimerization

A full CI treatment of all the electrons in such large systems will be required to accurately model the dispersive interactions responsible. We hope to have these results ready for a full-paper on this subject, via collaboration with our colleague Dr Joe MacDouall, but in lieu of this at present, and at the request of referees, it is possible to comment using simple electrostatics, literature values from analogous systems, and relatively inexpensive single-point calculations (9 hours on a PC) using the crystallographic geometry.

Using the graphical user interface Gaussview,[5] co-ordinates obtained from crystallographic cif files were input, minus anions and solvents of crystallization, to single-point energy calculations using Gaussian 09.[6] Both monomer cation and dimer dication crystallographic geometries were subjected to this total energy computation, at both Hartree-Fock-Self-Consistent Field (HF-SCF) and Density Functional (DF) levels, in both cases using a LANL2-DZ basis. It should be noted that Hartree-Fock contains no treatment of configuration interaction (CI), and DF contains only an indirect treatment of it. Accurate energies will have to wait for full all-electron treatments with CI. However, as a means to estimate the approximate charge on Tl+, in order to scale our estimates of coulombic repulsion, these methods should be adequate. To this end, we employed a Natural Population Analysis of charges,[7] which is known to give more realistic results than the crude Mulliken charge analysis, though both sets of data are presented for the reader. The results of these calculations are presented here as Table 2, and in the main text as table 1.

Table 2. Summary of computational results.

	$Tl_{q(M)}$	$Tl_{q(NPA)}$	*Energy /Hartrees*	ΔE_D /kcal mol^{-1}
HF-SCF				+ 47.4
Monomer	0.82	0.94	-1524.6289	
Dimer	0.84	0.87	-3049.18217	
DF-B3LYP				+39.9
Monomer	0.70	0.90	-1536.06077	
Dimer	0.65	0.82	-3072.05798	

Basis set: LANL2-DZ. $Tl_{q(M)}$ = Mulliken charge on Tl; $Tl_{q(NPA)}$ = Natural Population Analysis charge on Tl; ΔE_D = energy of dimerization, i.e. 2 x monomer energy – dimer energy.

The NPA charges are higher than the Mulliken charges, clustering around +0.9 across the methods and monomer/dimer range. They are systematically lower for dimer than for monomer, indicating the effect of π-aryl co-ordination, in all cases except the Mulliken DF-B3LYP case. This underlines the superiority of NPA charge analysis.[7] Taking the most conservative NPA estimate of true "Tl^+" charge, +0.82, the electrostatic repulsion between two such charges at the experimental Tl-Tl distance of 3.64 Å is calculated to be + 61.76 kcal mol^{-1}. The computed dimerization energies of the cation from **1** are +40 (B3-LYP) and +47 (SCF) kcal mol^{-1}. These smaller values (22 {B3-LYP} and 25{SCF} kcal mol^{-1} decreases) reflect the favourable effect of Tl-aryl interaction, which is modelled by these two methods. If one fully ascribes the decrease in repulsion to the effect of Tl-aryl attraction, this places a value of -11 to -12.5 kcal mol^{-1} per aryl, since there are two such interactions per dimer. This value lies within the lower part of the range found by others for such interactions.[8] However, these widely-used methods still fail to predict the formation of these dimers by some considerable margin. This failure is partially because of the single-point nature of the calculations, and partly because of the inability of SCF to model configuration interaction effects, only partially recovered by DF-B3LYP. Current understanding ascribes less than 10 kcal mol^{-1} to Tl-Tl attraction,[9] which leaves over 30 kcal mol^{-1} unaccounted for. The issue is ripe for investigation at the highest levels of theory not available to our computational resources. Either the assessment of the strength of Tl-Tl interactions is too low, the summation of multiple other small dispersive interactions in the crystal is unusually high in aggregate, or our dismissal of cation-diffuse anion interactions at distances approaching 6 Å is in error.

1 D. Barnes, G. L. Brown, M. Brownhill, I. German, C. J. Herbert, A. Jolleys, A. R. Kennedy, B. Liu, K. McBride, F. S. Mair, R. G. Pritchard, A. Sanders, J. E. Warren, *Eur. J. Inorg. Chem.* 2009, 1219.

2 H. Nishida, N. Takada, M. Yoshimura, *Bull. Chem. Soc. Jpn.* 1984, **57**, 2600.

3 *CrysAlis PRO and CrysAlis RED*, Oxford Diffraction Ltd, Abingdon, UK, 2007.

4 G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* 2008, **A64**, 112.

5 *GaussView, Version 5*, R. Dennington, T. Keith and J. Millam, *Semichem Inc*., Shawnee Mission KS, 2009.

6 *Gaussian 09, Revision B.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

7 A. E. Reed, R. B. Weinstock, F. Weinhold, *J. Chem. Phys.* 1985, **83** , 735–746.

8 T. Auel, E. L. Amma, *J. Am. Chem. Soc.*, 1968, **90**, 5941; H. Schmidbaur, W. Bublak, J. Riede, G. Müller, *Angew. Chem., Int. Ed. Engl.* 1985, **24**, 414; *Angew. Chem.* 1985, **97**, 402. Y. Sarazin, D. L. Hughes, N. Kaltsoyannis, J. A. Wright, M. Bochmann, *J. Am. Chem. Soc.* 2007, **129**, 881; Y. Sarazin, N. Kaltsoyannis, J. A. Wright, M. Bochmann, *Organometallics* 2007, **26**, 1881;

9 P. Pyykkö, M. Straka, T. Tamm, *Phys. Chem. Chem. Phys*. 1999, **1**, 3441; H. Schumann, C. Janiak, M. A. Khan and J. J. Zuckermann, *J. Organomet. Chem.* 1988, **354**, 7.

Appendix 1. Gaussian output for cation monomer, LANL2-DZ, HF-SCF.

Entering Link 1 = C:\G09W\l1.exe PID=   5392.

Cite this work as:
Gaussian 09, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
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P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

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Gaussian 09:  IA32W-G09RevB.01 12-Aug-2010
              15-Jan-2013
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# rhf/lanl2dz pop=npa geom=connectivity
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1/38=1,57=2/1;
2/12=2,17=6,18=5,40=1/2;
3/5=6,6=3,11=1,16=1,25=1,30=1,116=1/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1,40=-1/1,7;
99/5=1,9=1/99;
-----------------------
single-Point XRD Monomer
-----------------------
Symbolic Z-matrix:
Charge =  1 Multiplicity = 1
C                    -0.6205    11.0173   13.3488
H                    -1.1772    10.346    12.9002
C                    -0.7386    10.7853   14.8523
C                    -2.0146    10.1478   15.2951
H                    -2.0164    10.0668   16.2521
H                    -2.0905    9.2752    14.9004
H                    -2.7571    10.6899   15.0181
C                     0.1477    11.0887   17.0133
C                     0.985     10.2079   17.6933
C                     0.9712    10.2682   19.0865
C                     0.1757    11.1851   19.7698
C                    -0.6272    12.0471   19.0766
C                    -0.643     11.9981   17.6933
C                     1.8192    9.1837    16.9669
C                     1.2049    7.8117    17.0863
H                     1.2187    7.5343    18.0051
H                     1.706     7.1888    16.5556
H                     0.2964    7.8403    16.7745
C                     3.2525    9.155     17.4114
H                     3.6438    10.0232   17.287
H                     3.7359    8.5075    16.8939
H                     3.2939    8.9159    18.3418
C                    -1.123     12.3888   12.9283
C                    -1.6827    12.4638   11.5534
H                    -1.9518    13.3661   11.366
H                    -2.4428    11.8816   11.4854
H                    -1.0127    12.193    10.9198
C                    -1.289     14.7012   13.3745
C                    -2.2986    15.3891   14.0528
C                    -2.4429    16.7341   13.6979
C                    -1.6719    17.3532   12.804
C                    -0.6563    16.6662   12.1604
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C	-0.4748	15.3276	12.454
C	-3.1018	14.7409	15.1408
C	-4.5972	15.0605	15.0712
H	-4.7206	16.0118	15.0513
H	-5.0382	14.6958	15.8407
H	-4.9686	14.6725	14.2751
C	-2.5564	15.1673	16.5058
H	-1.6294	14.924	16.5705
H	-3.0515	14.7244	17.2008
H	-2.6467	16.1173	16.6053
C	0.8149	10.8036	12.8925
C	1.185	9.3929	12.5668
H	2.0832	9.368	12.2268
H	0.5821	9.0478	11.905
H	1.1288	8.8555	13.3612
C	2.9692	11.7205	12.532
C	3.4312	12.2928	11.3444
C	4.8043	12.3003	11.1454
C	5.6765	11.7802	12.0742
C	5.2031	11.2058	13.2236
C	3.8453	11.1763	13.4607
C	2.4476	12.825	10.3294
C	1.935	11.6972	9.4454
H	2.6628	11.3347	8.9346
H	1.2641	12.0378	8.8483
H	1.5553	11.0076	9.9944
C	3.0076	13.9575	9.4603
H	3.4149	14.6201	10.0242
H	2.2939	14.3599	8.9595
H	3.6632	13.6032	8.8566
H	1.5376	9.6958	19.6056
H	0.2777	11.1745	20.6986
H	-1.0785	12.5752	19.405
H	-1.1085	12.6356	17.1991
H	1.9153	9.4051	16.0879
H	-3.0335	17.0782	14.2137
H	-1.6683	18.2598	12.5386
H	-0.1278	17.0116	11.5932
H	0.1761	14.8424	12.0377
H	-3.0473	13.7776	15.0745
H	5.2053	12.7076	10.3908
H	6.5357	11.8968	11.8254
H	5.8118	10.8056	13.8323
H	3.5609	10.7602	14.2303
H	1.6499	13.1539	10.8187
N	0.2136	11.175	15.584
N	-0.9939	13.3524	13.7507
N	1.5756	11.8102	12.8487
Tl	1.3934	13.5394	14.8375

Stoichiometry C34H43N3Tl(1+)
Framework group C1[X(C34H43N3Tl)]
Deg. of freedom 237
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.018610	-0.083509	2.255965

2	1	0	0.004563	-0.122705	3.235795
3	6	0	1.475694	0.037251	1.819378
4	6	0	2.383293	0.678773	2.817058
5	1	0	3.268910	0.740388	2.450589
6	1	0	2.404998	0.148404	3.617819
7	1	0	2.060674	1.558898	3.024916
8	6	0	3.100261	-0.209698	0.131984
9	6	0	3.901979	-1.327516	-0.084833
10	6	0	5.120320	-1.118172	-0.730319
11	6	0	5.509287	0.147439	-1.163167
12	6	0	4.696747	1.225405	-0.948720
13	6	0	3.488421	1.047147	-0.297304
14	6	0	3.511043	-2.694884	0.415175
15	6	0	4.301631	-3.060222	1.646233
16	1	0	5.230767	-3.137415	1.418018
17	1	0	3.985941	-3.897280	1.993251
18	1	0	4.191528	-2.375482	2.311377
19	6	0	3.635796	-3.770424	-0.624249
20	1	0	3.091520	-3.546877	-1.383296
21	1	0	3.345446	-4.607581	-0.256005
22	1	0	4.554096	-3.843778	-0.899697
23	6	0	-0.819518	1.110863	1.830107
24	6	0	-1.963955	1.431667	2.722624
25	1	0	-2.448030	2.180175	2.366134
26	1	0	-1.635595	1.649364	3.597907
27	1	0	-2.549087	0.671305	2.778766
28	6	0	-1.338571	2.731076	0.193238
29	6	0	-0.817831	4.019156	0.044002
30	6	0	-1.657345	4.927439	-0.608713
31	6	0	-2.859380	4.613055	-1.091473
32	6	0	-3.350780	3.324906	-0.961731
33	6	0	-2.575807	2.384734	-0.308671
34	6	0	0.575307	4.362779	0.480037
35	6	0	0.677188	5.710898	1.197953
36	1	0	0.293384	6.396553	0.647347
37	1	0	1.598956	5.913988	1.367410
38	1	0	0.200933	5.664574	2.030595
39	6	0	1.507967	4.364168	-0.733490
40	1	0	1.482544	3.502822	-1.157927
41	1	0	2.406176	4.551802	-0.446567
42	1	0	1.224468	5.037208	-1.355743
43	6	0	-0.583107	-1.380062	1.735256
44	6	0	-0.367113	-2.582691	2.595582
45	1	0	-0.836795	-3.332532	2.221255
46	1	0	-0.695737	-2.407635	3.479846
47	1	0	0.571789	-2.782032	2.637478
48	6	0	-1.705379	-2.517673	-0.013464
49	6	0	-3.088728	-2.656069	-0.149691
50	6	0	-3.539864	-3.736897	-0.893565
51	6	0	-2.671563	-4.628305	-1.481231
52	6	0	-1.319113	-4.486814	-1.319917
53	6	0	-0.828045	-3.427120	-0.587380
54	6	0	-4.016761	-1.680893	0.534937
55	6	0	-4.239789	-2.088872	1.984061
56	1	0	-4.689360	-2.936869	2.012404
57	1	0	-4.778820	-1.426662	2.424024
58	1	0	-3.393081	-2.161062	2.430149
59	6	0	-5.365800	-1.509395	-0.173705
60	1	0	-5.216056	-1.346681	-1.108593
61	1	0	-5.836015	-0.764442	0.208441
62	1	0	-5.887201	-2.307161	-0.066446
63	1	0	5.705659	-1.852907	-0.918624

64	1	0	6.320426	0.169319	-1.626590
65	1	0	4.861412	1.941492	-1.173468
66	1	0	2.878627	1.747231	-0.224064
67	1	0	2.618643	-2.733005	0.597007
68	1	0	-1.222838	5.658391	-0.709589
69	1	0	-3.468463	5.144209	-1.580622
70	1	0	-4.101781	3.065483	-1.260104
71	1	0	-2.875714	1.530752	-0.193932
72	1	0	0.900886	3.712996	1.118076
73	1	0	-4.457959	-3.880782	-1.073882
74	1	0	-3.110430	-5.249296	-1.966502
75	1	0	-0.733023	-5.136672	-1.687849
76	1	0	0.084013	-3.377206	-0.477995
77	1	0	-3.558752	-0.802221	0.580520
78	7	0	1.779334	-0.372228	0.664361
79	7	0	-0.508284	1.706202	0.748331
80	7	0	-1.185303	-1.346835	0.626165
81	81	0	-0.088425	0.101083	-1.291919

Rotational constants (GHZ): 0.0954184 0.0934007 0.0606679
Standard basis: LANL2DZ (5D, 7F)
There are 437 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
437 basis functions, 1127 primitive gaussians, 439 cartesian basis functions
140 alpha electrons 140 beta electrons
nuclear repulsion energy 4616.8692399665 Hartrees.
NAtoms= 81 NActive= 81 NUniq= 81 SFac= 1.00D+00 NAtFMM= 50 NAOKFM=T Big=T
One-electron integrals computed using PRISM.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 38503 NPrTT= 272384 LenC2= 34176 LenP2D= 128614.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 437 RedAO= T NBF= 437
NBsUse= 437 1.00D-06 NBFU= 437
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 4.44D-02 ExpMax= 5.91D+03 ExpMxC= 2.05D+02 IAcc=2 IRadAn= 0 AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 0 IDoV= 1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Defaulting to unpruned grid for atomic number 81.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
Omega= 0.000000 0.000000 1.000000 0.000000 0.000000 ICntrl= 500 IOpCl= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
I1Cent= 4 NGrid= 0.
Petite list used in FoFCou.
Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RHF) = -1524.62886760 A.U. after 16 cycles
Convg = 0.3810D-08 -V/T = 2.0017

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.

Alpha occ. eigenvalues -- -15.69545 -15.69285 -15.69101 -11.44334 -11.44223
Alpha occ. eigenvalues -- -11.43735 -11.37944 -11.37357 -11.37327 -11.37219
Alpha occ. eigenvalues -- -11.33977 -11.33753 -11.33514 -11.32479 -11.32064
Alpha occ. eigenvalues -- -11.31928 -11.31902 -11.31387 -11.31285 -11.31262
Alpha occ. eigenvalues -- -11.31260 -11.31103 -11.31100 -11.31068 -11.31060
Alpha occ. eigenvalues -- -11.30857 -11.30792 -11.30619 -11.30582 -11.30572
Alpha occ. eigenvalues -- -11.29419 -11.26193 -11.25949 -11.25591 -11.25401
Alpha occ. eigenvalues -- -11.25323 -11.25024 -1.41927 -1.39225 -1.38938
Alpha occ. eigenvalues -- -1.28124 -1.27090 -1.26666 -1.21741 -1.21054
Alpha occ. eigenvalues -- -1.20509 -1.20309 -1.17484 -1.17114 -1.14115
Alpha occ. eigenvalues -- -1.13713 -1.13025 -1.12749 -1.11977 -1.11663
Alpha occ. eigenvalues -- -1.10627 -1.07323 -1.06999 -1.06985 -0.99357
Alpha occ. eigenvalues -- -0.99083 -0.98373 -0.98132 -0.97720 -0.96418
Alpha occ. eigenvalues -- -0.93971 -0.93813 -0.93556 -0.93541 -0.93330
Alpha occ. eigenvalues -- -0.91881 -0.91737 -0.91528 -0.90574 -0.89648
Alpha occ. eigenvalues -- -0.87661 -0.83521 -0.82815 -0.81142 -0.80511
Alpha occ. eigenvalues -- -0.79922 -0.79492 -0.77967 -0.77832 -0.76928
Alpha occ. eigenvalues -- -0.76663 -0.76349 -0.75988 -0.75099 -0.74892
Alpha occ. eigenvalues -- -0.74232 -0.73834 -0.73399 -0.72880 -0.72734
Alpha occ. eigenvalues -- -0.72427 -0.72202 -0.72082 -0.71584 -0.71145
Alpha occ. eigenvalues -- -0.70201 -0.68661 -0.68591 -0.68470 -0.68152
Alpha occ. eigenvalues -- -0.67660 -0.67445 -0.66973 -0.66730 -0.66665
Alpha occ. eigenvalues -- -0.65740 -0.65367 -0.64690 -0.63686 -0.63224
Alpha occ. eigenvalues -- -0.62087 -0.61281 -0.60909 -0.59962 -0.59119
Alpha occ. eigenvalues -- -0.58794 -0.58367 -0.57466 -0.57360 -0.57085
Alpha occ. eigenvalues -- -0.56855 -0.56291 -0.56121 -0.55100 -0.55014
Alpha occ. eigenvalues -- -0.53526 -0.53186 -0.53081 -0.45946 -0.43689
Alpha occ. eigenvalues -- -0.43298 -0.42519 -0.41720 -0.41446 -0.41255
Alpha virt. eigenvalues -- -0.02736 -0.02372 -0.00452 0.01295 0.01504
Alpha virt. eigenvalues -- 0.03098 0.03794 0.03870 0.03966 0.05549
Alpha virt. eigenvalues -- 0.05978 0.06600 0.11562 0.11930 0.12774
Alpha virt. eigenvalues -- 0.13722 0.14395 0.14422 0.16184 0.16612
Alpha virt. eigenvalues -- 0.16863 0.17218 0.17642 0.18091 0.18348
Alpha virt. eigenvalues -- 0.18696 0.18880 0.19058 0.19499 0.19565
Alpha virt. eigenvalues -- 0.19928 0.20146 0.20311 0.20908 0.21213
Alpha virt. eigenvalues -- 0.21740 0.22049 0.22250 0.22456 0.22849
Alpha virt. eigenvalues -- 0.23141 0.23363 0.23832 0.23875 0.24281
Alpha virt. eigenvalues -- 0.24565 0.24890 0.25247 0.25392 0.25560
Alpha virt. eigenvalues -- 0.26377 0.27100 0.27309 0.27702 0.28159
Alpha virt. eigenvalues -- 0.28739 0.28842 0.29696 0.29806 0.30299
Alpha virt. eigenvalues -- 0.30742 0.31244 0.31522 0.31778 0.31966
Alpha virt. eigenvalues -- 0.32312 0.33151 0.33385 0.34016 0.34154
Alpha virt. eigenvalues -- 0.34673 0.34779 0.35086 0.35281 0.35514
Alpha virt. eigenvalues -- 0.36047 0.36135 0.36621 0.37009 0.37104
Alpha virt. eigenvalues -- 0.38370 0.38382 0.38949 0.39181 0.39305
Alpha virt. eigenvalues -- 0.39500 0.39885 0.40070 0.40177 0.40630
Alpha virt. eigenvalues -- 0.40916 0.41405 0.41631 0.41905 0.42286
Alpha virt. eigenvalues -- 0.42513 0.42735 0.43150 0.43948 0.44300

```
Alpha virt. eigenvalues --    0.44547   0.45218   0.45458   0.45982   0.46454
Alpha virt. eigenvalues --    0.46649   0.46757   0.47255   0.47571   0.48182
Alpha virt. eigenvalues --    0.48561   0.48734   0.48913   0.49184   0.50141
Alpha virt. eigenvalues --    0.50355   0.50661   0.51151   0.51420   0.51739
Alpha virt. eigenvalues --    0.52270   0.52466   0.52729   0.53259   0.53498
Alpha virt. eigenvalues --    0.53976   0.54228   0.54569   0.55183   0.55344
Alpha virt. eigenvalues --    0.55793   0.55947   0.56197   0.56838   0.57395
Alpha virt. eigenvalues --    0.58106   0.58454   0.58770   0.59335   0.59673
Alpha virt. eigenvalues --    0.60028   0.60252   0.60920   0.61373   0.61910
Alpha virt. eigenvalues --    0.62093   0.62406   0.63021   0.63317   0.63686
Alpha virt. eigenvalues --    0.63894   0.64574   0.65034   0.65305   0.65509
Alpha virt. eigenvalues --    0.66736   0.67001   0.67135   0.67858   0.68215
Alpha virt. eigenvalues --    0.69072   0.69173   0.69894   0.70818   0.71558
Alpha virt. eigenvalues --    0.71933   0.72435   0.72933   0.73266   0.74107
Alpha virt. eigenvalues --    0.74307   0.74901   0.75413   0.75824   0.76353
Alpha virt. eigenvalues --    0.77226   0.77709   0.77920   0.78343   0.78798
Alpha virt. eigenvalues --    0.79022   0.80260   0.81273   0.81736   0.82644
Alpha virt. eigenvalues --    0.83736   0.84433   0.85352   0.86764   0.86915
Alpha virt. eigenvalues --    0.88273   0.89170   0.90176   0.90595   0.91465
Alpha virt. eigenvalues --    0.93717   0.94819   0.95354   0.95968   0.96578
Alpha virt. eigenvalues --    0.97356   0.98828   1.00323   1.00829   1.01930
Alpha virt. eigenvalues --    1.04415   1.04479   1.05394   1.05939   1.13032
Alpha virt. eigenvalues --    1.13831   1.14686   1.17587   1.18373   1.23972
Alpha virt. eigenvalues --    1.24588   1.25440   1.26996   1.27585   1.27857
Alpha virt. eigenvalues --    1.28825   1.31907   1.33103   1.34478   1.36889
Alpha virt. eigenvalues --    1.37397   1.38345   1.39133   1.40599   1.42132
Alpha virt. eigenvalues --    1.42695   1.43771   1.44109   1.44984   1.45663
Alpha virt. eigenvalues --    1.45963   1.46506   1.47093   1.47675   1.48510
Alpha virt. eigenvalues --    1.48962   1.49275   1.49960   1.50386   1.51142
Alpha virt. eigenvalues --    1.51934   1.52118   1.52891   1.53755   1.54182
Alpha virt. eigenvalues --    1.54510   1.54622   1.55066   1.56019   1.56282
Alpha virt. eigenvalues --    1.56775   1.57257   1.58125   1.59143   1.59282
Alpha virt. eigenvalues --    1.61028   1.61423   1.62270   1.62566   1.63915
Alpha virt. eigenvalues --    1.64459   1.65200   1.65467   1.66487   1.67284
Alpha virt. eigenvalues --    1.68403   1.68864   1.69926   1.71444   1.73576
Alpha virt. eigenvalues --    1.74680   1.76389   1.76662   1.77593   1.78656
Alpha virt. eigenvalues --    1.80414   1.81018   1.82436   1.84041   1.85190
Alpha virt. eigenvalues --    1.87574   1.88229   1.90183   1.92322   1.93228
Alpha virt. eigenvalues --    1.94952   1.97738   2.05464   2.08247   2.09727
Alpha virt. eigenvalues --    2.19730  10.97937
         Condensed to atoms (all electrons):
Mulliken atomic charges:
              1
     1  C   -0.266456
     2  H    0.247055
     3  C    0.225093
     4  C   -0.671943
     5  H    0.269294
     6  H    0.239787
     7  H    0.236633
     8  C    0.126187
     9  C    0.243147
    10  C   -0.364006
    11  C   -0.280345
    12  C   -0.389328
    13  C   -0.362305
    14  C   -0.207258
    15  C   -0.599509
    16  H    0.209296
    17  H    0.201303
    18  H    0.190710
    19  C   -0.615455
```

20	H	0.200198
21	H	0.203899
22	H	0.199163
23	C	0.248978
24	C	-0.681640
25	H	0.269910
26	H	0.245898
27	H	0.239839
28	C	0.129140
29	C	0.180959
30	C	-0.327214
31	C	-0.258605
32	C	-0.316622
33	C	-0.413412
34	C	-0.214630
35	C	-0.610529
36	H	0.197190
37	H	0.208723
38	H	0.207377
39	C	-0.601501
40	H	0.190155
41	H	0.202924
42	H	0.212686
43	C	0.239420
44	C	-0.674115
45	H	0.267285
46	H	0.240904
47	H	0.241408
48	C	0.162305
49	C	0.207318
50	C	-0.350868
51	C	-0.284701
52	C	-0.241217
53	C	-0.390864
54	C	-0.181342
55	C	-0.605355
56	H	0.217240
57	H	0.207211
58	H	0.185245
59	C	-0.628158
60	H	0.209962
61	H	0.210354
62	H	0.200921
63	H	0.261147
64	H	0.268813
65	H	0.431286
66	H	0.280742
67	H	0.217869
68	H	0.313502
69	H	0.263980
70	H	0.340896
71	H	0.303098
72	H	0.198037
73	H	0.267410
74	H	0.291434
75	H	0.265628
76	H	0.305115
77	H	0.180429
78	N	-0.442773
79	N	-0.465629
80	N	-0.478739
81	Tl	0.820015

Sum of Mulliken atomic charges = 1.00000
Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.019401
3	C	0.225093
4	C	0.073771
8	C	0.126187
9	C	0.243147
10	C	-0.102859
11	C	-0.011533
12	C	0.041958
13	C	-0.081563
14	C	0.010610
15	C	0.001801
19	C	-0.012195
23	C	0.248978
24	C	0.074007
28	C	0.129140
29	C	0.180959
30	C	-0.013712
31	C	0.005376
32	C	0.024274
33	C	-0.110314
34	C	-0.016593
35	C	0.002761
39	C	0.004264
43	C	0.239420
44	C	0.075482
48	C	0.162305
49	C	0.207318
50	C	-0.083458
51	C	0.006733
52	C	0.024411
53	C	-0.085749
54	C	-0.000913
55	C	0.004340
59	C	-0.006921
78	N	-0.442773
79	N	-0.465629
80	N	-0.478739
81	Tl	0.820015

Sum of Mulliken charges with hydrogens summed into heavy atoms = 1.00000
Electronic spatial extent (au): <R**2>= 18936.9244
Charge= 1.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -0.5128 Y= -0.4836 Z= 4.8570 Tot= 4.9079
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -195.1178 YY= -196.9825 ZZ= -216.2439
XY= 1.2165 XZ= 0.7221 YZ= -0.6321
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= 7.6636 YY= 5.7989 ZZ= -13.4625
XY= 1.2165 XZ= 0.7221 YZ= -0.6321
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -7.0397 YYY= 39.2490 ZZZ= -83.2349 XYY= -13.2635
XXY= -33.6174 XXZ= -93.8708 XZZ= -7.0497 YZZ= -0.2137
YYZ= -92.1043 XYZ= -0.7789
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -10506.0357 YYYY= -10422.7625 ZZZZ= -2657.5802 XXXY= 3.2769
XXXZ= -146.3972 YYYX= 53.9765 YYYZ= 15.4714 ZZZX= 25.3350
ZZZY= -14.9586 XXYY= -3455.9526 XXZZ= -2328.5186 YYZZ= -2262.0642
XXYZ= -30.5064 YYXZ= 168.1106 ZZXY= 11.5951
N-N= 4.616869239966D+03 E-N=-1.277307290042D+04 KE= 1.521968359954D+03

```
******************************Gaussian NBO Version 3.1******************************
      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
******************************Gaussian NBO Version 3.1******************************
 /RESON  / : Allow strongly delocalized NBO set

Analyzing the SCF density

Job title: single-Point XRD Monomer

Storage needed:    593108 in NPA (  33535799 available)


NATURAL POPULATIONS:  Natural atomic orbital occupancies

 NAO  Atom  No  lang   Type(AO)    Occupancy      Energy
---------------------------------------------------------
   1    C    1  S      Cor( 1S)     1.99896     -11.21738
   2    C    1  S      Val( 2S)     0.96255      -0.31219
   3    C    1  S      Ryd( 3S)     0.00100       1.63271
   4    C    1  px     Val( 2p)     1.07737      -0.20803
   5    C    1  px     Ryd( 3p)     0.00807       0.57089
   6    C    1  py     Val( 2p)     1.07383      -0.20718
   7    C    1  py     Ryd( 3p)     0.00748       0.55266
   8    C    1  pz     Val( 2p)     1.18308      -0.16343
   9    C    1  pz     Ryd( 3p)     0.02144       0.65750

  10    H    2  S      Val( 1S)     0.79434       0.13612
  11    H    2  S      Ryd( 2S)     0.00191       1.15690

  12    C    3  S      Cor( 1S)     1.99916     -11.29624
  13    C    3  S      Val( 2S)     0.85968      -0.24218
  14    C    3  S      Ryd( 3S)     0.00596       1.15904
  15    C    3  px     Val( 2p)     0.96022      -0.14022
  16    C    3  px     Ryd( 3p)     0.00816       0.70730
  17    C    3  py     Val( 2p)     0.79030      -0.13731
  18    C    3  py     Ryd( 3p)     0.00914       0.58202
  19    C    3  pz     Val( 2p)     0.87105      -0.07736
  20    C    3  pz     Ryd( 3p)     0.00732       0.62595

  21    C    4  S      Cor( 1S)     1.99921     -11.13375
  22    C    4  S      Val( 2S)     1.02185      -0.24205
  23    C    4  S      Ryd( 3S)     0.00051       1.32559
  24    C    4  px     Val( 2p)     1.18848      -0.14567
  25    C    4  px     Ryd( 3p)     0.00396       0.35355
  26    C    4  py     Val( 2p)     1.19978      -0.13893
  27    C    4  py     Ryd( 3p)     0.00212       0.35801
  28    C    4  pz     Val( 2p)     1.16897      -0.14591
  29    C    4  pz     Ryd( 3p)     0.00314       0.31548

  30    H    5  S      Val( 1S)     0.78586       0.17085
  31    H    5  S      Ryd( 2S)     0.00153       1.06392

  32    H    6  S      Val( 1S)     0.79377       0.14916
  33    H    6  S      Ryd( 2S)     0.00120       1.00152

  34    H    7  S      Val( 1S)     0.79380       0.14750
  35    H    7  S      Ryd( 2S)     0.00122       1.00289

  36    C    8  S      Cor( 1S)     1.99890     -11.22543
  37    C    8  S      Val( 2S)     0.84327      -0.16910
  38    C    8  S      Ryd( 3S)     0.00199       1.31378
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39	C	8	px	Val(2p)	0.88265	-0.06270
40	C	8	px	Ryd(3p)	0.00908	0.72071
41	C	8	py	Val(2p)	1.08277	-0.12648
42	C	8	py	Ryd(3p)	0.00547	0.63369
43	C	8	pz	Val(2p)	1.02612	-0.15413
44	C	8	pz	Ryd(3p)	0.01292	0.69144
45	C	9	S	Cor(1S)	1.99908	-11.18601
46	C	9	S	Val(2S)	0.89508	-0.18953
47	C	9	S	Ryd(3S)	0.00180	1.35160
48	C	9	px	Val(2p)	1.04707	-0.10842
49	C	9	px	Ryd(3p)	0.00697	0.67599
50	C	9	py	Val(2p)	1.05966	-0.10895
51	C	9	py	Ryd(3p)	0.01012	0.82766
52	C	9	pz	Val(2p)	0.99358	-0.12068
53	C	9	pz	Ryd(3p)	0.00780	0.63466
54	C	10	S	Cor(1S)	1.99920	-11.15647
55	C	10	S	Val(2S)	0.93906	-0.18289
56	C	10	S	Ryd(3S)	0.00094	1.22377
57	C	10	px	Val(2p)	1.08212	-0.07507
58	C	10	px	Ryd(3p)	0.00684	0.48508
59	C	10	py	Val(2p)	1.11698	-0.06049
60	C	10	py	Ryd(3p)	0.00537	0.61584
61	C	10	pz	Val(2p)	1.00490	-0.12198
62	C	10	pz	Ryd(3p)	0.00405	0.49701
63	C	11	S	Cor(1S)	1.99931	-11.15560
64	C	11	S	Val(2S)	0.94223	-0.16763
65	C	11	S	Ryd(3S)	0.00072	1.12297
66	C	11	px	Val(2p)	1.11283	-0.02777
67	C	11	px	Ryd(3p)	0.00673	0.47259
68	C	11	py	Val(2p)	1.04021	-0.07277
69	C	11	py	Ryd(3p)	0.00437	0.52064
70	C	11	pz	Val(2p)	1.02244	-0.09622
71	C	11	pz	Ryd(3p)	0.00486	0.47475
72	C	12	S	Cor(1S)	1.99872	-11.11016
73	C	12	S	Val(2S)	0.87779	-0.00910
74	C	12	S	Ryd(3S)	0.00040	1.12823
75	C	12	px	Val(2p)	1.04444	-0.08636
76	C	12	px	Ryd(3p)	0.00447	0.51413
77	C	12	py	Val(2p)	1.11242	0.09671
78	C	12	py	Ryd(3p)	0.00652	0.41551
79	C	12	pz	Val(2p)	1.00473	-0.10405
80	C	12	pz	Ryd(3p)	0.00491	0.46092
81	C	13	S	Cor(1S)	1.99919	-11.15959
82	C	13	S	Val(2S)	0.93244	-0.17220
83	C	13	S	Ryd(3S)	0.00092	1.28742
84	C	13	px	Val(2p)	1.09047	-0.07805
85	C	13	px	Ryd(3p)	0.00466	0.58451
86	C	13	py	Val(2p)	1.10737	-0.06218
87	C	13	py	Ryd(3p)	0.00884	0.54655
88	C	13	pz	Val(2p)	1.03829	-0.14522
89	C	13	pz	Ryd(3p)	0.00495	0.54949
90	C	14	S	Cor(1S)	1.99909	-11.13930
91	C	14	S	Val(2S)	0.92314	-0.16236
92	C	14	S	Ryd(3S)	0.00053	1.64593
93	C	14	px	Val(2p)	1.13334	-0.02294
94	C	14	px	Ryd(3p)	0.00984	0.55464

95	C	14	py	Val(2p)	1.01270	-0.09143
96	C	14	py	Ryd(3p)	0.00543	0.56238
97	C	14	pz	Val(2p)	1.02795	-0.09423
98	C	14	pz	Ryd(3p)	0.00431	0.56337
99	C	15	S	Cor(1S)	1.99932	-11.08290
100	C	15	S	Val(2S)	1.00987	-0.16901
101	C	15	S	Ryd(3S)	0.00064	1.28743
102	C	15	px	Val(2p)	1.18042	-0.07724
103	C	15	px	Ryd(3p)	0.00201	0.33307
104	C	15	py	Val(2p)	1.20271	-0.07056
105	C	15	py	Ryd(3p)	0.00330	0.38084
106	C	15	pz	Val(2p)	1.11491	-0.08250
107	C	15	pz	Ryd(3p)	0.00395	0.37799
108	H	16	S	Val(1S)	0.81826	0.19352
109	H	16	S	Ryd(2S)	0.00159	1.00540
110	H	17	S	Val(1S)	0.81945	0.19349
111	H	17	S	Ryd(2S)	0.00140	0.99496
112	H	18	S	Val(1S)	0.82757	0.18175
113	H	18	S	Ryd(2S)	0.00152	1.03787
114	C	19	S	Cor(1S)	1.99933	-11.07868
115	C	19	S	Val(2S)	1.00709	-0.16404
116	C	19	S	Ryd(3S)	0.00060	1.28919
117	C	19	px	Val(2p)	1.21549	-0.07256
118	C	19	px	Ryd(3p)	0.00265	0.37443
119	C	19	py	Val(2p)	1.14049	-0.07671
120	C	19	py	Ryd(3p)	0.00356	0.39561
121	C	19	pz	Val(2p)	1.14467	-0.07588
122	C	19	pz	Ryd(3p)	0.00329	0.37342
123	H	20	S	Val(1S)	0.82240	0.19136
124	H	20	S	Ryd(2S)	0.00141	1.00870
125	H	21	S	Val(1S)	0.81900	0.19499
126	H	21	S	Ryd(2S)	0.00139	1.01332
127	H	22	S	Val(1S)	0.82504	0.18688
128	H	22	S	Ryd(2S)	0.00170	1.04184
129	C	23	S	Cor(1S)	1.99917	-11.30124
130	C	23	S	Val(2S)	0.86141	-0.24823
131	C	23	S	Ryd(3S)	0.00579	1.17773
132	C	23	px	Val(2p)	0.90076	-0.14139
133	C	23	px	Ryd(3p)	0.00763	0.64982
134	C	23	py	Val(2p)	0.85856	-0.13087
135	C	23	py	Ryd(3p)	0.00959	0.62436
136	C	23	pz	Val(2p)	0.84806	-0.09106
137	C	23	pz	Ryd(3p)	0.00769	0.60891
138	C	24	S	Cor(1S)	1.99921	-11.13489
139	C	24	S	Val(2S)	1.01996	-0.24265
140	C	24	S	Ryd(3S)	0.00056	1.34798
141	C	24	px	Val(2p)	1.14450	-0.14931
142	C	24	px	Ryd(3p)	0.00351	0.35552
143	C	24	py	Val(2p)	1.23359	-0.14473
144	C	24	py	Ryd(3p)	0.00292	0.32992
145	C	24	pz	Val(2p)	1.18362	-0.14852
146	C	24	pz	Ryd(3p)	0.00309	0.33525

147	H	25	S	Val(1S)	0.78532	0.16801
148	H	25	S	Ryd(2S)	0.00162	1.06702
149	H	26	S	Val(1S)	0.79101	0.15093
150	H	26	S	Ryd(2S)	0.00124	1.00490
151	H	27	S	Val(1S)	0.79352	0.14151
152	H	27	S	Ryd(2S)	0.00146	1.06042
153	C	28	S	Cor(1S)	1.99891	-11.22584
154	C	28	S	Val(2S)	0.84416	-0.17373
155	C	28	S	Ryd(3S)	0.00200	1.27984
156	C	28	px	Val(2p)	0.99244	-0.10541
157	C	28	px	Ryd(3p)	0.00697	0.64057
158	C	28	py	Val(2p)	0.97864	-0.09709
159	C	28	py	Ryd(3p)	0.00780	0.72497
160	C	28	pz	Val(2p)	1.02469	-0.15625
161	C	28	pz	Ryd(3p)	0.01224	0.67129
162	C	29	S	Cor(1S)	1.99909	-11.18961
163	C	29	S	Val(2S)	0.89566	-0.19361
164	C	29	S	Ryd(3S)	0.00170	1.36059
165	C	29	px	Val(2p)	1.04943	-0.11475
166	C	29	px	Ryd(3p)	0.00986	0.77012
167	C	29	py	Val(2p)	1.03862	-0.09899
168	C	29	py	Ryd(3p)	0.00690	0.68174
169	C	29	pz	Val(2p)	0.98259	-0.12184
170	C	29	pz	Ryd(3p)	0.00890	0.63416
171	C	30	S	Cor(1S)	1.99902	-11.12759
172	C	30	S	Val(2S)	0.89570	-0.08675
173	C	30	S	Ryd(3S)	0.00083	1.21858
174	C	30	px	Val(2p)	1.08337	-0.06113
175	C	30	px	Ryd(3p)	0.00361	0.62701
176	C	30	py	Val(2p)	1.13066	-0.01125
177	C	30	py	Ryd(3p)	0.00848	0.43369
178	C	30	pz	Val(2p)	1.00757	-0.12270
179	C	30	pz	Ryd(3p)	0.00354	0.51639
180	C	31	S	Cor(1S)	1.99930	-11.15402
181	C	31	S	Val(2S)	0.93345	-0.15889
182	C	31	S	Ryd(3S)	0.00087	1.13726
183	C	31	px	Val(2p)	1.08411	-0.04446
184	C	31	px	Ryd(3p)	0.00498	0.49828
185	C	31	py	Val(2p)	1.08568	-0.06868
186	C	31	py	Ryd(3p)	0.00581	0.49120
187	C	31	pz	Val(2p)	1.02827	-0.09464
188	C	31	pz	Ryd(3p)	0.00474	0.47272
189	C	32	S	Cor(1S)	1.99915	-11.14048
190	C	32	S	Val(2S)	0.91349	-0.10672
191	C	32	S	Ryd(3S)	0.00059	1.11086
192	C	32	px	Val(2p)	1.10140	0.01266
193	C	32	px	Ryd(3p)	0.00716	0.41961
194	C	32	py	Val(2p)	1.04637	-0.07214
195	C	32	py	Ryd(3p)	0.00432	0.51368
196	C	32	pz	Val(2p)	1.00461	-0.10673
197	C	32	pz	Ryd(3p)	0.00528	0.45706
198	C	33	S	Cor(1S)	1.99917	-11.15596
199	C	33	S	Val(2S)	0.92510	-0.16432

200	C	33	S	Ryd(3S)	0.00090	1.24559
201	C	33	px	Val(2p)	1.06491	-0.11287
202	C	33	px	Ryd(3p)	0.00676	0.53553
203	C	33	py	Val(2p)	1.14621	-0.03820
204	C	33	py	Ryd(3p)	0.00694	0.52887
205	C	33	pz	Val(2p)	1.04926	-0.15138
206	C	33	pz	Ryd(3p)	0.00493	0.56800
207	C	34	S	Cor(1S)	1.99922	-11.16063
208	C	34	S	Val(2S)	0.94853	-0.21792
209	C	34	S	Ryd(3S)	0.00059	1.63561
210	C	34	px	Val(2p)	1.02029	-0.09048
211	C	34	px	Ryd(3p)	0.00451	0.48023
212	C	34	py	Val(2p)	1.08588	-0.08707
213	C	34	py	Ryd(3p)	0.00899	0.65200
214	C	34	pz	Val(2p)	1.06734	-0.07810
215	C	34	pz	Ryd(3p)	0.00563	0.53747
216	C	35	S	Cor(1S)	1.99931	-11.08317
217	C	35	S	Val(2S)	1.01070	-0.16993
218	C	35	S	Ryd(3S)	0.00059	1.28869
219	C	35	px	Val(2p)	1.21830	-0.07177
220	C	35	px	Ryd(3p)	0.00300	0.38020
221	C	35	py	Val(2p)	1.09477	-0.07930
222	C	35	py	Ryd(3p)	0.00297	0.35525
223	C	35	pz	Val(2p)	1.18154	-0.07516
224	C	35	pz	Ryd(3p)	0.00377	0.35743
225	H	36	S	Val(1S)	0.82656	0.18342
226	H	36	S	Ryd(2S)	0.00159	1.02838
227	H	37	S	Val(1S)	0.81619	0.19892
228	H	37	S	Ryd(2S)	0.00135	1.00210
229	H	38	S	Val(1S)	0.81866	0.19685
230	H	38	S	Ryd(2S)	0.00145	0.99191
231	C	39	S	Cor(1S)	1.99932	-11.08959
232	C	39	S	Val(2S)	1.01065	-0.17356
233	C	39	S	Ryd(3S)	0.00074	1.28898
234	C	39	px	Val(2p)	1.15953	-0.08406
235	C	39	px	Ryd(3p)	0.00391	0.44208
236	C	39	py	Val(2p)	1.20979	-0.07383
237	C	39	py	Ryd(3p)	0.00348	0.41832
238	C	39	pz	Val(2p)	1.12338	-0.08518
239	C	39	pz	Ryd(3p)	0.00276	0.38792
240	H	40	S	Val(1S)	0.83226	0.17453
241	H	40	S	Ryd(2S)	0.00146	1.06386
242	H	41	S	Val(1S)	0.81858	0.19029
243	H	41	S	Ryd(2S)	0.00142	0.99340
244	H	42	S	Val(1S)	0.81867	0.19501
245	H	42	S	Ryd(2S)	0.00152	1.05152
246	C	43	S	Cor(1S)	1.99915	-11.30115
247	C	43	S	Val(2S)	0.85970	-0.24551
248	C	43	S	Ryd(3S)	0.00607	1.15859
249	C	43	px	Val(2p)	0.77719	-0.12828
250	C	43	px	Ryd(3p)	0.00979	0.62257
251	C	43	py	Val(2p)	0.97872	-0.15045

252	C	43	py	Ryd(3p)	0.00739	0.71485
253	C	43	pz	Val(2p)	0.85124	-0.08553
254	C	43	pz	Ryd(3p)	0.00769	0.61376
255	C	44	S	Cor(1S)	1.99921	-11.13755
256	C	44	S	Val(2S)	1.02141	-0.24564
257	C	44	S	Ryd(3S)	0.00055	1.33011
258	C	44	px	Val(2p)	1.23264	-0.14309
259	C	44	px	Ryd(3p)	0.00194	0.36741
260	C	44	py	Val(2p)	1.14047	-0.15210
261	C	44	py	Ryd(3p)	0.00420	0.34940
262	C	44	pz	Val(2p)	1.18623	-0.14790
263	C	44	pz	Ryd(3p)	0.00300	0.33126
264	H	45	S	Val(1S)	0.78607	0.16603
265	H	45	S	Ryd(2S)	0.00159	1.05579
266	H	46	S	Val(1S)	0.79384	0.14865
267	H	46	S	Ryd(2S)	0.00116	1.00506
268	H	47	S	Val(1S)	0.79052	0.14676
269	H	47	S	Ryd(2S)	0.00126	1.03472
270	C	48	S	Cor(1S)	1.99891	-11.23310
271	C	48	S	Val(2S)	0.84185	-0.17606
272	C	48	S	Ryd(3S)	0.00205	1.30139
273	C	48	px	Val(2p)	1.06480	-0.12584
274	C	48	px	Ryd(3p)	0.00643	0.69110
275	C	48	py	Val(2p)	0.91246	-0.08417
276	C	48	py	Ryd(3p)	0.00759	0.67408
277	C	48	pz	Val(2p)	1.01439	-0.15206
278	C	48	pz	Ryd(3p)	0.01290	0.69470
279	C	49	S	Cor(1S)	1.99907	-11.18938
280	C	49	S	Val(2S)	0.89283	-0.19182
281	C	49	S	Ryd(3S)	0.00166	1.35157
282	C	49	px	Val(2p)	1.05934	-0.11053
283	C	49	px	Ryd(3p)	0.00815	0.77007
284	C	49	py	Val(2p)	1.04001	-0.11929
285	C	49	py	Ryd(3p)	0.00805	0.66664
286	C	49	pz	Val(2p)	1.00617	-0.12551
287	C	49	pz	Ryd(3p)	0.00821	0.65024
288	C	50	S	Cor(1S)	1.99918	-11.15241
289	C	50	S	Val(2S)	0.93112	-0.17034
290	C	50	S	Ryd(3S)	0.00090	1.22132
291	C	50	px	Val(2p)	1.15897	-0.03815
292	C	50	px	Ryd(3p)	0.00777	0.51081
293	C	50	py	Val(2p)	1.03615	-0.10177
294	C	50	py	Ryd(3p)	0.00428	0.55701
295	C	50	pz	Val(2p)	1.01152	-0.11806
296	C	50	pz	Ryd(3p)	0.00411	0.49569
297	C	51	S	Cor(1S)	1.99924	-11.14420
298	C	51	S	Val(2S)	0.92705	-0.14237
299	C	51	S	Ryd(3S)	0.00068	1.11403
300	C	51	px	Val(2p)	1.07049	-0.05103
301	C	51	px	Ryd(3p)	0.00446	0.51849
302	C	51	py	Val(2p)	1.08036	-0.05972
303	C	51	py	Ryd(3p)	0.00662	0.45000
304	C	51	pz	Val(2p)	1.03187	-0.08686
305	C	51	pz	Ryd(3p)	0.00506	0.45903

306	C	52	S	Cor(1S)	1.99931	-11.16278
307	C	52	S	Val(2S)	0.93967	-0.17717
308	C	52	S	Ryd(3S)	0.00071	1.11741
309	C	52	px	Val(2p)	1.09494	-0.05993
310	C	52	px	Ryd(3p)	0.00567	0.49621
311	C	52	py	Val(2p)	1.07377	-0.06464
312	C	52	py	Ryd(3p)	0.00570	0.48062
313	C	52	pz	Val(2p)	1.01882	-0.11068
314	C	52	pz	Ryd(3p)	0.00495	0.46300
315	C	53	S	Cor(1S)	1.99916	-11.16117
316	C	53	S	Val(2S)	0.92470	-0.16940
317	C	53	S	Ryd(3S)	0.00098	1.24410
318	C	53	px	Val(2p)	1.15625	-0.02874
319	C	53	px	Ryd(3p)	0.00870	0.51233
320	C	53	py	Val(2p)	1.05298	-0.13147
321	C	53	py	Ryd(3p)	0.00510	0.53736
322	C	53	pz	Val(2p)	1.04722	-0.14736
323	C	53	pz	Ryd(3p)	0.00469	0.54926
324	C	54	S	Cor(1S)	1.99926	-11.16784
325	C	54	S	Val(2S)	0.95266	-0.23196
326	C	54	S	Ryd(3S)	0.00054	1.66840
327	C	54	px	Val(2p)	1.04360	-0.09846
328	C	54	px	Ryd(3p)	0.00774	0.67171
329	C	54	py	Val(2p)	1.11131	-0.07389
330	C	54	py	Ryd(3p)	0.00757	0.48830
331	C	54	pz	Val(2p)	1.01030	-0.10208
332	C	54	pz	Ryd(3p)	0.00386	0.55663
333	C	55	S	Cor(1S)	1.99931	-11.09072
334	C	55	S	Val(2S)	1.00934	-0.17665
335	C	55	S	Ryd(3S)	0.00071	1.29404
336	C	55	px	Val(2p)	1.20209	-0.07479
337	C	55	px	Ryd(3p)	0.00341	0.37059
338	C	55	py	Val(2p)	1.21269	-0.08232
339	C	55	py	Ryd(3p)	0.00245	0.39029
340	C	55	pz	Val(2p)	1.08037	-0.09575
341	C	55	pz	Ryd(3p)	0.00395	0.38288
342	H	56	S	Val(1S)	0.81526	0.19529
343	H	56	S	Ryd(2S)	0.00167	1.01212
344	H	57	S	Val(1S)	0.81805	0.18757
345	H	57	S	Ryd(2S)	0.00142	0.98933
346	H	58	S	Val(1S)	0.83804	0.16315
347	H	58	S	Ryd(2S)	0.00201	1.14228
348	C	59	S	Cor(1S)	1.99931	-11.08574
349	C	59	S	Val(2S)	1.01089	-0.17410
350	C	59	S	Ryd(3S)	0.00061	1.29168
351	C	59	px	Val(2p)	1.10107	-0.08331
352	C	59	px	Ryd(3p)	0.00353	0.36976
353	C	59	py	Val(2p)	1.21815	-0.07460
354	C	59	py	Ryd(3p)	0.00286	0.38650
355	C	59	pz	Val(2p)	1.18633	-0.07688
356	C	59	pz	Ryd(3p)	0.00364	0.37847
357	H	60	S	Val(1S)	0.81664	0.19483
358	H	60	S	Ryd(2S)	0.00141	1.00246

359	H	61	S	Val(1S)	0.81385	0.19941
360	H	61	S	Ryd(2S)	0.00126	1.03169
361	H	62	S	Val(1S)	0.82113	0.18738
362	H	62	S	Ryd(2S)	0.00177	0.99167
363	H	63	S	Val(1S)	0.82230	0.23234
364	H	63	S	Ryd(2S)	0.00158	1.09232
365	H	64	S	Val(1S)	0.82834	0.26571
366	H	64	S	Ryd(2S)	0.00165	1.02888
367	H	65	S	Val(1S)	0.92010	0.37833
368	H	65	S	Ryd(2S)	0.00198	0.90874
369	H	66	S	Val(1S)	0.83533	0.23002
370	H	66	S	Ryd(2S)	0.00196	1.15377
371	H	67	S	Val(1S)	0.85201	0.25514
372	H	67	S	Ryd(2S)	0.00351	1.08711
373	H	68	S	Val(1S)	0.86157	0.31858
374	H	68	S	Ryd(2S)	0.00243	1.05958
375	H	69	S	Val(1S)	0.81815	0.25512
376	H	69	S	Ryd(2S)	0.00190	1.04313
377	H	70	S	Val(1S)	0.87321	0.32408
378	H	70	S	Ryd(2S)	0.00171	0.96935
379	H	71	S	Val(1S)	0.84284	0.24278
380	H	71	S	Ryd(2S)	0.00168	1.14368
381	H	72	S	Val(1S)	0.83095	0.20881
382	H	72	S	Ryd(2S)	0.00302	1.08942
383	H	73	S	Val(1S)	0.82389	0.24030
384	H	73	S	Ryd(2S)	0.00176	1.08862
385	H	74	S	Val(1S)	0.83921	0.29151
386	H	74	S	Ryd(2S)	0.00196	1.02026
387	H	75	S	Val(1S)	0.82091	0.24397
388	H	75	S	Ryd(2S)	0.00143	1.04097
389	H	76	S	Val(1S)	0.83338	0.24184
390	H	76	S	Ryd(2S)	0.00165	1.11496
391	H	77	S	Val(1S)	0.83161	0.17140
392	H	77	S	Ryd(2S)	0.00298	1.14521
393	N	78	S	Cor(1S)	1.99944	-15.49063
394	N	78	S	Val(2S)	1.36476	-0.77226
395	N	78	S	Ryd(3S)	0.00228	1.90474
396	N	78	px	Val(2p)	1.47578	-0.39863
397	N	78	px	Ryd(3p)	0.01145	1.09332
398	N	78	py	Val(2p)	1.35835	-0.36365
399	N	78	py	Ryd(3p)	0.00602	0.90509
400	N	78	pz	Val(2p)	1.44877	-0.42415
401	N	78	pz	Ryd(3p)	0.00745	0.85918

402	N	79	S	Cor(1S)	1.99945	-15.49327
403	N	79	S	Val(2S)	1.36950	-0.78097
404	N	79	S	Ryd(3S)	0.00230	1.90149
405	N	79	px	Val(2p)	1.56589	-0.43384
406	N	79	px	Ryd(3p)	0.00820	0.93586
407	N	79	py	Val(2p)	1.31816	-0.35689
408	N	79	py	Ryd(3p)	0.00901	1.06327
409	N	79	pz	Val(2p)	1.42152	-0.41515
410	N	79	pz	Ryd(3p)	0.00704	0.86335
411	N	80	S	Cor(1S)	1.99943	-15.49466
412	N	80	S	Val(2S)	1.36026	-0.77745
413	N	80	S	Ryd(3S)	0.00245	1.90334
414	N	80	px	Val(2p)	1.30119	-0.35544
415	N	80	px	Ryd(3p)	0.00673	0.96497
416	N	80	py	Val(2p)	1.60392	-0.44739
417	N	80	py	Ryd(3p)	0.01172	1.04050
418	N	80	pz	Val(2p)	1.41069	-0.41883
419	N	80	pz	Ryd(3p)	0.00708	0.87824
420	Tl	81	S	Val(6S)	1.94833	-0.48876
421	Tl	81	S	Ryd(7S)	0.00024	10.74317
422	Tl	81	px	Val(6p)	0.01963	0.01704
423	Tl	81	px	Ryd(7p)	0.00104	0.41618
424	Tl	81	py	Val(6p)	0.01942	0.02837
425	Tl	81	py	Ryd(7p)	0.00125	0.44119
426	Tl	81	pz	Val(6p)	0.08160	0.05170
427	Tl	81	pz	Ryd(7p)	0.00224	0.52466
428	Tl	81	dxy	Cor(5d)	1.99782	-0.93384
429	Tl	81	dxy	Ryd(6d)	0.00003	1.72920
430	Tl	81	dxz	Cor(5d)	1.99718	-0.92973
431	Tl	81	dxz	Ryd(6d)	0.00006	1.80849
432	Tl	81	dyz	Cor(5d)	1.99661	-0.92912
433	Tl	81	dyz	Ryd(6d)	0.00007	1.84361
434	Tl	81	dx2y2	Cor(5d)	1.99762	-0.93380
435	Tl	81	dx2y2	Ryd(6d)	0.00002	1.73393
436	Tl	81	dz2	Cor(5d)	1.99688	-0.92941
437	Tl	81	dz2	Ryd(6d)	0.00004	1.77140

[68 electrons found in the effective core potential]

WARNING: 1 low occupancy (<1.9990e) core orbital found on C   1
1 low occupancy (<1.9990e) core orbital found on C   8
1 low occupancy (<1.9990e) core orbital found on C   12
1 low occupancy (<1.9990e) core orbital found on C   28
1 low occupancy (<1.9990e) core orbital found on C   48
5 low occupancy (<1.9990e) core orbitals found on Tl   81

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.33377	1.99896	4.29682	0.03799	6.33377
H	2	0.20374	0.00000	0.79434	0.00191	0.79626
C	3	0.48900	1.99916	3.48126	0.03058	5.51100
C	4	-0.58802	1.99921	4.57909	0.00973	6.58802
H	5	0.21261	0.00000	0.78586	0.00153	0.78739
H	6	0.20502	0.00000	0.79377	0.00120	0.79498
H	7	0.20498	0.00000	0.79380	0.00122	0.79502

C	8	0.13684	1.99890	3.83481	0.02945	5.86316
C	9	-0.02117	1.99908	3.99539	0.02670	6.02117
C	10	-0.15946	1.99920	4.14306	0.01720	6.15946
C	11	-0.13372	1.99931	4.11772	0.01669	6.13372
C	12	-0.05440	1.99872	4.03939	0.01630	6.05440
C	13	-0.18714	1.99919	4.16857	0.01938	6.18714
C	14	-0.11632	1.99909	4.09712	0.02011	6.11632
C	15	-0.51714	1.99932	4.50791	0.00990	6.51714
H	16	0.18014	0.00000	0.81826	0.00159	0.81986
H	17	0.17915	0.00000	0.81945	0.00140	0.82085
H	18	0.17090	0.00000	0.82757	0.00152	0.82910
C	19	-0.51718	1.99933	4.50775	0.01010	6.51718
H	20	0.17619	0.00000	0.82240	0.00141	0.82381
H	21	0.17960	0.00000	0.81900	0.00139	0.82040
H	22	0.17326	0.00000	0.82504	0.00170	0.82674
C	23	0.50134	1.99917	3.46879	0.03071	5.49866
C	24	-0.59095	1.99921	4.58166	0.01008	6.59095
H	25	0.21306	0.00000	0.78532	0.00162	0.78694
H	26	0.20775	0.00000	0.79101	0.00124	0.79225
H	27	0.20503	0.00000	0.79352	0.00146	0.79497
C	28	0.13215	1.99891	3.83993	0.02901	5.86785
C	29	0.00725	1.99909	3.96630	0.02736	5.99275
C	30	-0.13278	1.99902	4.11730	0.01645	6.13278
C	31	-0.14722	1.99930	4.13151	0.01640	6.14722
C	32	-0.08237	1.99915	4.06586	0.01735	6.08237
C	33	-0.20418	1.99917	4.18549	0.01952	6.20418
C	34	-0.14098	1.99922	4.12204	0.01973	6.14098
C	35	-0.51495	1.99931	4.50531	0.01033	6.51495
H	36	0.17185	0.00000	0.82656	0.00159	0.82815
H	37	0.18245	0.00000	0.81619	0.00135	0.81755
H	38	0.17989	0.00000	0.81866	0.00145	0.82011
C	39	-0.51355	1.99932	4.50335	0.01088	6.51355
H	40	0.16629	0.00000	0.83226	0.00146	0.83371
H	41	0.18000	0.00000	0.81858	0.00142	0.82000
H	42	0.17981	0.00000	0.81867	0.00152	0.82019
C	43	0.50307	1.99915	3.46685	0.03093	5.49693
C	44	-0.58965	1.99921	4.58076	0.00968	6.58965
H	45	0.21234	0.00000	0.78607	0.00159	0.78766
H	46	0.20500	0.00000	0.79384	0.00116	0.79500
H	47	0.20822	0.00000	0.79052	0.00126	0.79178
C	48	0.13862	1.99891	3.83350	0.02897	5.86138
C	49	-0.02350	1.99907	3.99835	0.02608	6.02350
C	50	-0.15399	1.99918	4.13776	0.01705	6.15399
C	51	-0.12581	1.99924	4.10975	0.01681	6.12581
C	52	-0.14352	1.99931	4.12719	0.01703	6.14352
C	53	-0.19979	1.99916	4.18115	0.01947	6.19979
C	54	-0.13683	1.99926	4.11786	0.01970	6.13683
C	55	-0.51431	1.99931	4.50448	0.01052	6.51431
H	56	0.18307	0.00000	0.81526	0.00167	0.81693
H	57	0.18053	0.00000	0.81805	0.00142	0.81947
H	58	0.15994	0.00000	0.83804	0.00201	0.84006
C	59	-0.52641	1.99931	4.51645	0.01065	6.52641
H	60	0.18195	0.00000	0.81664	0.00141	0.81805
H	61	0.18489	0.00000	0.81385	0.00126	0.81511
H	62	0.17710	0.00000	0.82113	0.00177	0.82290
H	63	0.17612	0.00000	0.82230	0.00158	0.82388
H	64	0.17001	0.00000	0.82834	0.00165	0.82999
H	65	0.07793	0.00000	0.92010	0.00198	0.92207
H	66	0.16271	0.00000	0.83533	0.00196	0.83729
H	67	0.14448	0.00000	0.85201	0.00351	0.85552
H	68	0.13599	0.00000	0.86157	0.00243	0.86401
H	69	0.17995	0.00000	0.81815	0.00190	0.82005

H	70	0.12508	0.00000	0.87321	0.00171	0.87492
H	71	0.15548	0.00000	0.84284	0.00168	0.84452
H	72	0.16603	0.00000	0.83095	0.00302	0.83397
H	73	0.17435	0.00000	0.82389	0.00176	0.82565
H	74	0.15883	0.00000	0.83921	0.00196	0.84117
H	75	0.17766	0.00000	0.82091	0.00143	0.82234
H	76	0.16497	0.00000	0.83338	0.00165	0.83503
H	77	0.16540	0.00000	0.83161	0.00298	0.83460
N	78	-0.67429	1.99944	5.64765	0.02720	7.67429
N	79	-0.70109	1.99945	5.67508	0.02655	7.70109
N	80	-0.70347	1.99943	5.67606	0.02798	7.70347
Tl	81	0.93991	77.98612	2.06898	0.00499	80.06009
* Total *		1.00000	151.95588	195.22580	0.81832	348.00000

Natural Population

Effective Core	68.00000
Core	83.95588 (99.9475% of 84)
Valence	195.22580 (99.6050% of 196)
Natural Minimal Basis	347.18168 (99.7649% of 348)
Natural Rydberg Basis	0.81832 (0.2351% of 348)

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.96)2p(3.33)3p(0.04)
H	2	1S(0.79)
C	3	[core]2S(0.86)2p(2.62)3S(0.01)3p(0.02)
C	4	[core]2S(1.02)2p(3.56)3p(0.01)
H	5	1S(0.79)
H	6	1S(0.79)
H	7	1S(0.79)
C	8	[core]2S(0.84)2p(2.99)3p(0.03)
C	9	[core]2S(0.90)2p(3.10)3p(0.02)
C	10	[core]2S(0.94)2p(3.20)3p(0.02)
C	11	[core]2S(0.94)2p(3.18)3p(0.02)
C	12	[core]2S(0.88)2p(3.16)3p(0.02)
C	13	[core]2S(0.93)2p(3.24)3p(0.02)
C	14	[core]2S(0.92)2p(3.17)3p(0.02)
C	15	[core]2S(1.01)2p(3.50)3p(0.01)
H	16	1S(0.82)
H	17	1S(0.82)
H	18	1S(0.83)
C	19	[core]2S(1.01)2p(3.50)3p(0.01)
H	20	1S(0.82)
H	21	1S(0.82)
H	22	1S(0.83)
C	23	[core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C	24	[core]2S(1.02)2p(3.56)3p(0.01)
H	25	1S(0.79)
H	26	1S(0.79)
H	27	1S(0.79)
C	28	[core]2S(0.84)2p(3.00)3p(0.03)
C	29	[core]2S(0.90)2p(3.07)3p(0.03)
C	30	[core]2S(0.90)2p(3.22)3p(0.02)
C	31	[core]2S(0.93)2p(3.20)3p(0.02)
C	32	[core]2S(0.91)2p(3.15)3p(0.02)
C	33	[core]2S(0.93)2p(3.26)3p(0.02)
C	34	[core]2S(0.95)2p(3.17)3p(0.02)
C	35	[core]2S(1.01)2p(3.49)3p(0.01)
H	36	1S(0.83)

H 37 1S(0.82)
H 38 1S(0.82)
C 39 [core]2S(1.01)2p(3.49)3p(0.01)
H 40 1S(0.83)
H 41 1S(0.82)
H 42 1S(0.82)
C 43 [core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C 44 [core]2S(1.02)2p(3.56)3p(0.01)
H 45 1S(0.79)
H 46 1S(0.79)
H 47 1S(0.79)
C 48 [core]2S(0.84)2p(2.99)3p(0.03)
C 49 [core]2S(0.89)2p(3.11)3p(0.02)
C 50 [core]2S(0.93)2p(3.21)3p(0.02)
C 51 [core]2S(0.93)2p(3.18)3p(0.02)
C 52 [core]2S(0.94)2p(3.19)3p(0.02)
C 53 [core]2S(0.92)2p(3.26)3p(0.02)
C 54 [core]2S(0.95)2p(3.17)3p(0.02)
C 55 [core]2S(1.01)2p(3.50)3p(0.01)
H 56 1S(0.82)
H 57 1S(0.82)
H 58 1S(0.84)
C 59 [core]2S(1.01)2p(3.51)3p(0.01)
H 60 1S(0.82)
H 61 1S(0.81)
H 62 1S(0.82)
H 63 1S(0.82)
H 64 1S(0.83)
H 65 1S(0.92)
H 66 1S(0.84)
H 67 1S(0.85)
H 68 1S(0.86)
H 69 1S(0.82)
H 70 1S(0.87)
H 71 1S(0.84)
H 72 1S(0.83)
H 73 1S(0.82)
H 74 1S(0.84)
H 75 1S(0.82)
H 76 1S(0.83)
H 77 1S(0.83)
N 78 [core]2S(1.36)2p(4.28)3p(0.02)
N 79 [core]2S(1.37)2p(4.31)3p(0.02)
N 80 [core]2S(1.36)2p(4.32)3p(0.03)
Tl 81 [core]6S(1.95)6p(0.12)

NBO analysis skipped by request.

1|1|UNPC-E-C07CYG43063|SP|RHF|LANL2DZ|C34H43N3Tl1(1+)|MCDSTFM|15-Jan-2
013|0||# rhf/lanl2dz pop=npa geom=connectivity||single-Point XRD Monom
er||1,1|C,0,-0.6205,11.0173,13.3488|H,0,-1.1772,10.346,12.9002|C,0,-0.
7386,10.7853,14.8523|C,0,-2.0146,10.1478,15.2951|H,0,-2.0164,10.0668,1
6.2521|H,0,-2.0905,9.2752,14.9004|H,0,-2.7571,10.6899,15.0181|C,0,0.14
77,11.0887,17.0133|C,0,0.985,10.2079,17.6933|C,0,0.9712,10.2682,19.086
5|C,0,0.1757,11.1851,19.7698|C,0,-0.6272,12.0471,19.0766|C,0,-0.643,11
.9981,17.6933|C,0,1.8192,9.1837,16.9669|C,0,1.2049,7.8117,17.0863|H,0,
1.2187,7.5343,18.0051|H,0,1.706,7.1888,16.5556|H,0,0.2964,7.8403,16.77
45|C,0,3.2525,9.155,17.4114|H,0,3.6438,10.0232,17.287|H,0,3.7359,8.507
5,16.8939|H,0,3.2939,8.9159,18.3418|C,0,-1.123,12.3888,12.9283|C,0,-1.
6827,12.4638,11.5534|H,0,-1.9518,13.3661,11.366|H,0,-2.4428,11.8816,11
.4854|H,0,-1.0127,12.193,10.9198|C,0,-1.289,14.7012,13.3745|C,0,-2.298
6,15.3891,14.0528|C,0,-2.4429,16.7341,13.6979|C,0,-1.6719,17.3532,12.8

04|C,0,-0.6563,16.6662,12.1604|C,0,-0.4748,15.3276,12.454|C,0,-3.1018,
14.7409,15.1408|C,0,-4.5972,15.0605,15.0712|H,0,-4.7206,16.0118,15.051
3|H,0,-5.0382,14.6958,15.8407|H,0,-4.9686,14.6725,14.2751|C,0,-2.5564,
15.1673,16.5058|H,0,-1.6294,14.924,16.5705|H,0,-3.0515,14.7244,17.2008
|H,0,-2.6467,16.1173,16.6053|C,0,0.8149,10.8036,12.8925|C,0,1.185,9.39
29,12.5668|H,0,2.0832,9.368,12.2268|H,0,0.5821,9.0478,11.905|H,0,1.128
8,8.8555,13.3612|C,0,2.9692,11.7205,12.532|C,0,3.4312,12.2928,11.3444|
C,0,4.8043,12.3003,11.1454|C,0,5.6765,11.7802,12.0742|C,0,5.2031,11.20
58,13.2236|C,0,3.8453,11.1763,13.4607|C,0,2.4476,12.825,10.3294|C,0,1.
935,11.6972,9.4454|H,0,2.6628,11.3347,8.9346|H,0,1.2641,12.0378,8.8483
|H,0,1.5553,11.0076,9.9944|C,0,3.0076,13.9575,9.4603|H,0,3.4149,14.620
1,10.0242|H,0,2.2939,14.3599,8.9595|H,0,3.6632,13.6032,8.8566|H,0,1.53
76,9.6958,19.6056|H,0,0.2777,11.1745,20.6986|H,0,-1.0785,12.5752,19.40
5|H,0,-1.1085,12.6356,17.1991|H,0,1.9153,9.4051,16.0879|H,0,-3.0335,17
.0782,14.2137|H,0,-1.6683,18.2598,12.5386|H,0,-0.1278,17.0116,11.5932|
H,0,0.1761,14.8424,12.0377|H,0,-3.0473,13.7776,15.0745|H,0,5.2053,12.7
076,10.3908|H,0,6.5357,11.8968,11.8254|H,0,5.8118,10.8056,13.8323|H,0,
3.5609,10.7602,14.2303|H,0,1.6499,13.1539,10.8187|N,0,0.2136,11.175,15
.584|N,0,-0.9939,13.3524,13.7507|N,0,1.5756,11.8102,12.8487|Tl,0,1.393
4,13.5394,14.8375||Version=IA32W-G09RevB.01|State=1-A|HF=-1524.6288676
|RMSD=3.810e-009|Dipole=-0.9632388,-1.3085232,-1.0432729|Quadrupole=-0
.8575993,-1.5876609,2.4452602,-5.316211,-5.0523255,-4.305488|PG=C01 [X
(C34H43N3Tl1)]||@

GARLIC THEN HAVE POWER TO SAVE FROM DEATH
BEAR WITH IT THOUGH IT MAKETH UNSAVORY BREATH,
AND SCORN NOT GARLIC LIKE SOME THAT THINK
IT ONLY MAKETH MEN WINK AND DRINK AND STINK.
-- SIR JOHN HARRINGTON,
"THE ENGLISHMAN'S DOCTOR", 1609
Job cpu time: 0 days 1 hours 2 minutes 47.0 seconds.
File lengths (MBytes): RWF= 105 Int= 0 D2E= 0 Chk= 8 Scr= 1
Normal termination of Gaussian 09 at Tue Jan 15 12:19:55 2013.

Appendix 2. Gaussian output for cation monomer, LANL2-DZ, DF-B3-LYP.

```
******************************************
Gaussian 09:  IA32W-G09RevB.01 12-Aug-2010
              03-Apr-2013
******************************************
%chk=\\vdm09-g1.ds.man.ac.uk\HOME\Desktop\cationOnly_1_1.chk
----------------------------------------
# rb3lyp/lanl2dz pop=npa geom=connectivity
----------------------------------------
1/38=1,57=2/1;
2/12=2,17=6,18=5,40=1/2;
3/5=6,6=3,11=2,16=1,25=1,30=1,74=-5,116=1/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1,40=-1/1,7;
99/5=1,9=1/99;
-----------------------
single-Point XRD Monomer
```

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

C	0.01861	-0.08351	2.25597
H	0.00456	-0.12271	3.2358
C	1.47569	0.03725	1.81938
C	2.38329	0.67877	2.81706
H	3.26891	0.74039	2.45059
H	2.405	0.1484	3.61782
H	2.06067	1.5589	3.02492
C	3.10026	-0.2097	0.13198
C	3.90198	-1.32752	-0.08483
C	5.12032	-1.11817	-0.73032
C	5.50929	0.14744	-1.16317
C	4.69675	1.22541	-0.94872
C	3.48842	1.04715	-0.2973
C	3.51104	-2.69488	0.41518
C	4.30163	-3.06022	1.64623
H	5.23077	-3.13741	1.41802
H	3.98594	-3.89728	1.99325
H	4.19153	-2.37548	2.31138
C	3.6358	-3.77042	-0.62425
H	3.09152	-3.54688	-1.3833
H	3.34545	-4.60758	-0.25601
H	4.5541	-3.84378	-0.8997
C	-0.81952	1.11086	1.83011
C	-1.96396	1.43167	2.72262
H	-2.44803	2.18018	2.36613
H	-1.6356	1.64936	3.59791
H	-2.54909	0.67131	2.77877
C	-1.33857	2.73108	0.19324
C	-0.81783	4.01916	0.044
C	-1.65735	4.92744	-0.60871
C	-2.85938	4.61306	-1.09147
C	-3.35078	3.32491	-0.96173
C	-2.57581	2.38473	-0.30867
C	0.57531	4.36278	0.48004
C	0.67719	5.7109	1.19795
H	0.29338	6.39655	0.64735
H	1.59896	5.91399	1.36741
H	0.20093	5.66457	2.03059
C	1.50797	4.36417	-0.73349
H	1.48254	3.50282	-1.15793
H	2.40618	4.5518	-0.44657
H	1.22447	5.03721	-1.35574
C	-0.58311	-1.38006	1.73526
C	-0.36711	-2.58269	2.59558
H	-0.8368	-3.33253	2.22126
H	-0.69574	-2.40764	3.47985
H	0.57179	-2.78203	2.63748
C	-1.70538	-2.51767	-0.01346
C	-3.08873	-2.65607	-0.14969
C	-3.53986	-3.7369	-0.89357
C	-2.67156	-4.62831	-1.48123
C	-1.31911	-4.48681	-1.31992
C	-0.82805	-3.42712	-0.58738
C	-4.01676	-1.68089	0.53494
C	-4.23979	-2.08887	1.98406
H	-4.68936	-2.93687	2.0124
H	-4.77882	-1.42666	2.42402
H	-3.39308	-2.16106	2.43015
C	-5.3658	-1.5094	-0.17371

H	-5.21606	-1.34668	-1.10859
H	-5.83602	-0.76444	0.20844
H	-5.8872	-2.30716	-0.06645
H	5.70566	-1.85291	-0.91862
H	6.32043	0.16932	-1.62659
H	4.86141	1.94149	-1.17347
H	2.87863	1.74723	-0.22406
H	2.61864	-2.73301	0.59701
H	-1.22284	5.65839	-0.70959
H	-3.46846	5.14421	-1.58062
H	-4.10178	3.06548	-1.2601
H	-2.87571	1.53075	-0.19393
H	0.90089	3.713	1.11808
H	-4.45796	-3.88078	-1.07388
H	-3.11043	-5.2493	-1.9665
H	-0.73302	-5.13667	-1.68785
H	0.08401	-3.37721	-0.478
H	-3.55875	-0.80222	0.58052
N	1.77933	-0.37223	0.66436
N	-0.50828	1.7062	0.74833
N	-1.1853	-1.34684	0.62617
Tl	-0.08843	0.10108	-1.29192

Stoichiometry C34H43N3Tl(1+)
Framework group C1[X(C34H43N3Tl)]
Deg. of freedom 237
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.018610	-0.083509	2.255965
2	1	0	0.004563	-0.122705	3.235795
3	6	0	1.475694	0.037252	1.819378
4	6	0	2.383292	0.678775	2.817058
5	1	0	3.268909	0.740391	2.450589
6	1	0	2.404998	0.148406	3.617819
7	1	0	2.060673	1.558900	3.024916
8	6	0	3.100261	-0.209695	0.131984
9	6	0	3.901980	-1.327513	-0.084833
10	6	0	5.120321	-1.118168	-0.730319
11	6	0	5.509287	0.147444	-1.163167
12	6	0	4.696746	1.225409	-0.948720
13	6	0	3.488420	1.047150	-0.297304
14	6	0	3.511045	-2.694881	0.415175
15	6	0	4.301634	-3.060218	1.646233
16	1	0	5.230770	-3.137411	1.418018
17	1	0	3.985944	-3.897277	1.993251
18	1	0	4.191530	-2.375478	2.311377
19	6	0	3.635799	-3.770421	-0.624249
20	1	0	3.091523	-3.546874	-1.383296
21	1	0	3.345450	-4.607578	-0.256005
22	1	0	4.554099	-3.843774	-0.899697
23	6	0	-0.819519	1.110862	1.830107
24	6	0	-1.963956	1.431665	2.722624
25	1	0	-2.448032	2.180173	2.366134
26	1	0	-1.635596	1.649363	3.597907
27	1	0	-2.549088	0.671303	2.778766
28	6	0	-1.338573	2.731075	0.193238

29	6	0	-0.817834	4.019155	0.044002
30	6	0	-1.657349	4.927438	-0.608713
31	6	0	-2.859384	4.613053	-1.091473
32	6	0	-3.350783	3.324903	-0.961731
33	6	0	-2.575809	2.384732	-0.308671
34	6	0	0.575303	4.362779	0.480037
35	6	0	0.677183	5.710899	1.197953
36	1	0	0.293379	6.396553	0.647347
37	1	0	1.598951	5.913989	1.367410
38	1	0	0.200928	5.664574	2.030595
39	6	0	1.507963	4.364169	-0.733490
40	1	0	1.482541	3.502823	-1.157927
41	1	0	2.406172	4.551804	-0.446567
42	1	0	1.224464	5.037209	-1.355743
43	6	0	-0.583106	-1.380063	1.735256
44	6	0	-0.367111	-2.582691	2.595582
45	1	0	-0.836792	-3.332533	2.221255
46	1	0	-0.695735	-2.407636	3.479846
47	1	0	0.571791	-2.782032	2.637478
48	6	0	-1.705377	-2.517674	-0.013464
49	6	0	-3.088726	-2.656072	-0.149691
50	6	0	-3.539861	-3.736900	-0.893565
51	6	0	-2.671559	-4.628307	-1.481231
52	6	0	-1.319109	-4.486815	-1.319917
53	6	0	-0.828042	-3.427121	-0.587380
54	6	0	-4.016760	-1.680896	0.534937
55	6	0	-4.239787	-2.088876	1.984061
56	1	0	-4.689357	-2.936873	2.012404
57	1	0	-4.778819	-1.426666	2.424024
58	1	0	-3.393079	-2.161065	2.430149
59	6	0	-5.365799	-1.509400	-0.173705
60	1	0	-5.216055	-1.346686	-1.108593
61	1	0	-5.836014	-0.764447	0.208441
62	1	0	-5.887199	-2.307166	-0.066446
63	1	0	5.705661	-1.852902	-0.918624
64	1	0	6.320426	0.169324	-1.626590
65	1	0	4.861410	1.941496	-1.173468
66	1	0	2.878626	1.747233	-0.224064
67	1	0	2.618645	-2.733003	0.597007
68	1	0	-1.222843	5.658390	-0.709589
69	1	0	-3.468467	5.144206	-1.580622
70	1	0	-4.101784	3.065479	-1.260104
71	1	0	-2.875715	1.530750	-0.193932
72	1	0	0.900883	3.712997	1.118076
73	1	0	-4.457956	-3.880786	-1.073882
74	1	0	-3.110425	-5.249299	-1.966502
75	1	0	-0.733019	-5.136673	-1.687849
76	1	0	0.084016	-3.377206	-0.477995
77	1	0	-3.558751	-0.802224	0.580520
78	7	0	1.779334	-0.372226	0.664361
79	7	0	-0.508285	1.706202	0.748331
80	7	0	-1.185302	-1.346836	0.626165
81	81	0	-0.088425	0.101083	-1.291919

Rotational constants (GHZ): 0.0954184 0.0934007 0.0606679
Standard basis: LANL2DZ (5D, 7F)
There are 437 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
437 basis functions, 1127 primitive gaussians, 439 cartesian basis functions
140 alpha electrons 140 beta electrons

```
     nuclear repulsion energy      4616.8692356483 Hartrees.
NAtoms=   81 NActive=   81 NUniq=   81 SFac= 1.00D+00 NAtFMM=   50 NAOKFM=T Big=T
One-electron integrals computed using PRISM.
  1 Symmetry operations used in ECPInt.
ECPInt:  NShTT=   38503 NPrTT=  272384 LenC2=   34176 LenP2D=  128614.
LDataN:  DoStor=T MaxTD1= 6 Len=  172
NBasis=   437 RedAO= T  NBF=   437
NBsUse=   437 1.00D-06 NBFU=   437
Defaulting to unpruned grid for atomic number  81.
Harris functional with IExCor=  402 diagonalized for initial guess.
ExpMin= 4.44D-02 ExpMax= 5.91D+03 ExpMxC= 2.05D+02 IAcc=2 IRadAn=         0 AccDes= 0.00D+00
HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=         0 IDoV= 1
ScaDFX=  1.000000  1.000000  1.000000  1.000000
Defaulting to unpruned grid for atomic number  81.
FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=        2001
        NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
        Omega=  0.000000  0.000000  1.000000  0.000000  0.000000 ICntrl=     500 IOpCl=  0
        NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1 NMtDS0=    0 NMtDT0=    0
        I1Cent=           4 NGrid=           0.
Petite list used in FoFCou.
Initial guess orbital symmetries:
     Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
```

No special actions if energy rises.
Defaulting to unpruned grid for atomic number 81.
SCF Done: E(RB3LYP) = -1536.06076743 A.U. after 14 cycles
Convg = 0.5589D-08 -V/T = 2.0091

****

Population analysis using the SCF density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.
Alpha occ. eigenvalues -- -14.46067 -14.45824 -14.45645 -10.38160 -10.38047
Alpha occ. eigenvalues -- -10.37703 -10.32761 -10.32320 -10.32200 -10.32120
Alpha occ. eigenvalues -- -10.29136 -10.28950 -10.28710 -10.27688 -10.27382
Alpha occ. eigenvalues -- -10.27249 -10.27164 -10.26991 -10.26863 -10.26757
Alpha occ. eigenvalues -- -10.26713 -10.26651 -10.26532 -10.26529 -10.26523
Alpha occ. eigenvalues -- -10.26456 -10.26411 -10.26143 -10.25969 -10.25902
Alpha occ. eigenvalues -- -10.25497 -10.22364 -10.22258 -10.21747 -10.21616
Alpha occ. eigenvalues -- -10.21543 -10.21273 -1.09888 -1.07768 -1.07515
Alpha occ. eigenvalues -- -0.97988 -0.97020 -0.96615 -0.93410 -0.92095
Alpha occ. eigenvalues -- -0.91799 -0.91596 -0.89930 -0.89613 -0.87129
Alpha occ. eigenvalues -- -0.86528 -0.86029 -0.85551 -0.85250 -0.84931
Alpha occ. eigenvalues -- -0.84228 -0.83386 -0.83370 -0.83134 -0.83108

Alpha occ. eigenvalues -- -0.82961 -0.81238 -0.81015 -0.80919 -0.75881
Alpha occ. eigenvalues -- -0.75331 -0.75287 -0.74923 -0.74651 -0.73862
Alpha occ. eigenvalues -- -0.70213 -0.69936 -0.69586 -0.68926 -0.68556
Alpha occ. eigenvalues -- -0.67186 -0.64341 -0.63771 -0.62364 -0.61353
Alpha occ. eigenvalues -- -0.60977 -0.60604 -0.59802 -0.59567 -0.58748
Alpha occ. eigenvalues -- -0.58585 -0.58294 -0.58039 -0.57679 -0.57470
Alpha occ. eigenvalues -- -0.56805 -0.56258 -0.55887 -0.55484 -0.55374
Alpha occ. eigenvalues -- -0.54972 -0.54881 -0.54741 -0.54456 -0.54040
Alpha occ. eigenvalues -- -0.53818 -0.52262 -0.52162 -0.52051 -0.51507
Alpha occ. eigenvalues -- -0.51455 -0.51214 -0.50445 -0.50319 -0.50135
Alpha occ. eigenvalues -- -0.49836 -0.49228 -0.48623 -0.48160 -0.47994
Alpha occ. eigenvalues -- -0.47144 -0.46770 -0.46114 -0.45912 -0.44877
Alpha occ. eigenvalues -- -0.44805 -0.44278 -0.43648 -0.43575 -0.43314
Alpha occ. eigenvalues -- -0.43155 -0.42754 -0.42409 -0.42109 -0.42014
Alpha occ. eigenvalues -- -0.40928 -0.40198 -0.39886 -0.37125 -0.35063
Alpha occ. eigenvalues -- -0.34857 -0.34211 -0.33300 -0.33024 -0.32804
Alpha virt. eigenvalues -- -0.14977 -0.14661 -0.13090 -0.11933 -0.11442
Alpha virt. eigenvalues -- -0.10316 -0.09478 -0.09295 -0.09130 -0.08763
Alpha virt. eigenvalues -- -0.08370 -0.06297 -0.01248 -0.00560 0.00139
Alpha virt. eigenvalues -- 0.01182 0.01961 0.02306 0.03099 0.04151
Alpha virt. eigenvalues -- 0.04620 0.04931 0.05030 0.05235 0.05422
Alpha virt. eigenvalues -- 0.05442 0.05788 0.06135 0.06318 0.06491
Alpha virt. eigenvalues -- 0.06837 0.07171 0.07224 0.07552 0.07816
Alpha virt. eigenvalues -- 0.08369 0.08579 0.08703 0.08820 0.09152
Alpha virt. eigenvalues -- 0.09394 0.09728 0.10175 0.10257 0.10731
Alpha virt. eigenvalues -- 0.10823 0.11221 0.11674 0.12086 0.12297
Alpha virt. eigenvalues -- 0.12611 0.12701 0.13299 0.13486 0.13632
Alpha virt. eigenvalues -- 0.13998 0.14384 0.14627 0.15202 0.15380
Alpha virt. eigenvalues -- 0.15763 0.16150 0.16196 0.16286 0.16872
Alpha virt. eigenvalues -- 0.17077 0.17163 0.17556 0.17684 0.18048
Alpha virt. eigenvalues -- 0.18403 0.18621 0.18846 0.19176 0.19576
Alpha virt. eigenvalues -- 0.19864 0.20184 0.20359 0.20866 0.21274
Alpha virt. eigenvalues -- 0.21708 0.22049 0.22365 0.22672 0.22925
Alpha virt. eigenvalues -- 0.23048 0.23263 0.23440 0.23792 0.24144
Alpha virt. eigenvalues -- 0.24227 0.24576 0.24938 0.25115 0.25219
Alpha virt. eigenvalues -- 0.25732 0.25910 0.26061 0.26454 0.26499
Alpha virt. eigenvalues -- 0.26784 0.27133 0.27493 0.27631 0.27863
Alpha virt. eigenvalues -- 0.28059 0.28407 0.28685 0.29211 0.29491
Alpha virt. eigenvalues -- 0.29972 0.30500 0.30672 0.30934 0.31175
Alpha virt. eigenvalues -- 0.31847 0.32216 0.32269 0.32401 0.33070
Alpha virt. eigenvalues -- 0.33181 0.33434 0.33822 0.34169 0.34230
Alpha virt. eigenvalues -- 0.34329 0.34802 0.35044 0.35131 0.35506
Alpha virt. eigenvalues -- 0.35957 0.36399 0.36778 0.36982 0.37290
Alpha virt. eigenvalues -- 0.37799 0.38038 0.38378 0.38596 0.39124
Alpha virt. eigenvalues -- 0.39251 0.39596 0.40316 0.40809 0.40962
Alpha virt. eigenvalues -- 0.41847 0.42258 0.42351 0.42515 0.42983
Alpha virt. eigenvalues -- 0.43427 0.43731 0.43947 0.44310 0.44589
Alpha virt. eigenvalues -- 0.45032 0.45482 0.45864 0.46323 0.46587
Alpha virt. eigenvalues -- 0.47086 0.47543 0.47697 0.48599 0.48987
Alpha virt. eigenvalues -- 0.49653 0.49970 0.50163 0.50584 0.50862
Alpha virt. eigenvalues -- 0.51231 0.51568 0.52517 0.53020 0.53522
Alpha virt. eigenvalues -- 0.53962 0.54683 0.55257 0.55561 0.56374
Alpha virt. eigenvalues -- 0.56741 0.57299 0.58660 0.59333 0.59578
Alpha virt. eigenvalues -- 0.61403 0.61981 0.62558 0.63364 0.64047
Alpha virt. eigenvalues -- 0.65097 0.65368 0.65987 0.66496 0.66786
Alpha virt. eigenvalues -- 0.67583 0.68066 0.68895 0.70132 0.71150
Alpha virt. eigenvalues -- 0.72163 0.72993 0.73964 0.75243 0.77078
Alpha virt. eigenvalues -- 0.78203 0.78872 0.79450 0.80986 0.88598
Alpha virt. eigenvalues -- 0.89478 0.90222 0.93047 0.93470 1.02039
Alpha virt. eigenvalues -- 1.02501 1.03175 1.04839 1.05491 1.05564
Alpha virt. eigenvalues -- 1.06202 1.09208 1.09851 1.11271 1.11841
Alpha virt. eigenvalues -- 1.12786 1.14247 1.14556 1.15717 1.16070

```
Alpha virt. eigenvalues --    1.16952   1.17061   1.17570   1.17834   1.18255
Alpha virt. eigenvalues --    1.18643   1.19527   1.20019   1.20163   1.21065
Alpha virt. eigenvalues --    1.21391   1.21914   1.22282   1.22659   1.23423
Alpha virt. eigenvalues --    1.24163   1.24724   1.25368   1.25506   1.25771
Alpha virt. eigenvalues --    1.26097   1.26424   1.26936   1.27358   1.27997
Alpha virt. eigenvalues --    1.28841   1.29158   1.29931   1.30502   1.30852
Alpha virt. eigenvalues --    1.32262   1.32373   1.33183   1.34285   1.35148
Alpha virt. eigenvalues --    1.35451   1.36376   1.37381   1.37857   1.38553
Alpha virt. eigenvalues --    1.39648   1.40729   1.41538   1.42766   1.44595
Alpha virt. eigenvalues --    1.46057   1.47175   1.47921   1.49048   1.50881
Alpha virt. eigenvalues --    1.51643   1.52937   1.54545   1.55253   1.56392
Alpha virt. eigenvalues --    1.58906   1.60527   1.60807   1.63041   1.65167
Alpha virt. eigenvalues --    1.66316   1.68111   1.73415   1.80676   1.81752
Alpha virt. eigenvalues --    1.91630  10.57886
          Condensed to atoms (all electrons):
Mulliken atomic charges:
              1
     1  C   -0.345637
     2  H    0.261845
     3  C    0.136261
     4  C   -0.784317
     5  H    0.300981
     6  H    0.277472
     7  H    0.275783
     8  C    0.042686
     9  C    0.359054
    10  C   -0.458715
    11  C   -0.324979
    12  C   -0.475370
    13  C   -0.436250
    14  C   -0.276589
    15  C   -0.736780
    16  H    0.252459
    17  H    0.242144
    18  H    0.235857
    19  C   -0.751775
    20  H    0.240684
    21  H    0.245516
    22  H    0.242444
    23  C    0.150880
    24  C   -0.791223
    25  H    0.300635
    26  H    0.281527
    27  H    0.282342
    28  C    0.057885
    29  C    0.291357
    30  C   -0.455316
    31  C   -0.302448
    32  C   -0.381474
    33  C   -0.496997
    34  C   -0.267020
    35  C   -0.747159
    36  H    0.241692
    37  H    0.248789
    38  H    0.248500
    39  C   -0.740936
    40  H    0.232808
    41  H    0.243249
    42  H    0.258595
    43  C    0.141358
    44  C   -0.786800
    45  H    0.298653
```

46 H 0.278258
47 H 0.279146
48 C 0.082634
49 C 0.302155
50 C -0.442070
51 C -0.337277
52 C -0.283531
53 C -0.479015
54 C -0.227188
55 C -0.747564
56 H 0.259140
57 H 0.247543
58 H 0.239839
59 C -0.755739
60 H 0.248076
61 H 0.249937
62 H 0.239505
63 H 0.312922
64 H 0.314465
65 H 0.506990
66 H 0.335561
67 H 0.266570
68 H 0.381039
69 H 0.306198
70 H 0.407852
71 H 0.367801
72 H 0.239102
73 H 0.319739
74 H 0.345635
75 H 0.311077
76 H 0.365662
77 H 0.215004
78 N -0.212215
79 N -0.231154
80 N -0.237550
81 Tl 0.699781
Sum of Mulliken atomic charges = 1.00000
Mulliken charges with hydrogens summed into heavy atoms:
1
1 C -0.083792
3 C 0.136261
4 C 0.069918
8 C 0.042686
9 C 0.359054
10 C -0.145793
11 C -0.010514
12 C 0.031620
13 C -0.100689
14 C -0.010019
15 C -0.006320
19 C -0.023130
23 C 0.150880
24 C 0.073281
28 C 0.057885
29 C 0.291357
30 C -0.074276
31 C 0.003751
32 C 0.026377
33 C -0.129195
34 C -0.027918
35 C -0.008178
39 C -0.006284

43	C	0.141358
44	C	0.069258
48	C	0.082634
49	C	0.302155
50	C	-0.122331
51	C	0.008357
52	C	0.027546
53	C	-0.113353
54	C	-0.012185
55	C	-0.001043
59	C	-0.018221
78	N	-0.212215
79	N	-0.231154
80	N	-0.237550
81	Tl	0.699781

Sum of Mulliken charges with hydrogens summed into heavy atoms = 1.00000
Electronic spatial extent (au): <R**2>= 18924.6193
Charge= 1.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -0.4921 Y= -0.4135 Z= 4.0742 Tot= 4.1246
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -189.5188 YY= -191.1702 ZZ= -211.1044
XY= 1.1969 XZ= 0.6882 YZ= -0.4394
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= 7.7457 YY= 6.0943 ZZ= -13.8400
XY= 1.1969 XZ= 0.6882 YZ= -0.4394
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -4.6716 YYY= 38.0961 ZZZ= -89.2270 XYY= -14.7519
XXY= -33.5144 XXZ= -90.0328 XZZ= -7.2190 YZZ= 0.2380
YYZ= -88.2014 XYZ= -0.9132
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -10242.4267 YYYY= -10157.7575 ZZZZ= -2606.0210 XXXY= 3.1792
XXXZ= -142.0794 YYYX= 56.6727 YYYZ= 19.1741 ZZZX= 25.6691
ZZZY= -11.6704 XXYY= -3366.2900 XXZZ= -2274.1099 YYZZ= -2210.0402
XXYZ= -29.9268 YYXZ= 161.6365 ZZXY= 10.2778
N-N= 4.616869235648D+03 E-N=-1.277907172422D+04 KE= 1.522227716595D+03
******************************Gaussian NBO Version 3.1******************************
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
******************************Gaussian NBO Version 3.1******************************
/RESON / : Allow strongly delocalized NBO set

Analyzing the SCF density

Job title: single-Point XRD Monomer

Storage needed: 593108 in NPA (33535799 available)

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	S	Cor(1S)	1.99885	-10.17823
2	C	1	S	Val(2S)	0.96147	-0.30265
3	C	1	S	Ryd(3S)	0.00107	1.40050
4	C	1	px	Val(2p)	1.07544	-0.22540
5	C	1	px	Ryd(3p)	0.00635	0.40913
6	C	1	py	Val(2p)	1.07282	-0.22533
7	C	1	py	Ryd(3p)	0.00593	0.39310
8	C	1	pz	Val(2p)	1.19714	-0.17447
9	C	1	pz	Ryd(3p)	0.01811	0.49910

10	H	2	S	Val(1S)	0.77396	0.06461
11	H	2	S	Ryd(2S)	0.00191	0.95067
12	C	3	S	Cor(1S)	1.99906	-10.24722
13	C	3	S	Val(2S)	0.85454	-0.26383
14	C	3	S	Ryd(3S)	0.00473	0.96572
15	C	3	px	Val(2p)	0.96585	-0.18186
16	C	3	px	Ryd(3p)	0.00693	0.52953
17	C	3	py	Val(2p)	0.83907	-0.21953
18	C	3	py	Ryd(3p)	0.00837	0.40414
19	C	3	pz	Val(2p)	0.88277	-0.13674
20	C	3	pz	Ryd(3p)	0.00676	0.45364
21	C	4	S	Cor(1S)	1.99907	-10.10342
22	C	4	S	Val(2S)	1.02364	-0.23373
23	C	4	S	Ryd(3S)	0.00054	1.10653
24	C	4	px	Val(2p)	1.20795	-0.16145
25	C	4	px	Ryd(3p)	0.00339	0.23328
26	C	4	py	Val(2p)	1.21658	-0.15400
27	C	4	py	Ryd(3p)	0.00185	0.23721
28	C	4	pz	Val(2p)	1.18886	-0.16520
29	C	4	pz	Ryd(3p)	0.00296	0.20000
30	H	5	S	Val(1S)	0.76986	0.09223
31	H	5	S	Ryd(2S)	0.00123	0.86155
32	H	6	S	Val(1S)	0.77304	0.07660
33	H	6	S	Ryd(2S)	0.00104	0.79982
34	H	7	S	Val(1S)	0.77323	0.07481
35	H	7	S	Ryd(2S)	0.00103	0.80112
36	C	8	S	Cor(1S)	1.99881	-10.18644
37	C	8	S	Val(2S)	0.84527	-0.20242
38	C	8	S	Ryd(3S)	0.00186	1.10551
39	C	8	px	Val(2p)	0.88888	-0.12982
40	C	8	px	Ryd(3p)	0.00886	0.54268
41	C	8	py	Val(2p)	1.08534	-0.14524
42	C	8	py	Ryd(3p)	0.00444	0.46859
43	C	8	pz	Val(2p)	1.03212	-0.19712
44	C	8	pz	Ryd(3p)	0.01015	0.50054
45	C	9	S	Cor(1S)	1.99899	-10.15023
46	C	9	S	Val(2S)	0.89236	-0.20644
47	C	9	S	Ryd(3S)	0.00146	1.13947
48	C	9	px	Val(2p)	1.05073	-0.13701
49	C	9	px	Ryd(3p)	0.00612	0.49689
50	C	9	py	Val(2p)	1.05462	-0.13202
51	C	9	py	Ryd(3p)	0.00935	0.63543
52	C	9	pz	Val(2p)	0.99956	-0.16951
53	C	9	pz	Ryd(3p)	0.00671	0.44914
54	C	10	S	Cor(1S)	1.99909	-10.12148
55	C	10	S	Val(2S)	0.94051	-0.19459
56	C	10	S	Ryd(3S)	0.00098	1.02364
57	C	10	px	Val(2p)	1.08594	-0.10559
58	C	10	px	Ryd(3p)	0.00564	0.34590
59	C	10	py	Val(2p)	1.12159	-0.08377
60	C	10	py	Ryd(3p)	0.00452	0.47351
61	C	10	pz	Val(2p)	1.00561	-0.16770
62	C	10	pz	Ryd(3p)	0.00287	0.33541

63	C	11	S	Cor(1S)	1.99922	-10.12108
64	C	11	S	Val(2S)	0.94300	-0.17917
65	C	11	S	Ryd(3S)	0.00073	0.92872
66	C	11	px	Val(2p)	1.11961	-0.06035
67	C	11	px	Ryd(3p)	0.00595	0.34696
68	C	11	py	Val(2p)	1.04428	-0.10144
69	C	11	py	Ryd(3p)	0.00304	0.37339
70	C	11	pz	Val(2p)	1.02710	-0.14414
71	C	11	pz	Ryd(3p)	0.00341	0.32163
72	C	12	S	Cor(1S)	1.99860	-10.07897
73	C	12	S	Val(2S)	0.87686	-0.04148
74	C	12	S	Ryd(3S)	0.00046	0.93356
75	C	12	px	Val(2p)	1.04962	-0.11940
76	C	12	px	Ryd(3p)	0.00305	0.37150
77	C	12	py	Val(2p)	1.12539	0.06061
78	C	12	py	Ryd(3p)	0.00590	0.30891
79	C	12	pz	Val(2p)	1.01127	-0.15385
80	C	12	pz	Ryd(3p)	0.00315	0.30871
81	C	13	S	Cor(1S)	1.99908	-10.12502
82	C	13	S	Val(2S)	0.93220	-0.18576
83	C	13	S	Ryd(3S)	0.00101	1.08246
84	C	13	px	Val(2p)	1.09385	-0.10538
85	C	13	px	Ryd(3p)	0.00373	0.44158
86	C	13	py	Val(2p)	1.11245	-0.08955
87	C	13	py	Ryd(3p)	0.00742	0.40928
88	C	13	pz	Val(2p)	1.04538	-0.18510
89	C	13	pz	Ryd(3p)	0.00355	0.38011
90	C	14	S	Cor(1S)	1.99897	-10.11174
91	C	14	S	Val(2S)	0.92086	-0.17825
92	C	14	S	Ryd(3S)	0.00049	1.40005
93	C	14	px	Val(2p)	1.14888	-0.05590
94	C	14	px	Ryd(3p)	0.00842	0.39511
95	C	14	py	Val(2p)	1.02246	-0.13614
96	C	14	py	Ryd(3p)	0.00437	0.39590
97	C	14	pz	Val(2p)	1.03006	-0.13302
98	C	14	pz	Ryd(3p)	0.00304	0.39497
99	C	15	S	Cor(1S)	1.99918	-10.05755
100	C	15	S	Val(2S)	1.01189	-0.17118
101	C	15	S	Ryd(3S)	0.00044	1.06938
102	C	15	px	Val(2p)	1.20146	-0.10145
103	C	15	px	Ryd(3p)	0.00181	0.20982
104	C	15	py	Val(2p)	1.22679	-0.09212
105	C	15	py	Ryd(3p)	0.00255	0.25477
106	C	15	pz	Val(2p)	1.13137	-0.11532
107	C	15	pz	Ryd(3p)	0.00335	0.25078
108	H	16	S	Val(1S)	0.79807	0.12125
109	H	16	S	Ryd(2S)	0.00154	0.80588
110	H	17	S	Val(1S)	0.79812	0.12164
111	H	17	S	Ryd(2S)	0.00132	0.79396
112	H	18	S	Val(1S)	0.80593	0.11278
113	H	18	S	Ryd(2S)	0.00127	0.83343
114	C	19	S	Cor(1S)	1.99919	-10.05368
115	C	19	S	Val(2S)	1.00883	-0.16711

116	C	19	S	Ryd(3S)	0.00042	1.07018
117	C	19	px	Val(2p)	1.24151	-0.09272
118	C	19	px	Ryd(3p)	0.00220	0.24474
119	C	19	py	Val(2p)	1.15832	-0.10646
120	C	19	py	Ryd(3p)	0.00279	0.26979
121	C	19	pz	Val(2p)	1.16343	-0.10498
122	C	19	pz	Ryd(3p)	0.00285	0.24722
123	H	20	S	Val(1S)	0.80214	0.11945
124	H	20	S	Ryd(2S)	0.00122	0.80525
125	H	21	S	Val(1S)	0.79798	0.12269
126	H	21	S	Ryd(2S)	0.00133	0.80984
127	H	22	S	Val(1S)	0.80417	0.11611
128	H	22	S	Ryd(2S)	0.00160	0.83814
129	C	23	S	Cor(1S)	1.99907	-10.25071
130	C	23	S	Val(2S)	0.85588	-0.26859
131	C	23	S	Ryd(3S)	0.00466	0.98341
132	C	23	px	Val(2p)	0.92426	-0.19745
133	C	23	px	Ryd(3p)	0.00692	0.47526
134	C	23	py	Val(2p)	0.88814	-0.19480
135	C	23	py	Ryd(3p)	0.00866	0.44836
136	C	23	pz	Val(2p)	0.86846	-0.15560
137	C	23	pz	Ryd(3p)	0.00699	0.43547
138	C	24	S	Cor(1S)	1.99907	-10.10434
139	C	24	S	Val(2S)	1.02132	-0.23408
140	C	24	S	Ryd(3S)	0.00058	1.12788
141	C	24	px	Val(2p)	1.16285	-0.17238
142	C	24	px	Ryd(3p)	0.00324	0.23615
143	C	24	py	Val(2p)	1.25110	-0.15304
144	C	24	py	Ryd(3p)	0.00232	0.21037
145	C	24	pz	Val(2p)	1.20291	-0.16481
146	C	24	pz	Ryd(3p)	0.00284	0.21778
147	H	25	S	Val(1S)	0.76964	0.08941
148	H	25	S	Ryd(2S)	0.00129	0.86432
149	H	26	S	Val(1S)	0.77072	0.07769
150	H	26	S	Ryd(2S)	0.00109	0.80310
151	H	27	S	Val(1S)	0.77325	0.06896
152	H	27	S	Ryd(2S)	0.00119	0.85552
153	C	28	S	Cor(1S)	1.99882	-10.18747
154	C	28	S	Val(2S)	0.84601	-0.20681
155	C	28	S	Ryd(3S)	0.00189	1.07416
156	C	28	px	Val(2p)	0.99718	-0.14674
157	C	28	px	Ryd(3p)	0.00604	0.47160
158	C	28	py	Val(2p)	0.98233	-0.14024
159	C	28	py	Ryd(3p)	0.00764	0.54521
160	C	28	pz	Val(2p)	1.02870	-0.19937
161	C	28	pz	Ryd(3p)	0.00975	0.48189
162	C	29	S	Cor(1S)	1.99900	-10.15377
163	C	29	S	Val(2S)	0.89260	-0.21042
164	C	29	S	Ryd(3S)	0.00137	1.14676
165	C	29	px	Val(2p)	1.04372	-0.14084
166	C	29	px	Ryd(3p)	0.00896	0.58575
167	C	29	py	Val(2p)	1.04222	-0.12811

168	C	29	py	Ryd(3p)	0.00617	0.50000
169	C	29	pz	Val(2p)	0.99109	-0.17322
170	C	29	pz	Ryd(3p)	0.00758	0.44859
171	C	30	S	Cor(1S)	1.99889	-10.09573
172	C	30	S	Val(2S)	0.89521	-0.11227
173	C	30	S	Ryd(3S)	0.00094	1.01922
174	C	30	px	Val(2p)	1.08726	-0.08983
175	C	30	px	Ryd(3p)	0.00273	0.48146
176	C	30	py	Val(2p)	1.14060	-0.04083
177	C	30	py	Ryd(3p)	0.00767	0.31273
178	C	30	pz	Val(2p)	1.00960	-0.16918
179	C	30	pz	Ryd(3p)	0.00250	0.35710
180	C	31	S	Cor(1S)	1.99922	-10.12066
181	C	31	S	Val(2S)	0.93378	-0.17285
182	C	31	S	Ryd(3S)	0.00085	0.94226
183	C	31	px	Val(2p)	1.08831	-0.07598
184	C	31	px	Ryd(3p)	0.00408	0.36262
185	C	31	py	Val(2p)	1.09262	-0.09623
186	C	31	py	Ryd(3p)	0.00477	0.35313
187	C	31	pz	Val(2p)	1.03172	-0.14245
188	C	31	pz	Ryd(3p)	0.00355	0.32151
189	C	32	S	Cor(1S)	1.99905	-10.10748
190	C	32	S	Val(2S)	0.91324	-0.12777
191	C	32	S	Ryd(3S)	0.00065	0.91603
192	C	32	px	Val(2p)	1.11127	-0.02434
193	C	32	px	Ryd(3p)	0.00619	0.30306
194	C	32	py	Val(2p)	1.05079	-0.10265
195	C	32	py	Ryd(3p)	0.00312	0.37342
196	C	32	pz	Val(2p)	1.01109	-0.15632
197	C	32	pz	Ryd(3p)	0.00353	0.30318
198	C	33	S	Cor(1S)	1.99906	-10.12239
199	C	33	S	Val(2S)	0.92454	-0.17958
200	C	33	S	Ryd(3S)	0.00100	1.04310
201	C	33	px	Val(2p)	1.06634	-0.14035
202	C	33	px	Ryd(3p)	0.00537	0.38826
203	C	33	py	Val(2p)	1.15410	-0.06357
204	C	33	py	Ryd(3p)	0.00611	0.39889
205	C	33	pz	Val(2p)	1.05604	-0.18926
206	C	33	pz	Ryd(3p)	0.00339	0.39788
207	C	34	S	Cor(1S)	1.99911	-10.13177
208	C	34	S	Val(2S)	0.94745	-0.22701
209	C	34	S	Ryd(3S)	0.00051	1.39024
210	C	34	px	Val(2p)	1.03163	-0.13494
211	C	34	px	Ryd(3p)	0.00381	0.32257
212	C	34	py	Val(2p)	1.09350	-0.12043
213	C	34	py	Ryd(3p)	0.00729	0.47413
214	C	34	pz	Val(2p)	1.07296	-0.11484
215	C	34	pz	Ryd(3p)	0.00446	0.37496
216	C	35	S	Cor(1S)	1.99917	-10.05775
217	C	35	S	Val(2S)	1.01282	-0.17233
218	C	35	S	Ryd(3S)	0.00039	1.07031
219	C	35	px	Val(2p)	1.24284	-0.09062
220	C	35	px	Ryd(3p)	0.00232	0.25314
221	C	35	py	Val(2p)	1.10951	-0.11659
222	C	35	py	Ryd(3p)	0.00259	0.23107
223	C	35	pz	Val(2p)	1.20399	-0.09909

224	C	35	pz	Ryd(3p)	0.00313	0.23186
225	H	36	S	Val(1S)	0.80633	0.11297
226	H	36	S	Ryd(2S)	0.00142	0.82686
227	H	37	S	Val(1S)	0.79566	0.12557
228	H	37	S	Ryd(2S)	0.00128	0.80111
229	H	38	S	Val(1S)	0.79783	0.12467
230	H	38	S	Ryd(2S)	0.00122	0.79038
231	C	39	S	Cor(1S)	1.99918	-10.06503
232	C	39	S	Val(2S)	1.01292	-0.17710
233	C	39	S	Ryd(3S)	0.00049	1.07002
234	C	39	px	Val(2p)	1.17954	-0.11224
235	C	39	px	Ryd(3p)	0.00296	0.30469
236	C	39	py	Val(2p)	1.23437	-0.09555
237	C	39	py	Ryd(3p)	0.00274	0.28344
238	C	39	pz	Val(2p)	1.14023	-0.11852
239	C	39	pz	Ryd(3p)	0.00245	0.25918
240	H	40	S	Val(1S)	0.81209	0.10457
241	H	40	S	Ryd(2S)	0.00119	0.85759
242	H	41	S	Val(1S)	0.79679	0.11740
243	H	41	S	Ryd(2S)	0.00131	0.79134
244	H	42	S	Val(1S)	0.79808	0.12158
245	H	42	S	Ryd(2S)	0.00143	0.84430
246	C	43	S	Cor(1S)	1.99905	-10.25074
247	C	43	S	Val(2S)	0.85403	-0.26639
248	C	43	S	Ryd(3S)	0.00485	0.96548
249	C	43	px	Val(2p)	0.82861	-0.21204
250	C	43	px	Ryd(3p)	0.00906	0.43831
251	C	43	py	Val(2p)	0.98184	-0.18769
252	C	43	py	Ryd(3p)	0.00627	0.53732
253	C	43	pz	Val(2p)	0.86941	-0.14923
254	C	43	pz	Ryd(3p)	0.00696	0.44083
255	C	44	S	Cor(1S)	1.99907	-10.10650
256	C	44	S	Val(2S)	1.02293	-0.23659
257	C	44	S	Ryd(3S)	0.00057	1.11131
258	C	44	px	Val(2p)	1.24905	-0.15192
259	C	44	px	Ryd(3p)	0.00152	0.24298
260	C	44	py	Val(2p)	1.16004	-0.17522
261	C	44	py	Ryd(3p)	0.00381	0.23140
262	C	44	pz	Val(2p)	1.20613	-0.16383
263	C	44	pz	Ryd(3p)	0.00271	0.21375
264	H	45	S	Val(1S)	0.76997	0.08805
265	H	45	S	Ryd(2S)	0.00125	0.85407
266	H	46	S	Val(1S)	0.77360	0.07630
267	H	46	S	Ryd(2S)	0.00101	0.80367
268	H	47	S	Val(1S)	0.77039	0.07366
269	H	47	S	Ryd(2S)	0.00108	0.83039
270	C	48	S	Cor(1S)	1.99882	-10.19319
271	C	48	S	Val(2S)	0.84400	-0.20950
272	C	48	S	Ryd(3S)	0.00193	1.09493

273	C	48	px	Val(2p)	1.06694	-0.14786
274	C	48	px	Ryd(3p)	0.00570	0.51649
275	C	48	py	Val(2p)	0.91875	-0.14584
276	C	48	py	Ryd(3p)	0.00701	0.50163
277	C	48	pz	Val(2p)	1.02050	-0.19595
278	C	48	pz	Ryd(3p)	0.01031	0.50461
279	C	49	S	Cor(1S)	1.99897	-10.15331
280	C	49	S	Val(2S)	0.89025	-0.20885
281	C	49	S	Ryd(3S)	0.00134	1.13968
282	C	49	px	Val(2p)	1.05840	-0.13353
283	C	49	px	Ryd(3p)	0.00740	0.58215
284	C	49	py	Val(2p)	1.04189	-0.15077
285	C	49	py	Ryd(3p)	0.00713	0.49129
286	C	49	pz	Val(2p)	1.00988	-0.16944
287	C	49	pz	Ryd(3p)	0.00720	0.46459
288	C	50	S	Cor(1S)	1.99907	-10.11805
289	C	50	S	Val(2S)	0.93192	-0.18389
290	C	50	S	Ryd(3S)	0.00094	1.02161
291	C	50	px	Val(2p)	1.16585	-0.06050
292	C	50	px	Ryd(3p)	0.00690	0.38882
293	C	50	py	Val(2p)	1.03835	-0.13542
294	C	50	py	Ryd(3p)	0.00308	0.40103
295	C	50	pz	Val(2p)	1.01331	-0.16137
296	C	50	pz	Ryd(3p)	0.00302	0.33869
297	C	51	S	Cor(1S)	1.99915	-10.11084
298	C	51	S	Val(2S)	0.92699	-0.15757
299	C	51	S	Ryd(3S)	0.00068	0.92099
300	C	51	px	Val(2p)	1.07423	-0.07802
301	C	51	px	Ryd(3p)	0.00331	0.38517
302	C	51	py	Val(2p)	1.08793	-0.09476
303	C	51	py	Ryd(3p)	0.00552	0.31619
304	C	51	pz	Val(2p)	1.03803	-0.13268
305	C	51	pz	Ryd(3p)	0.00369	0.31218
306	C	52	S	Cor(1S)	1.99921	-10.12840
307	C	52	S	Val(2S)	0.94036	-0.18890
308	C	52	S	Ryd(3S)	0.00075	0.92157
309	C	52	px	Val(2p)	1.10138	-0.08499
310	C	52	px	Ryd(3p)	0.00477	0.36204
311	C	52	py	Val(2p)	1.07820	-0.10031
312	C	52	py	Ryd(3p)	0.00455	0.34307
313	C	52	pz	Val(2p)	1.02182	-0.15580
314	C	52	pz	Ryd(3p)	0.00352	0.30907
315	C	53	S	Cor(1S)	1.99906	-10.12647
316	C	53	S	Val(2S)	0.92450	-0.18435
317	C	53	S	Ryd(3S)	0.00106	1.04226
318	C	53	px	Val(2p)	1.16421	-0.05392
319	C	53	px	Ryd(3p)	0.00756	0.39307
320	C	53	py	Val(2p)	1.05528	-0.16014
321	C	53	py	Ryd(3p)	0.00379	0.38611
322	C	53	pz	Val(2p)	1.05467	-0.18423
323	C	53	pz	Ryd(3p)	0.00335	0.38415
324	C	54	S	Cor(1S)	1.99915	-10.13769
325	C	54	S	Val(2S)	0.95187	-0.23911
326	C	54	S	Ryd(3S)	0.00052	1.42055
327	C	54	px	Val(2p)	1.04990	-0.13657
328	C	54	px	Ryd(3p)	0.00613	0.48979

329	C	54	py	Val(2p)	1.12775	-0.10814
330	C	54	py	Ryd(3p)	0.00664	0.33244
331	C	54	pz	Val(2p)	1.01167	-0.14255
332	C	54	pz	Ryd(3p)	0.00274	0.38700
333	C	55	S	Cor(1S)	1.99916	-10.06492
334	C	55	S	Val(2S)	1.01167	-0.17896
335	C	55	S	Ryd(3S)	0.00047	1.07575
336	C	55	px	Val(2p)	1.22696	-0.09705
337	C	55	px	Ryd(3p)	0.00267	0.24345
338	C	55	py	Val(2p)	1.23709	-0.10166
339	C	55	py	Ryd(3p)	0.00202	0.26222
340	C	55	pz	Val(2p)	1.09211	-0.13308
341	C	55	pz	Ryd(3p)	0.00330	0.25454
342	H	56	S	Val(1S)	0.79505	0.12187
343	H	56	S	Ryd(2S)	0.00160	0.81022
344	H	57	S	Val(1S)	0.79665	0.11565
345	H	57	S	Ryd(2S)	0.00133	0.78894
346	H	58	S	Val(1S)	0.81619	0.09712
347	H	58	S	Ryd(2S)	0.00157	0.92973
348	C	59	S	Cor(1S)	1.99917	-10.05966
349	C	59	S	Val(2S)	1.01302	-0.17565
350	C	59	S	Ryd(3S)	0.00044	1.07304
351	C	59	px	Val(2p)	1.11690	-0.11876
352	C	59	px	Ryd(3p)	0.00292	0.24587
353	C	59	py	Val(2p)	1.24309	-0.09318
354	C	59	py	Ryd(3p)	0.00225	0.25650
355	C	59	pz	Val(2p)	1.20860	-0.09957
356	C	59	pz	Ryd(3p)	0.00302	0.25099
357	H	60	S	Val(1S)	0.79638	0.12210
358	H	60	S	Ryd(2S)	0.00119	0.80085
359	H	61	S	Val(1S)	0.79349	0.12590
360	H	61	S	Ryd(2S)	0.00116	0.82659
361	H	62	S	Val(1S)	0.80066	0.11624
362	H	62	S	Ryd(2S)	0.00161	0.79331
363	H	63	S	Val(1S)	0.81171	0.14245
364	H	63	S	Ryd(2S)	0.00156	0.91368
365	H	64	S	Val(1S)	0.81722	0.17625
366	H	64	S	Ryd(2S)	0.00163	0.85488
367	H	65	S	Val(1S)	0.90275	0.31958
368	H	65	S	Ryd(2S)	0.00193	0.74535
369	H	66	S	Val(1S)	0.82490	0.14493
370	H	66	S	Ryd(2S)	0.00173	0.96546
371	H	67	S	Val(1S)	0.83380	0.18341
372	H	67	S	Ryd(2S)	0.00308	0.88845
373	H	68	S	Val(1S)	0.84735	0.23812
374	H	68	S	Ryd(2S)	0.00227	0.88681
375	H	69	S	Val(1S)	0.80755	0.16359

376	H	69	S	Ryd(2S)	0.00187	0.86588
377	H	70	S	Val(1S)	0.85901	0.24626
378	H	70	S	Ryd(2S)	0.00166	0.80358
379	H	71	S	Val(1S)	0.83087	0.16039
380	H	71	S	Ryd(2S)	0.00160	0.95580
381	H	72	S	Val(1S)	0.81340	0.13279
382	H	72	S	Ryd(2S)	0.00271	0.88587
383	H	73	S	Val(1S)	0.81282	0.15077
384	H	73	S	Ryd(2S)	0.00165	0.91122
385	H	74	S	Val(1S)	0.82711	0.20420
386	H	74	S	Ryd(2S)	0.00188	0.84901
387	H	75	S	Val(1S)	0.81024	0.15343
388	H	75	S	Ryd(2S)	0.00142	0.86362
389	H	76	S	Val(1S)	0.82192	0.15694
390	H	76	S	Ryd(2S)	0.00157	0.93041
391	H	77	S	Val(1S)	0.81379	0.09645
392	H	77	S	Ryd(2S)	0.00261	0.93724
393	N	78	S	Cor(1S)	1.99936	-14.27015
394	N	78	S	Val(2S)	1.35906	-0.64535
395	N	78	S	Ryd(3S)	0.00212	1.64127
396	N	78	px	Val(2p)	1.45024	-0.33403
397	N	78	px	Ryd(3p)	0.01087	0.84700
398	N	78	py	Val(2p)	1.32774	-0.33066
399	N	78	py	Ryd(3p)	0.00533	0.66485
400	N	78	pz	Val(2p)	1.43505	-0.35864
401	N	78	pz	Ryd(3p)	0.00688	0.63682
402	N	79	S	Cor(1S)	1.99938	-14.27255
403	N	79	S	Val(2S)	1.36445	-0.65274
404	N	79	S	Ryd(3S)	0.00219	1.63845
405	N	79	px	Val(2p)	1.52834	-0.34979
406	N	79	px	Ryd(3p)	0.00763	0.69805
407	N	79	py	Val(2p)	1.29796	-0.32967
408	N	79	py	Ryd(3p)	0.00796	0.81545
409	N	79	pz	Val(2p)	1.40540	-0.35811
410	N	79	pz	Ryd(3p)	0.00643	0.63748
411	N	80	S	Cor(1S)	1.99935	-14.27397
412	N	80	S	Val(2S)	1.35429	-0.65040
413	N	80	S	Ryd(3S)	0.00228	1.64037
414	N	80	px	Val(2p)	1.27512	-0.33382
415	N	80	px	Ryd(3p)	0.00582	0.72062
416	N	80	py	Val(2p)	1.57002	-0.35366
417	N	80	py	Ryd(3p)	0.01116	0.79622
418	N	80	pz	Val(2p)	1.39683	-0.36244
419	N	80	pz	Ryd(3p)	0.00643	0.65260
420	Tl	81	S	Val(6S)	1.95204	-0.41212
421	Tl	81	S	Ryd(7S)	0.00019	10.33245
422	Tl	81	px	Val(6p)	0.03081	-0.07738
423	Tl	81	px	Ryd(7p)	0.00144	0.28427
424	Tl	81	py	Val(6p)	0.02918	-0.06861
425	Tl	81	py	Ryd(7p)	0.00168	0.30558

426	Tl	81	pz	Val(6p)	0.09308	-0.03013
427	Tl	81	pz	Ryd(7p)	0.00234	0.38458
428	Tl	81	dxy	Cor(5d)	1.99814	-0.83170
429	Tl	81	dxy	Ryd(6d)	0.00007	1.40745
430	Tl	81	dxz	Cor(5d)	1.99759	-0.82763
431	Tl	81	dxz	Ryd(6d)	0.00016	1.48405
432	Tl	81	dyz	Cor(5d)	1.99709	-0.82704
433	Tl	81	dyz	Ryd(6d)	0.00018	1.51843
434	Tl	81	dx2y2	Cor(5d)	1.99798	-0.83182
435	Tl	81	dx2y2	Ryd(6d)	0.00005	1.41231
436	Tl	81	dz2	Cor(5d)	1.99743	-0.82763
437	Tl	81	dz2	Ryd(6d)	0.00010	1.44805

[68 electrons found in the effective core potential]

WARNING: 1 low occupancy (<1.9990e) core orbital found on C 1
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 12
1 low occupancy (<1.9990e) core orbital found on C 14
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 48
1 low occupancy (<1.9990e) core orbital found on C 49
5 low occupancy (<1.9990e) core orbitals found on Tl 81

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.33719	1.99885	4.30687	0.03147	6.33719
H	2	0.22412	0.00000	0.77396	0.00191	0.77588
C	3	0.43191	1.99906	3.54223	0.02679	5.56809
C	4	-0.64484	1.99907	4.63703	0.00874	6.64484
H	5	0.22891	0.00000	0.76986	0.00123	0.77109
H	6	0.22592	0.00000	0.77304	0.00104	0.77408
H	7	0.22574	0.00000	0.77323	0.00103	0.77426
C	8	0.12429	1.99881	3.85161	0.02530	5.87571
C	9	-0.01989	1.99899	3.99728	0.02363	6.01989
C	10	-0.16676	1.99909	4.15365	0.01401	6.16676
C	11	-0.14635	1.99922	4.13400	0.01313	6.14635
C	12	-0.07429	1.99860	4.06313	0.01256	6.07429
C	13	-0.19868	1.99908	4.18389	0.01571	6.19868
C	14	-0.13756	1.99897	4.12227	0.01632	6.13756
C	15	-0.57883	1.99918	4.57151	0.00814	6.57883
H	16	0.20040	0.00000	0.79807	0.00154	0.79960
H	17	0.20056	0.00000	0.79812	0.00132	0.79944
H	18	0.19280	0.00000	0.80593	0.00127	0.80720
C	19	-0.57953	1.99919	4.57209	0.00826	6.57953
H	20	0.19664	0.00000	0.80214	0.00122	0.80336
H	21	0.20069	0.00000	0.79798	0.00133	0.79931
H	22	0.19423	0.00000	0.80417	0.00160	0.80577
C	23	0.43696	1.99907	3.53673	0.02723	5.56304
C	24	-0.64623	1.99907	4.63819	0.00898	6.64623
H	25	0.22907	0.00000	0.76964	0.00129	0.77093
H	26	0.22819	0.00000	0.77072	0.00109	0.77181
H	27	0.22556	0.00000	0.77325	0.00119	0.77444
C	28	0.12165	1.99882	3.85421	0.02532	5.87835

C	29	0.00730	1.99900	3.96963	0.02408	5.99270
C	30	-0.14541	1.99889	4.13267	0.01384	6.14541
C	31	-0.15889	1.99922	4.14642	0.01325	6.15889
C	32	-0.09894	1.99905	4.08639	0.01350	6.09894
C	33	-0.21596	1.99906	4.20102	0.01588	6.21596
C	34	-0.16073	1.99911	4.14555	0.01607	6.16073
C	35	-0.57676	1.99917	4.56917	0.00843	6.57676
H	36	0.19225	0.00000	0.80633	0.00142	0.80775
H	37	0.20307	0.00000	0.79566	0.00128	0.79693
H	38	0.20095	0.00000	0.79783	0.00122	0.79905
C	39	-0.57488	1.99918	4.56705	0.00865	6.57488
H	40	0.18672	0.00000	0.81209	0.00119	0.81328
H	41	0.20190	0.00000	0.79679	0.00131	0.79810
H	42	0.20049	0.00000	0.79808	0.00143	0.79951
C	43	0.43993	1.99905	3.53389	0.02713	5.56007
C	44	-0.64582	1.99907	4.63814	0.00860	6.64582
H	45	0.22878	0.00000	0.76997	0.00125	0.77122
H	46	0.22539	0.00000	0.77360	0.00101	0.77461
H	47	0.22854	0.00000	0.77039	0.00108	0.77146
C	48	0.12604	1.99882	3.85019	0.02495	5.87396
C	49	-0.02245	1.99897	4.00041	0.02307	6.02245
C	50	-0.16245	1.99907	4.14942	0.01395	6.16245
C	51	-0.13953	1.99915	4.12719	0.01320	6.13953
C	52	-0.15456	1.99921	4.14176	0.01359	6.15456
C	53	-0.21348	1.99906	4.19867	0.01575	6.21348
C	54	-0.15637	1.99915	4.14119	0.01602	6.15637
C	55	-0.57545	1.99916	4.56782	0.00847	6.57545
H	56	0.20335	0.00000	0.79505	0.00160	0.79665
H	57	0.20202	0.00000	0.79665	0.00133	0.79798
H	58	0.18224	0.00000	0.81619	0.00157	0.81776
C	59	-0.58943	1.99917	4.58161	0.00864	6.58943
H	60	0.20243	0.00000	0.79638	0.00119	0.79757
H	61	0.20535	0.00000	0.79349	0.00116	0.79465
H	62	0.19773	0.00000	0.80066	0.00161	0.80227
H	63	0.18673	0.00000	0.81171	0.00156	0.81327
H	64	0.18115	0.00000	0.81722	0.00163	0.81885
H	65	0.09531	0.00000	0.90275	0.00193	0.90469
H	66	0.17337	0.00000	0.82490	0.00173	0.82663
H	67	0.16312	0.00000	0.83380	0.00308	0.83688
H	68	0.15038	0.00000	0.84735	0.00227	0.84962
H	69	0.19058	0.00000	0.80755	0.00187	0.80942
H	70	0.13933	0.00000	0.85901	0.00166	0.86067
H	71	0.16753	0.00000	0.83087	0.00160	0.83247
H	72	0.18389	0.00000	0.81340	0.00271	0.81611
H	73	0.18553	0.00000	0.81282	0.00165	0.81447
H	74	0.17101	0.00000	0.82711	0.00188	0.82899
H	75	0.18834	0.00000	0.81024	0.00142	0.81166
H	76	0.17651	0.00000	0.82192	0.00157	0.82349
H	77	0.18360	0.00000	0.81379	0.00261	0.81640
N	78	-0.59663	1.99936	5.57207	0.02520	7.59663
N	79	-0.61974	1.99938	5.59615	0.02421	7.61974
N	80	-0.62132	1.99935	5.59627	0.02571	7.62132
Tl	81	0.90046	77.98823	2.10511	0.00620	80.09954
* Total *		1.00000	151.95394	195.34617	0.69989	348.00000

	Natural Population
Effective Core	68.00000
Core	83.95394 (99.9452% of 84)
Valence	195.34617 (99.6664% of 196)
Natural Minimal Basis	347.30011 (99.7989% of 348)

Natural Rydberg Basis 0.69989 (0.2011% of 348)

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.96)2p(3.35)3p(0.03)
H	2	1S(0.77)
C	3	[core]2S(0.85)2p(2.69)3p(0.02)
C	4	[core]2S(1.02)2p(3.61)3p(0.01)
H	5	1S(0.77)
H	6	1S(0.77)
H	7	1S(0.77)
C	8	[core]2S(0.85)2p(3.01)3p(0.02)
C	9	[core]2S(0.89)2p(3.10)3p(0.02)
C	10	[core]2S(0.94)2p(3.21)3p(0.01)
C	11	[core]2S(0.94)2p(3.19)3p(0.01)
C	12	[core]2S(0.88)2p(3.19)3p(0.01)
C	13	[core]2S(0.93)2p(3.25)3p(0.01)
C	14	[core]2S(0.92)2p(3.20)3p(0.02)
C	15	[core]2S(1.01)2p(3.56)3p(0.01)
H	16	1S(0.80)
H	17	1S(0.80)
H	18	1S(0.81)
C	19	[core]2S(1.01)2p(3.56)3p(0.01)
H	20	1S(0.80)
H	21	1S(0.80)
H	22	1S(0.80)
C	23	[core]2S(0.86)2p(2.68)3p(0.02)
C	24	[core]2S(1.02)2p(3.62)3p(0.01)
H	25	1S(0.77)
H	26	1S(0.77)
H	27	1S(0.77)
C	28	[core]2S(0.85)2p(3.01)3p(0.02)
C	29	[core]2S(0.89)2p(3.08)3p(0.02)
C	30	[core]2S(0.90)2p(3.24)3p(0.01)
C	31	[core]2S(0.93)2p(3.21)3p(0.01)
C	32	[core]2S(0.91)2p(3.17)3p(0.01)
C	33	[core]2S(0.92)2p(3.28)3p(0.01)
C	34	[core]2S(0.95)2p(3.20)3p(0.02)
C	35	[core]2S(1.01)2p(3.56)3p(0.01)
H	36	1S(0.81)
H	37	1S(0.80)
H	38	1S(0.80)
C	39	[core]2S(1.01)2p(3.55)3p(0.01)
H	40	1S(0.81)
H	41	1S(0.80)
H	42	1S(0.80)
C	43	[core]2S(0.85)2p(2.68)3p(0.02)
C	44	[core]2S(1.02)2p(3.62)3p(0.01)
H	45	1S(0.77)
H	46	1S(0.77)
H	47	1S(0.77)
C	48	[core]2S(0.84)2p(3.01)3p(0.02)
C	49	[core]2S(0.89)2p(3.11)3p(0.02)
C	50	[core]2S(0.93)2p(3.22)3p(0.01)
C	51	[core]2S(0.93)2p(3.20)3p(0.01)
C	52	[core]2S(0.94)2p(3.20)3p(0.01)
C	53	[core]2S(0.92)2p(3.27)3p(0.01)
C	54	[core]2S(0.95)2p(3.19)3p(0.02)
C	55	[core]2S(1.01)2p(3.56)3p(0.01)
H	56	1S(0.80)
H	57	1S(0.80)

H	58	1S(0.82)
C	59	[core]2S(1.01)2p(3.57)3p(0.01)
H	60	1S(0.80)
H	61	1S(0.79)
H	62	1S(0.80)
H	63	1S(0.81)
H	64	1S(0.82)
H	65	1S(0.90)
H	66	1S(0.82)
H	67	1S(0.83)
H	68	1S(0.85)
H	69	1S(0.81)
H	70	1S(0.86)
H	71	1S(0.83)
H	72	1S(0.81)
H	73	1S(0.81)
H	74	1S(0.83)
H	75	1S(0.81)
H	76	1S(0.82)
H	77	1S(0.81)
N	78	[core]2S(1.36)2p(4.21)3p(0.02)
N	79	[core]2S(1.36)2p(4.23)3p(0.02)
N	80	[core]2S(1.35)2p(4.24)3p(0.02)
Tl	81	[core]6S(1.95)6p(0.15)7p(0.01)

NBO analysis skipped by request.

1|1|UNPC-E-C07CYG43054|SP|RB3LYP|LANL2DZ|C34H43N3Tl1(1+)|MCDSTFM|03-Ap
r-2013|0||# rb3lyp/lanl2dz pop=npa geom=connectivity||single-Point XRD
 Monomer||1,1|C,0,0.01861,-0.083509,2.255965|H,0,0.004563,-0.122705,3.
235795|C,0,1.475694,0.037251,1.819378|C,0,2.383293,0.678773,2.817058|H
,0,3.26891,0.740388,2.450589|H,0,2.404998,0.148404,3.617819|H,0,2.0606
74,1.558898,3.024916|C,0,3.100261,-0.209698,0.131984|C,0,3.901979,-1.3
27516,-0.084833|C,0,5.12032,-1.118172,-0.730319|C,0,5.509287,0.147439,
-1.163167|C,0,4.696747,1.225405,-0.94872|C,0,3.488421,1.047147,-0.2973
04|C,0,3.511043,-2.694884,0.415175|C,0,4.301631,-3.060222,1.646233|H,0
,5.230767,-3.137415,1.418018|H,0,3.985941,-3.89728,1.993251|H,0,4.1915
28,-2.375482,2.311377|C,0,3.635796,-3.770424,-0.624249|H,0,3.09152,-3.
546877,-1.383296|H,0,3.345446,-4.607581,-0.256005|H,0,4.554096,-3.8437
78,-0.899697|C,0,-0.819518,1.110863,1.830107|C,0,-1.963955,1.431667,2.
722624|H,0,-2.44803,2.180175,2.366134|H,0,-1.635595,1.649364,3.597907|
H,0,-2.549087,0.671305,2.778766|C,0,-1.338571,2.731076,0.193238|C,0,-0
.817831,4.019156,0.044002|C,0,-1.657345,4.927439,-0.608713|C,0,-2.8593
8,4.613055,-1.091473|C,0,-3.35078,3.324906,-0.961731|C,0,-2.575807,2.3
84734,-0.308671|C,0,0.575307,4.362779,0.480037|C,0,0.677188,5.710898,1
.197953|H,0,0.293384,6.396553,0.647347|H,0,1.598956,5.913988,1.36741|H
,0,0.200933,5.664574,2.030595|C,0,1.507967,4.364168,-0.73349|H,0,1.482
544,3.502822,-1.157927|H,0,2.406176,4.551802,-0.446567|H,0,1.224468,5.
037208,-1.355743|C,0,-0.583107,-1.380062,1.735256|C,0,-0.367113,-2.582
691,2.595582|H,0,-0.836795,-3.332532,2.221255|H,0,-0.695737,-2.407635,
3.479846|H,0,0.571789,-2.782032,2.637478|C,0,-1.705379,-2.517673,-0.01
3464|C,0,-3.088728,-2.656069,-0.149691|C,0,-3.539864,-3.736897,-0.8935
65|C,0,-2.671563,-4.628305,-1.481231|C,0,-1.319113,-4.486814,-1.319917
|C,0,-0.828045,-3.42712,-0.58738|C,0,-4.016761,-1.680893,0.534937|C,0,
-4.239789,-2.088872,1.984061|H,0,-4.68936,-2.936869,2.012404|H,0,-4.77
882,-1.426662,2.424024|H,0,-3.393081,-2.161062,2.430149|C,0,-5.3658,-1
.509395,-0.173705|H,0,-5.216056,-1.346681,-1.108593|H,0,-5.836015,-0.7
64442,0.208441|H,0,-5.887201,-2.307161,-0.066446|H,0,5.705659,-1.85290
7,-0.918624|H,0,6.320426,0.169319,-1.62659|H,0,4.861412,1.941492,-1.17
3468|H,0,2.878627,1.747231,-0.224064|H,0,2.618643,-2.733005,0.597007|H
,0,-1.222838,5.658391,-0.709589|H,0,-3.468463,5.144209,-1.580622|H,0,-
4.101781,3.065483,-1.260104|H,0,-2.875714,1.530752,-0.193932|H,0,0.900

886,3.712996,1.118076|H,0,-4.457959,-3.880782,-1.073882|H,0,-3.11043,-
5.249296,-1.966502|H,0,-0.733023,-5.136672,-1.687849|H,0,0.084013,-3.3
77206,-0.477995|H,0,-3.558752,-0.802221,0.58052|N,0,1.779334,-0.372228
,0.664361|N,0,-0.508284,1.706202,0.748331|N,0,-1.185303,-1.346835,0.62
6165|Tl,0,-0.088425,0.101083,-1.291919||Version=IA32W-G09RevB.01|State
=1-A|HF=-1536.0607674|RMSD=5.589e-009|Dipole=-0.1935887,-0.162696,1.60
29179|Quadrupole=5.7587195,4.5309503,-10.2896698,0.8898621,0.5116285,-
0.3266483|PG=C01 [X(C34H43N3Tl1)]||@

TRUST EVERYONE, BUT CUT THE CARDS.
Job cpu time: 0 days 1 hours 15 minutes 27.0 seconds.
File lengths (MBytes): RWF=   106 Int=   0 D2E=   0 Chk=   8 Scr=   1
Normal termination of Gaussian 09 at Wed Apr 03 11:13:36 2013.

Appendix 3. Gaussian output for dication dimer, LANL2-DZ, HF-SCF.

```
 ******************************************
 Gaussian 09:  IA32W-G09RevB.01 12-Aug-2010
              28-Mar-2013
 ******************************************
 %chk=\\vdm09-g1.ds.man.ac.uk\HOME\Desktop\cation_only_edited.chk
 ----------------------------------------------------
 # hf/lanl2dz guess=local pop=npa geom=connectivity
 ----------------------------------------------------
 1/38=1,57=2/1;
 2/12=2,17=6,18=5,40=1/2;
 3/5=6,6=3,11=9,16=1,25=1,30=1/1,2,3;
 4/9=10/1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1,40=-1/1,7;
 99/5=1,9=1/99;
 ------------------
 CSD ENTRY ofm27p-1
 ------------------
 Symbolic Z-matrix:
 Charge =  2 Multiplicity = 1
 C(PDBName=C1,ResName=UNK,ResNum=1) -0.621     11.017    13.349
 H(PDBName=H1,ResName=UNK,ResNum=1) -1.177     10.346    12.9
 C(PDBName=C2,ResName=UNK,ResNum=1) -0.739     10.785    14.852
 C(PDBName=C3,ResName=UNK,ResNum=1) -2.015     10.148    15.295
 H(PDBName=H3A,ResName=UNK,ResNum=1) -2.016     10.067    16.252
 H(PDBName=H3B,ResName=UNK,ResNum=1) -2.09      9.275     14.9
 H(PDBName=H3C,ResName=UNK,ResNum=1) -2.757     10.69     15.018
 C(PDBName=C4,ResName=UNK,ResNum=1)  0.148     11.089    17.013
 C(PDBName=C5,ResName=UNK,ResNum=1)  0.985     10.208    17.693
 C(PDBName=C6,ResName=UNK,ResNum=1)  0.971     10.268    19.087
 C(PDBName=C7,ResName=UNK,ResNum=1)  0.176     11.185    19.77
 C(PDBName=C8,ResName=UNK,ResNum=1) -0.627     12.047    19.077
 C(PDBName=C9,ResName=UNK,ResNum=1) -0.643     11.998    17.693
 C(PDBName=C10,ResName=UNK,ResNum=1)  1.819     9.184     16.967
 C(PDBName=C11,ResName=UNK,ResNum=1)  1.205     7.812     17.086
 H(PDBName=H11A,ResName=UNK,ResNum=1)  1.219     7.534     18.005
 H(PDBName=H11B,ResName=UNK,ResNum=1)  1.706     7.189     16.556
```

H(PDBName=H11C,ResName=UNK,ResNum=1) 0.296 7.84 16.775
C(PDBName=C12,ResName=UNK,ResNum=1) 3.252 9.155 17.411
H(PDBName=H12A,ResName=UNK,ResNum=1) 3.644 10.023 17.287
H(PDBName=H12B,ResName=UNK,ResNum=1) 3.736 8.508 16.894
H(PDBName=H12C,ResName=UNK,ResNum=1) 3.294 8.916 18.342
C(PDBName=C13,ResName=UNK,ResNum=1) -1.123 12.389 12.928
C(PDBName=C14,ResName=UNK,ResNum=1) -1.683 12.464 11.553
H(PDBName=H14A,ResName=UNK,ResNum=1) -1.952 13.366 11.366
H(PDBName=H14B,ResName=UNK,ResNum=1) -2.443 11.882 11.485
H(PDBName=H14C,ResName=UNK,ResNum=1) -1.013 12.193 10.92
C(PDBName=C15,ResName=UNK,ResNum=1) -1.289 14.701 13.374
C(PDBName=C16,ResName=UNK,ResNum=1) -2.299 15.389 14.053
C(PDBName=C17,ResName=UNK,ResNum=1) -2.443 16.734 13.698
C(PDBName=C18,ResName=UNK,ResNum=1) -1.672 17.353 12.804
C(PDBName=C19,ResName=UNK,ResNum=1) -0.656 16.666 12.16
C(PDBName=C20,ResName=UNK,ResNum=1) -0.475 15.328 12.454
C(PDBName=C21,ResName=UNK,ResNum=1) -3.102 14.741 15.141
C(PDBName=C22,ResName=UNK,ResNum=1) -4.597 15.06 15.071
H(PDBName=H22A,ResName=UNK,ResNum=1) -4.721 16.012 15.051
H(PDBName=H22B,ResName=UNK,ResNum=1) -5.038 14.696 15.841
H(PDBName=H22C,ResName=UNK,ResNum=1) -4.969 14.672 14.275
C(PDBName=C23,ResName=UNK,ResNum=1) -2.556 15.167 16.506
H(PDBName=H23A,ResName=UNK,ResNum=1) -1.629 14.924 16.571
H(PDBName=H23B,ResName=UNK,ResNum=1) -3.051 14.724 17.201
H(PDBName=H23C,ResName=UNK,ResNum=1) -2.647 16.117 16.605
C(PDBName=C24,ResName=UNK,ResNum=1) 0.815 10.804 12.893
C(PDBName=C25,ResName=UNK,ResNum=1) 1.185 9.393 12.567
H(PDBName=H25A,ResName=UNK,ResNum=1) 2.083 9.368 12.227
H(PDBName=H25B,ResName=UNK,ResNum=1) 0.582 9.048 11.905
H(PDBName=H25C,ResName=UNK,ResNum=1) 1.129 8.856 13.361
C(PDBName=C26,ResName=UNK,ResNum=1) 2.969 11.72 12.532
C(PDBName=C27,ResName=UNK,ResNum=1) 3.431 12.293 11.344
C(PDBName=C28,ResName=UNK,ResNum=1) 4.804 12.3 11.145
C(PDBName=C29,ResName=UNK,ResNum=1) 5.677 11.78 12.074
C(PDBName=C30,ResName=UNK,ResNum=1) 5.203 11.206 13.224
C(PDBName=C31,ResName=UNK,ResNum=1) 3.845 11.176 13.461
C(PDBName=C32,ResName=UNK,ResNum=1) 2.448 12.825 10.329
C(PDBName=C33,ResName=UNK,ResNum=1) 1.935 11.697 9.445
H(PDBName=H33A,ResName=UNK,ResNum=1) 2.663 11.335 8.935
H(PDBName=H33B,ResName=UNK,ResNum=1) 1.264 12.038 8.848
H(PDBName=H33C,ResName=UNK,ResNum=1) 1.555 11.008 9.994
C(PDBName=C34,ResName=UNK,ResNum=1) 3.008 13.957 9.46
H(PDBName=H34A,ResName=UNK,ResNum=1) 3.415 14.62 10.024
H(PDBName=H34B,ResName=UNK,ResNum=1) 2.294 14.36 8.959
H(PDBName=H34C,ResName=UNK,ResNum=1) 3.663 13.603 8.857
H(PDBName=H6,ResName=UNK,ResNum=1) 1.538 9.696 19.606
H(PDBName=H7,ResName=UNK,ResNum=1) 0.278 11.174 20.699
H(PDBName=H8,ResName=UNK,ResNum=1) -1.078 12.575 19.405
H(PDBName=H9,ResName=UNK,ResNum=1) -1.108 12.636 17.199
H(PDBName=H10,ResName=UNK,ResNum=1) 1.915 9.405 16.088
H(PDBName=H17,ResName=UNK,ResNum=1) -3.034 17.078 14.214
H(PDBName=H18,ResName=UNK,ResNum=1) -1.668 18.26 12.539
H(PDBName=H19,ResName=UNK,ResNum=1) -0.128 17.012 11.593
H(PDBName=H20,ResName=UNK,ResNum=1) 0.176 14.842 12.038
H(PDBName=H21,ResName=UNK,ResNum=1) -3.047 13.778 15.075
H(PDBName=H28,ResName=UNK,ResNum=1) 5.205 12.708 10.391
H(PDBName=H29,ResName=UNK,ResNum=1) 6.536 11.897 11.825
H(PDBName=H30,ResName=UNK,ResNum=1) 5.812 10.806 13.832
H(PDBName=H31,ResName=UNK,ResNum=1) 3.561 10.76 14.23
H(PDBName=H32,ResName=UNK,ResNum=1) 1.65 13.154 10.819
N(PDBName=N1,ResName=UNK,ResNum=1) 0.214 11.175 15.584
N(PDBName=N2,ResName=UNK,ResNum=1) -0.994 13.352 13.751

N(PDBName=N3,ResName=UNK,ResNum=1)	1.576	11.81	12.849
Tl(PDBName=Tl1,ResName=UNK,ResNum=1)	1.393	13.539	14.838
Tl(PDBName=Tl1,ResName=UNK,ResNum=1)	2.419	13.341	18.333
C(PDBName=C4,ResName=UNK,ResNum=1)	3.665	15.791	16.158
C(PDBName=C5,ResName=UNK,ResNum=1)	2.828	16.672	15.478
C(PDBName=C6,ResName=UNK,ResNum=1)	2.842	16.612	14.084
C(PDBName=C7,ResName=UNK,ResNum=1)	3.637	15.695	13.401
C(PDBName=C8,ResName=UNK,ResNum=1)	4.44	14.833	14.094
C(PDBName=C9,ResName=UNK,ResNum=1)	4.456	14.882	15.478
C(PDBName=C1,ResName=UNK,ResNum=1)	4.433	15.863	19.822
H(PDBName=H1,ResName=UNK,ResNum=1)	4.99	16.534	20.271
C(PDBName=C2,ResName=UNK,ResNum=1)	4.551	16.095	18.319
C(PDBName=C3,ResName=UNK,ResNum=1)	5.827	16.732	17.876
H(PDBName=H3A,ResName=UNK,ResNum=1)	5.829	16.813	16.919
H(PDBName=H3B,ResName=UNK,ResNum=1)	5.903	17.605	18.271
H(PDBName=H3C,ResName=UNK,ResNum=1)	6.57	16.19	18.153
C(PDBName=C10,ResName=UNK,ResNum=1)	1.994	17.696	16.204
C(PDBName=C11,ResName=UNK,ResNum=1)	2.608	19.068	16.085
H(PDBName=H11A,ResName=UNK,ResNum=1)	2.594	19.346	15.166
H(PDBName=H11B,ResName=UNK,ResNum=1)	2.107	19.691	16.615
H(PDBName=H11C,ResName=UNK,ResNum=1)	3.516	19.04	16.396
C(PDBName=C12,ResName=UNK,ResNum=1)	0.56	17.725	15.759
H(PDBName=H12A,ResName=UNK,ResNum=1)	0.169	16.857	15.884
H(PDBName=H12B,ResName=UNK,ResNum=1)	0.077	18.373	16.277
H(PDBName=H12C,ResName=UNK,ResNum=1)	0.519	17.964	14.829
C(PDBName=C13,ResName=UNK,ResNum=1)	4.936	14.491	20.243
C(PDBName=C14,ResName=UNK,ResNum=1)	5.496	14.416	21.617
H(PDBName=H14A,ResName=UNK,ResNum=1)	5.765	13.514	21.805
H(PDBName=H14B,ResName=UNK,ResNum=1)	6.256	14.998	21.685
H(PDBName=H14C,ResName=UNK,ResNum=1)	4.825	14.687	22.251
C(PDBName=C15,ResName=UNK,ResNum=1)	5.102	12.179	19.796
C(PDBName=C16,ResName=UNK,ResNum=1)	6.111	11.491	19.118
C(PDBName=C17,ResName=UNK,ResNum=1)	6.256	10.146	19.473
C(PDBName=C18,ResName=UNK,ResNum=1)	5.485	9.527	20.367
C(PDBName=C19,ResName=UNK,ResNum=1)	4.469	10.214	21.01
C(PDBName=C20,ResName=UNK,ResNum=1)	4.288	11.552	20.717
C(PDBName=C21,ResName=UNK,ResNum=1)	6.915	12.139	18.03
C(PDBName=C22,ResName=UNK,ResNum=1)	8.41	11.82	18.1
H(PDBName=H22A,ResName=UNK,ResNum=1)	8.533	10.868	18.12
H(PDBName=H22B,ResName=UNK,ResNum=1)	8.851	12.184	17.33
H(PDBName=H22C,ResName=UNK,ResNum=1)	8.781	12.208	18.896
C(PDBName=C23,ResName=UNK,ResNum=1)	6.369	11.713	16.665
H(PDBName=H23A,ResName=UNK,ResNum=1)	5.442	11.956	16.6
H(PDBName=H23B,ResName=UNK,ResNum=1)	6.864	12.156	15.97
H(PDBName=H23C,ResName=UNK,ResNum=1)	6.46	10.763	16.566
C(PDBName=C24,ResName=UNK,ResNum=1)	2.998	16.076	20.278
C(PDBName=C25,ResName=UNK,ResNum=1)	2.628	17.487	20.604
H(PDBName=H25A,ResName=UNK,ResNum=1)	1.73	17.512	20.944
H(PDBName=H25B,ResName=UNK,ResNum=1)	3.231	17.832	21.266
H(PDBName=H25C,ResName=UNK,ResNum=1)	2.684	18.025	19.81
C(PDBName=C26,ResName=UNK,ResNum=1)	0.844	15.16	20.639
C(PDBName=C27,ResName=UNK,ResNum=1)	0.382	14.587	21.826
C(PDBName=C28,ResName=UNK,ResNum=1)	-0.992	14.58	22.025
C(PDBName=C29,ResName=UNK,ResNum=1)	-1.864	15.1	21.097
C(PDBName=C30,ResName=UNK,ResNum=1)	-1.39	15.674	19.947
C(PDBName=C31,ResName=UNK,ResNum=1)	-0.032	15.704	19.71
C(PDBName=C32,ResName=UNK,ResNum=1)	1.365	14.055	22.841
C(PDBName=C33,ResName=UNK,ResNum=1)	1.878	15.183	23.725
H(PDBName=H33A,ResName=UNK,ResNum=1)	1.15	15.545	24.236
H(PDBName=H33B,ResName=UNK,ResNum=1)	2.549	14.842	24.323
H(PDBName=H33C,ResName=UNK,ResNum=1)	2.257	15.872	23.176
C(PDBName=C34,ResName=UNK,ResNum=1)	0.805	12.923	23.711

H(PDBName=H34A,ResName=UNK,ResNum=1) 0.398 12.26 23.147
H(PDBName=H34B,ResName=UNK,ResNum=1) 1.519 12.52 24.211
H(PDBName=H34C,ResName=UNK,ResNum=1) 0.15 13.277 24.314
H(PDBName=H6,ResName=UNK,ResNum=1) 2.275 17.184 13.565
H(PDBName=H7,ResName=UNK,ResNum=1) 3.535 15.706 12.472
H(PDBName=H8,ResName=UNK,ResNum=1) 4.891 14.305 13.766
H(PDBName=H9,ResName=UNK,ResNum=1) 4.921 14.244 15.972
H(PDBName=H10,ResName=UNK,ResNum=1) 1.898 17.475 17.083
H(PDBName=H17,ResName=UNK,ResNum=1) 6.846 9.802 18.957
H(PDBName=H18,ResName=UNK,ResNum=1) 5.481 8.62 20.632
H(PDBName=H19,ResName=UNK,ResNum=1) 3.941 9.868 21.578
H(PDBName=H20,ResName=UNK,ResNum=1) 3.637 12.038 21.133
H(PDBName=H21,ResName=UNK,ResNum=1) 6.86 13.102 18.096
H(PDBName=H28,ResName=UNK,ResNum=1) -1.392 14.172 22.78
H(PDBName=H29,ResName=UNK,ResNum=1) -2.723 14.983 21.345
H(PDBName=H30,ResName=UNK,ResNum=1) -1.999 16.074 19.339
H(PDBName=H31,ResName=UNK,ResNum=1) 0.252 16.12 18.941
H(PDBName=H32,ResName=UNK,ResNum=1) 2.163 13.726 22.352
N(PDBName=N1,ResName=UNK,ResNum=1) 3.599 15.705 17.587
N(PDBName=N2,ResName=UNK,ResNum=1) 4.807 13.528 19.42
N(PDBName=N3,ResName=UNK,ResNum=1) 2.237 15.07 20.322

Residue 1 PDB Number 1_0 UNK charge 0.00000000 ave dist 0.000
Stoichiometry C68H86N6Tl2(2+)
Framework group C1[X(C68H86N6Tl2)]
Deg. of freedom 480
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.903023	0.051295	-2.737981
2	1	0	-4.514533	0.085596	-3.503394
3	6	0	-2.503247	-0.227432	-3.276213
4	6	0	-2.460164	-0.972930	-4.569492
5	1	0	-1.545611	-1.129417	-4.817515
6	1	0	-2.892297	-0.452722	-5.252444
7	1	0	-2.914133	-1.812707	-4.470777
8	6	0	-0.170439	-0.150782	-2.958032
9	6	0	0.684185	0.872376	-3.360395
10	6	0	2.019408	0.533222	-3.582174
11	6	0	2.485112	-0.764383	-3.385337
12	6	0	1.626865	-1.746963	-2.977845
13	6	0	0.293215	-1.440024	-2.765050
14	6	0	0.184239	2.270912	-3.616048
15	6	0	0.075302	2.538076	-5.096013
16	1	0	0.950346	2.513578	-5.490651
17	1	0	-0.315350	3.402468	-5.238301
18	1	0	-0.477148	1.865062	-5.502998
19	6	0	1.011329	3.333035	-2.953263
20	1	0	1.034524	3.177106	-2.005839
21	1	0	0.627484	4.194823	-3.126870
22	1	0	1.907183	3.306084	-3.303069
23	6	0	-4.397058	-1.039420	-1.801017
24	6	0	-5.870231	-1.237389	-1.780559
25	1	0	-6.091786	-1.924870	-1.148722
26	1	0	-6.170325	-1.496216	-2.654573
27	1	0	-6.299217	-0.417141	-1.523277
28	6	0	-3.930526	-2.580467	-0.074942

29	6	0	-3.537481	-3.917900	-0.181117
30	6	0	-3.868700	-4.722562	0.913689
31	6	0	-4.486773	-4.273217	2.005895
32	6	0	-4.844529	-2.938962	2.109501
33	6	0	-4.561165	-2.096006	1.051875
34	6	0	-2.743405	-4.417091	-1.351036
35	6	0	-3.218501	-5.772304	-1.879589
36	1	0	-3.237334	-6.408158	-1.160273
37	1	0	-2.617282	-6.078198	-2.561382
38	1	0	-4.100692	-5.679533	-2.247930
39	6	0	-1.265249	-4.513108	-0.965484
40	1	0	-0.951616	-3.651630	-0.678966
41	1	0	-0.754039	-4.801185	-1.727045
42	1	0	-1.160762	-5.146678	-0.252564
43	6	0	-3.945046	1.410207	-2.054612
44	6	0	-4.205935	2.575653	-2.953371
45	1	0	-4.280814	3.375466	-2.426758
46	1	0	-5.022881	2.432070	-3.435929
47	1	0	-3.479994	2.669176	-3.574825
48	6	0	-3.652669	2.677734	-0.075475
49	6	0	-4.641162	2.969572	0.868363
50	6	0	-4.446268	4.099082	1.650030
51	6	0	-3.329395	4.893029	1.516565
52	6	0	-2.380753	4.600231	0.572637
53	6	0	-2.535840	3.487717	-0.227047
54	6	0	-5.870955	2.099481	0.968797
55	6	0	-6.904465	2.519616	-0.066748
56	1	0	-7.202563	3.411803	0.123697
57	1	0	-7.652825	1.918078	-0.034507
58	1	0	-6.510077	2.493668	-0.940994
59	6	0	-6.505344	2.084019	2.364325
60	1	0	-5.825671	1.911567	3.021302
61	1	0	-7.171417	1.392791	2.406236
62	1	0	-6.912835	2.933227	2.539671
63	1	0	2.655230	1.199916	-3.845393
64	1	0	3.404316	-0.872897	-3.515165
65	1	0	1.834315	-2.474982	-2.848538
66	1	0	-0.287553	-2.068439	-2.397481
67	1	0	-0.623664	2.406848	-3.216657
68	1	0	-3.527049	-5.496860	0.780988
69	1	0	-4.706301	-4.730062	2.803385
70	1	0	-5.227296	-2.596463	2.784907
71	1	0	-4.795310	-1.214323	1.081259
72	1	0	-2.826831	-3.811705	-2.100233
73	1	0	-5.041747	4.344775	2.343442
74	1	0	-3.322704	5.561882	2.121677
75	1	0	-1.641429	5.183719	0.456500
76	1	0	-1.893421	3.336427	-0.866954
77	1	0	-5.612911	1.174631	0.717379
78	7	0	-1.519237	0.154047	-2.581712
79	7	0	-3.535959	-1.658124	-1.095997
80	7	0	-3.736426	1.452274	-0.810506
81	81	0	-1.816362	-0.095993	0.135685
82	81	0	1.816323	0.095450	-0.136066
83	6	0	0.170681	0.151034	2.958188
84	6	0	-0.683944	-0.872124	3.360551
85	6	0	-2.019167	-0.532970	3.582331
86	6	0	-2.484871	0.764635	3.385494
87	6	0	-1.626623	1.747215	2.978002
88	6	0	-0.292974	1.440276	2.765207
89	6	0	3.902984	-0.051837	2.737600
90	1	0	4.514774	-0.085344	3.503551

91	6	0	2.503207	0.226889	3.275832
92	6	0	2.460125	0.972387	4.569111
93	1	0	1.545852	1.129669	4.817671
94	1	0	2.892539	0.452974	5.252601
95	1	0	2.914375	1.812959	4.470934
96	6	0	-0.183997	-2.270660	3.616204
97	6	0	-0.075061	-2.537824	5.096170
98	1	0	-0.950105	-2.513326	5.490807
99	1	0	0.315592	-3.402216	5.238458
100	1	0	0.477109	-1.865605	5.502617
101	6	0	-1.012327	-3.333367	2.953071
102	1	0	-1.034283	-3.176854	2.005995
103	1	0	-0.627206	-4.195139	3.127848
104	1	0	-1.906942	-3.305832	3.303225
105	6	0	4.397299	1.039672	1.801173
106	6	0	5.869514	1.237852	1.780905
107	1	0	6.092028	1.925122	1.148879
108	1	0	6.169608	1.496679	2.654918
109	1	0	6.299178	0.416598	1.522896
110	6	0	3.929808	2.580930	0.075287
111	6	0	3.537442	3.917358	0.180736
112	6	0	3.868942	4.722814	-0.913532
113	6	0	4.487014	4.273469	-2.005739
114	6	0	4.843811	2.939425	-2.109156
115	6	0	4.561407	2.096258	-1.051719
116	6	0	2.743647	4.417343	1.351192
117	6	0	3.218742	5.772556	1.879746
118	1	0	3.237295	6.407615	1.159892
119	1	0	2.617523	6.078450	2.561539
120	1	0	4.100653	5.678990	2.247549
121	6	0	1.265490	4.513361	0.965640
122	1	0	0.951858	3.651882	0.679122
123	1	0	0.754281	4.801437	1.727201
124	1	0	1.161003	5.146930	0.252721
125	6	0	3.945288	-1.409955	2.054769
126	6	0	4.206177	-2.575401	2.953528
127	1	0	4.281056	-3.375214	2.426914
128	1	0	5.023122	-2.431818	3.436086
129	1	0	3.480273	-2.669493	3.575803
130	6	0	3.652911	-2.677482	0.075632
131	6	0	4.640444	-2.969109	-0.868017
132	6	0	4.445269	-4.099414	-1.650222
133	6	0	3.329636	-4.892777	-1.516408
134	6	0	2.380994	-4.599979	-0.572480
135	6	0	2.536082	-3.487465	0.227203
136	6	0	5.870238	-2.099018	-0.968451
137	6	0	6.903748	-2.519153	0.067093
138	1	0	7.202804	-3.411550	-0.123541
139	1	0	7.653067	-1.917826	0.034663
140	1	0	6.509079	-2.494000	0.940802
141	6	0	6.505586	-2.083767	-2.364168
142	1	0	5.825913	-1.911315	-3.021146
143	1	0	7.170699	-1.392328	-2.405890
144	1	0	6.913077	-2.932975	-2.539515
145	1	0	-2.654988	-1.199664	3.845550
146	1	0	-3.404074	0.873149	3.515322
147	1	0	-1.834074	2.475234	2.848695
148	1	0	0.287795	2.068691	2.397638
149	1	0	0.623905	-2.406596	3.216814
150	1	0	3.527009	5.496317	-0.781369
151	1	0	4.706543	4.730314	-2.803228
152	1	0	5.227537	2.596715	-2.784751

153	1	0	4.795551	1.214575	-1.081102
154	1	0	2.827073	3.811957	2.100390
155	1	0	5.041988	-4.344523	-2.343285
156	1	0	3.321986	-5.561420	-2.121332
157	1	0	1.641671	-5.183467	-0.456343
158	1	0	1.893663	-3.336175	0.867111
159	1	0	5.613153	-1.174379	-0.717222
160	7	0	1.519479	-0.153795	2.581869
161	7	0	3.536200	1.658376	1.096154
162	7	0	3.736668	-1.452022	0.810662

Rotational constants (GHZ): 0.0363398 0.0248776 0.0221224
Standard basis: LANL2DZ (5D, 7F)
There are 874 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 1 integral format.
Two-electron integral symmetry is turned on.
874 basis functions, 2254 primitive gaussians, 878 cartesian basis functions
280 alpha electrons 280 beta electrons
nuclear repulsion energy 14838.1292451976 Hartrees.
NAtoms= 162 NActive= 162 NUniq= 162 SFac= 1.00D+00 NAtFMM= 50 NAOKFM=T Big=T
One-electron integrals computed using PRISM.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 153735 NPrTT= 1086464 LenC2= 123334 LenP2D= 411860.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 874 RedAO= T NBF= 874
NBsUse= 874 1.00D-06 NBFU= 874
Initial guess orbitals will be localized using method 0.
Harris functional with IExCor= 205 diagonalized for initial guess.
ExpMin= 4.44D-02 ExpMax= 5.91D+03 ExpMxC= 2.05D+02 IAcc=2 IRadAn= 0 AccDes= 0.00D+00
HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 0 IDoV= 1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Defaulting to unpruned grid for atomic number 81.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
Omega= 0.000000 0.000000 1.000000 0.000000 0.000000 ICntrl= 500 IOpCl= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
I1Cent= 4 NGrid= 0.
Petite list used in FoFCou.
LocMO: Using Boys method
Initial Trace= 0.32263912D-01 Initial TraceA= 0.26228830D+04
RMSG= 0.21826247D-06
LocMO: Using Boys method
Initial Trace= 0.61616713D-01 Initial TraceA= 0.76698294D+02
Initial Trace= 0.61616713D-01 Initial TraceA= 0.76698294D+02
Initial Trace= 0.61616713D-01 Initial TraceA= 0.76698294D+02
Localization failed after 3 tries of 1000 iterations each. Last change= 0.81024714D-05
RMSG= 0.12953000D-03
Initial guess orbital symmetries:
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The electronic state of the initial guess is 1-A.

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Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on             energy=1.00D-06.
No special actions if energy rises.
Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
SCF Done:  E(RHF) =  -3049.18216743     A.U. after   15 cycles
           Convg  =    0.8302D-08             -V/T =  2.0017

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          Population analysis using the SCF density.

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Orbital symmetries:
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The electronic state is 1-A.
Alpha occ. eigenvalues -- -15.75088 -15.75084 -15.75023 -15.75015 -15.74633
Alpha occ. eigenvalues -- -15.74624 -11.49845 -11.49838 -11.49679 -11.49667
Alpha occ. eigenvalues -- -11.49597 -11.49591 -11.44399 -11.44398 -11.43842
Alpha occ. eigenvalues -- -11.43830 -11.43004 -11.42998 -11.42821 -11.42815
Alpha occ. eigenvalues -- -11.40729 -11.40726 -11.39819 -11.39819 -11.39439
Alpha occ. eigenvalues -- -11.39425 -11.39100 -11.39097 -11.38849 -11.38846
Alpha occ. eigenvalues -- -11.38650 -11.38646 -11.38473 -11.38472 -11.37972
Alpha occ. eigenvalues -- -11.37969 -11.37955 -11.37955 -11.37737 -11.37736
Alpha occ. eigenvalues -- -11.37179 -11.37175 -11.37041 -11.37034 -11.36766
Alpha occ. eigenvalues -- -11.36761 -11.36756 -11.36754 -11.36543 -11.36540
Alpha occ. eigenvalues -- -11.36513 -11.36511 -11.36471 -11.36468 -11.36399
Alpha occ. eigenvalues -- -11.36394 -11.36219 -11.36216 -11.36149 -11.36143
Alpha occ. eigenvalues -- -11.35875 -11.35871 -11.32319 -11.32313 -11.31504
Alpha occ. eigenvalues -- -11.31501 -11.31440 -11.31429 -11.31286 -11.31281
Alpha occ. eigenvalues -- -11.31066 -11.31064 -11.30741 -11.30734 -1.47608
Alpha occ. eigenvalues --   -1.47597 -1.45042 -1.45028 -1.44600 -1.44598
Alpha occ. eigenvalues --   -1.34550 -1.34443 -1.33424 -1.33306 -1.32896
Alpha occ. eigenvalues --   -1.32881 -1.27838 -1.27826 -1.27503 -1.27470
Alpha occ. eigenvalues --   -1.26333 -1.26326 -1.25890 -1.25883 -1.22966
Alpha occ. eigenvalues --   -1.22954 -1.22827 -1.22827 -1.20135 -1.20117
Alpha occ. eigenvalues --   -1.19700 -1.19660 -1.19485 -1.19453 -1.19076
Alpha occ. eigenvalues --   -1.19060 -1.18146 -1.18120 -1.17449 -1.17391
Alpha occ. eigenvalues --   -1.16494 -1.16473 -1.13302 -1.13298 -1.12896
Alpha occ. eigenvalues --   -1.12892 -1.12636 -1.12631 -1.06038 -1.06036
Alpha occ. eigenvalues --   -1.05080 -1.05072 -1.04212 -1.04188 -1.04024
Alpha occ. eigenvalues --   -1.03971 -1.03852 -1.03814 -1.02684 -1.02679
Alpha occ. eigenvalues --   -0.99562 -0.99407 -0.99394 -0.99386 -0.99243
Alpha occ. eigenvalues --   -0.98999 -0.98998 -0.98886 -0.98856 -0.98839
Alpha occ. eigenvalues --   -0.98600 -0.98588 -0.97492 -0.97462 -0.97315
Alpha occ. eigenvalues --   -0.97302 -0.96670 -0.96650 -0.95746 -0.95732
Alpha occ. eigenvalues --   -0.93575 -0.93563 -0.89620 -0.89584 -0.88652
Alpha occ. eigenvalues --   -0.88619 -0.86860 -0.86797 -0.86578 -0.86477
Alpha occ. eigenvalues --   -0.85877 -0.85855 -0.85508 -0.85497 -0.84084
Alpha occ. eigenvalues --   -0.84071 -0.83729 -0.83672 -0.82916 -0.82862

Alpha occ. eigenvalues --   -0.82486 -0.82475 -0.82172 -0.82137 -0.81959
Alpha occ. eigenvalues --   -0.81944 -0.80653 -0.80617 -0.80424 -0.80409
Alpha occ. eigenvalues --   -0.79960 -0.79941 -0.79866 -0.79836 -0.79419
Alpha occ. eigenvalues --   -0.79408 -0.79190 -0.79163 -0.78524 -0.78510
Alpha occ. eigenvalues --   -0.78404 -0.78325 -0.78203 -0.78088 -0.77971
Alpha occ. eigenvalues --   -0.77966 -0.77560 -0.77535 -0.76965 -0.76950
Alpha occ. eigenvalues --   -0.75954 -0.75814 -0.75002 -0.74988 -0.74392
Alpha occ. eigenvalues --   -0.74358 -0.74083 -0.74069 -0.73975 -0.73942
Alpha occ. eigenvalues --   -0.73336 -0.73334 -0.73221 -0.73182 -0.72941
Alpha occ. eigenvalues --   -0.72896 -0.72617 -0.72607 -0.72505 -0.72498
Alpha occ. eigenvalues --   -0.72264 -0.72248 -0.71716 -0.71176 -0.70742
Alpha occ. eigenvalues --   -0.70652 -0.70188 -0.70103 -0.69421 -0.68977
Alpha occ. eigenvalues --   -0.68526 -0.68422 -0.67861 -0.67389 -0.66677
Alpha occ. eigenvalues --   -0.66619 -0.66054 -0.65860 -0.65342 -0.65264
Alpha occ. eigenvalues --   -0.64990 -0.64707 -0.64308 -0.64160 -0.63742
Alpha occ. eigenvalues --   -0.63666 -0.63308 -0.63154 -0.63102 -0.62911
Alpha occ. eigenvalues --   -0.62858 -0.62781 -0.62475 -0.62222 -0.61801
Alpha occ. eigenvalues --   -0.61765 -0.61241 -0.61078 -0.60814 -0.60772
Alpha occ. eigenvalues --   -0.59364 -0.59202 -0.59015 -0.58975 -0.58936
Alpha occ. eigenvalues --   -0.58893 -0.53377 -0.50446 -0.50333 -0.50006
Alpha occ. eigenvalues --   -0.49328 -0.49317 -0.49097 -0.48996 -0.48929
Alpha occ. eigenvalues --   -0.47901 -0.47640 -0.47141 -0.46997 -0.46472
Alpha virt. eigenvalues --   -0.09331 -0.09302 -0.06106 -0.05745 -0.04694
Alpha virt. eigenvalues --   -0.04613 -0.04321 -0.04315 -0.03390 -0.03381
Alpha virt. eigenvalues --   -0.03221 -0.02677 -0.02484 -0.01903 -0.01763
Alpha virt. eigenvalues --   -0.01260 -0.00873 -0.00799 -0.00186 -0.00034
Alpha virt. eigenvalues --   0.00170   0.01132   0.03232   0.04732   0.05269
Alpha virt. eigenvalues --   0.05957   0.05971   0.06623   0.06991   0.07401
Alpha virt. eigenvalues --   0.07405   0.08013   0.08023   0.09214   0.09332
Alpha virt. eigenvalues --   0.09642   0.09957   0.09972   0.10562   0.10808
Alpha virt. eigenvalues --   0.11008   0.11108   0.11261   0.11331   0.11912
Alpha virt. eigenvalues --   0.12028   0.12297   0.12396   0.12853   0.12904
Alpha virt. eigenvalues --   0.12953   0.13059   0.13218   0.13472   0.13771
Alpha virt. eigenvalues --   0.13907   0.14103   0.14186   0.14482   0.14509
Alpha virt. eigenvalues --   0.14682   0.14877   0.15002   0.15188   0.15244
Alpha virt. eigenvalues --   0.15529   0.15810   0.16049   0.16119   0.16121
Alpha virt. eigenvalues --   0.16255   0.16331   0.16666   0.16900   0.17241
Alpha virt. eigenvalues --   0.17474   0.17608   0.17750   0.18189   0.18247
Alpha virt. eigenvalues --   0.18286   0.18441   0.18507   0.18782   0.18789
Alpha virt. eigenvalues --   0.18905   0.19263   0.19363   0.19602   0.19740
Alpha virt. eigenvalues --   0.19765   0.19932   0.20419   0.20508   0.21098
Alpha virt. eigenvalues --   0.21246   0.21390   0.21575   0.21619   0.21690
Alpha virt. eigenvalues --   0.22012   0.22093   0.22390   0.22464   0.22483
Alpha virt. eigenvalues --   0.22885   0.22987   0.23196   0.23242   0.23770
Alpha virt. eigenvalues --   0.24017   0.24211   0.24383   0.24555   0.24618
Alpha virt. eigenvalues --   0.24737   0.24801   0.25335   0.25434   0.25515
Alpha virt. eigenvalues --   0.25721   0.25845   0.26132   0.26430   0.26443
Alpha virt. eigenvalues --   0.26493   0.26770   0.26805   0.27074   0.27363
Alpha virt. eigenvalues --   0.27632   0.28015   0.28155   0.28449   0.28499
Alpha virt. eigenvalues --   0.28536   0.28781   0.28873   0.28949   0.29064
Alpha virt. eigenvalues --   0.29497   0.29502   0.29756   0.29769   0.29951
Alpha virt. eigenvalues --   0.30347   0.30419   0.30475   0.30744   0.30995
Alpha virt. eigenvalues --   0.31041   0.31769   0.31967   0.32171   0.32402
Alpha virt. eigenvalues --   0.32568   0.32700   0.32722   0.32870   0.32894
Alpha virt. eigenvalues --   0.33374   0.33413   0.33723   0.33799   0.33872
Alpha virt. eigenvalues --   0.33938   0.34121   0.34220   0.34299   0.34712
Alpha virt. eigenvalues --   0.35170   0.35338   0.35515   0.35661   0.35811
Alpha virt. eigenvalues --   0.35852   0.36105   0.36277   0.36357   0.36526
Alpha virt. eigenvalues --   0.36772   0.36833   0.37338   0.37479   0.37620
Alpha virt. eigenvalues --   0.37867   0.38097   0.38180   0.38241   0.38410
Alpha virt. eigenvalues --   0.38537   0.38578   0.38863   0.39104   0.39187
Alpha virt. eigenvalues --   0.39503   0.39779   0.39943   0.40312   0.40421

Alpha virt. eigenvalues -- 0.40705 0.41010 0.41151 0.41298 0.41509
Alpha virt. eigenvalues -- 0.41540 0.41853 0.41980 0.42295 0.42471
Alpha virt. eigenvalues -- 0.42474 0.42720 0.43032 0.43134 0.43309
Alpha virt. eigenvalues -- 0.43411 0.43652 0.43778 0.44063 0.44439
Alpha virt. eigenvalues -- 0.44518 0.44727 0.44960 0.45034 0.45369
Alpha virt. eigenvalues -- 0.45560 0.45844 0.46069 0.46123 0.46151
Alpha virt. eigenvalues -- 0.46351 0.46524 0.46593 0.46792 0.47413
Alpha virt. eigenvalues -- 0.47528 0.47845 0.47879 0.48061 0.48274
Alpha virt. eigenvalues -- 0.48562 0.48898 0.49426 0.49543 0.49663
Alpha virt. eigenvalues -- 0.49667 0.49902 0.50145 0.50405 0.50540
Alpha virt. eigenvalues -- 0.50758 0.51013 0.51134 0.51169 0.51528
Alpha virt. eigenvalues -- 0.51636 0.51912 0.52047 0.52319 0.52588
Alpha virt. eigenvalues -- 0.52700 0.52842 0.53147 0.53285 0.53427
Alpha virt. eigenvalues -- 0.53590 0.53845 0.53981 0.54173 0.54198
Alpha virt. eigenvalues -- 0.55025 0.55334 0.55507 0.55575 0.55635
Alpha virt. eigenvalues -- 0.56209 0.56320 0.56712 0.56782 0.57397
Alpha virt. eigenvalues -- 0.57573 0.57618 0.57858 0.58232 0.58375
Alpha virt. eigenvalues -- 0.58461 0.58708 0.58718 0.59226 0.59548
Alpha virt. eigenvalues -- 0.59733 0.59943 0.60186 0.60639 0.60759
Alpha virt. eigenvalues -- 0.60986 0.61144 0.61269 0.61854 0.62084
Alpha virt. eigenvalues -- 0.62211 0.62447 0.62780 0.62935 0.63194
Alpha virt. eigenvalues -- 0.63424 0.63446 0.63749 0.63936 0.64115
Alpha virt. eigenvalues -- 0.64393 0.64596 0.64635 0.65179 0.65466
Alpha virt. eigenvalues -- 0.65794 0.66062 0.66169 0.66414 0.66633
Alpha virt. eigenvalues -- 0.66686 0.66836 0.67144 0.67297 0.67706
Alpha virt. eigenvalues -- 0.67835 0.68238 0.68621 0.68728 0.68791
Alpha virt. eigenvalues -- 0.69179 0.69189 0.69551 0.69590 0.70057
Alpha virt. eigenvalues -- 0.70622 0.70636 0.71069 0.71196 0.71750
Alpha virt. eigenvalues -- 0.71921 0.72246 0.72270 0.72556 0.72818
Alpha virt. eigenvalues -- 0.73124 0.73133 0.73575 0.73882 0.73968
Alpha virt. eigenvalues -- 0.74386 0.74707 0.74743 0.75460 0.75709
Alpha virt. eigenvalues -- 0.75967 0.76000 0.76771 0.76899 0.77451
Alpha virt. eigenvalues -- 0.77500 0.77853 0.78321 0.78683 0.78729
Alpha virt. eigenvalues -- 0.79126 0.80095 0.80108 0.80460 0.81081
Alpha virt. eigenvalues -- 0.81414 0.81601 0.82021 0.82660 0.82853
Alpha virt. eigenvalues -- 0.83223 0.83503 0.83878 0.84953 0.85425
Alpha virt. eigenvalues -- 0.85785 0.86277 0.86398 0.87373 0.88317
Alpha virt. eigenvalues -- 0.88361 0.88574 0.89227 0.89667 0.89926
Alpha virt. eigenvalues -- 0.90148 0.90585 0.91349 0.91483 0.91798
Alpha virt. eigenvalues -- 0.92350 0.92760 0.92972 0.93887 0.94374
Alpha virt. eigenvalues -- 0.94823 0.96183 0.96978 0.97136 0.97275
Alpha virt. eigenvalues -- 0.97432 0.98346 0.98655 0.99130 0.99769
Alpha virt. eigenvalues -- 1.00296 1.00628 1.00865 1.01814 1.02757
Alpha virt. eigenvalues -- 1.04318 1.05952 1.08030 1.09066 1.09234
Alpha virt. eigenvalues -- 1.09642 1.12297 1.13442 1.13620 1.14103
Alpha virt. eigenvalues -- 1.16232 1.16783 1.16892 1.18859 1.21355
Alpha virt. eigenvalues -- 1.21982 1.22293 1.22734 1.22892 1.22957
Alpha virt. eigenvalues -- 1.23305 1.23510 1.24306 1.24838 1.25693
Alpha virt. eigenvalues -- 1.25921 1.26932 1.27269 1.28373 1.28803
Alpha virt. eigenvalues -- 1.29143 1.31460 1.31718 1.31767 1.32328
Alpha virt. eigenvalues -- 1.32673 1.33087 1.34621 1.35238 1.35996
Alpha virt. eigenvalues -- 1.36035 1.37513 1.38027 1.38089 1.38657
Alpha virt. eigenvalues -- 1.38770 1.38961 1.39263 1.39272 1.39895
Alpha virt. eigenvalues -- 1.40550 1.40710 1.41287 1.41496 1.41839
Alpha virt. eigenvalues -- 1.42011 1.42391 1.42515 1.42709 1.42735
Alpha virt. eigenvalues -- 1.43241 1.43410 1.43817 1.44272 1.44410
Alpha virt. eigenvalues -- 1.44662 1.44726 1.44944 1.45059 1.45426
Alpha virt. eigenvalues -- 1.45859 1.46335 1.46648 1.46673 1.47546
Alpha virt. eigenvalues -- 1.47651 1.48010 1.48379 1.48542 1.48953
Alpha virt. eigenvalues -- 1.49329 1.49693 1.49749 1.50642 1.50730
Alpha virt. eigenvalues -- 1.51148 1.51167 1.51586 1.51720 1.52164
Alpha virt. eigenvalues -- 1.52178 1.52416 1.52603 1.53687 1.53768

```
 Alpha virt. eigenvalues --    1.54347   1.54387   1.55288   1.55421   1.55820
 Alpha virt. eigenvalues --    1.56069   1.56622   1.56904   1.57221   1.57494
 Alpha virt. eigenvalues --    1.58083   1.58523   1.58545   1.58863   1.59323
 Alpha virt. eigenvalues --    1.59603   1.60139   1.60507   1.60771   1.61000
 Alpha virt. eigenvalues --    1.61110   1.61464   1.62028   1.62308   1.63412
 Alpha virt. eigenvalues --    1.63742   1.64264   1.64439   1.64682   1.65232
 Alpha virt. eigenvalues --    1.65442   1.66726   1.67039   1.67645   1.68252
 Alpha virt. eigenvalues --    1.68797   1.69084   1.69282   1.70001   1.70716
 Alpha virt. eigenvalues --    1.71119   1.71767   1.72397   1.72433   1.74789
 Alpha virt. eigenvalues --    1.75517   1.76024   1.76056   1.77146   1.77785
 Alpha virt. eigenvalues --    1.78425   1.79487   1.80623   1.80675   1.81787
 Alpha virt. eigenvalues --    1.81862   1.82416   1.82621   1.84087   1.84388
 Alpha virt. eigenvalues --    1.85199   1.85368   1.86986   1.87814   1.88056
 Alpha virt. eigenvalues --    1.88411   1.89587   1.90192   1.90529   1.92132
 Alpha virt. eigenvalues --    1.95009   1.95599   1.95696   1.97487   2.04621
 Alpha virt. eigenvalues --    2.05814   2.06451   2.06695   2.09298   2.09788
 Alpha virt. eigenvalues --    2.16137   2.17473  11.53991  11.57164
          Condensed to atoms (all electrons):
 Mulliken atomic charges:
              1
     1  C   -0.252190
     2  H    0.250828
     3  C    0.216690
     4  C   -0.669704
     5  H    0.265583
     6  H    0.246625
     7  H    0.241505
     8  C    0.107307
     9  C    0.209248
    10  C   -0.372072
    11  C   -0.306830
    12  C   -0.435532
    13  C   -0.386803
    14  C   -0.219147
    15  C   -0.594735
    16  H    0.206865
    17  H    0.207936
    18  H    0.194467
    19  C   -0.609538
    20  H    0.196345
    21  H    0.216148
    22  H    0.206132
    23  C    0.231423
    24  C   -0.679376
    25  H    0.270524
    26  H    0.251100
    27  H    0.241855
    28  C    0.111095
    29  C    0.192873
    30  C   -0.340852
    31  C   -0.265355
    32  C   -0.348456
    33  C   -0.392464
    34  C   -0.218081
    35  C   -0.605227
    36  H    0.196501
    37  H    0.208089
    38  H    0.213872
    39  C   -0.613371
    40  H    0.189681
    41  H    0.211336
    42  H    0.209494
```

43	C	0.222424
44	C	-0.670828
45	H	0.267531
46	H	0.247170
47	H	0.239748
48	C	0.169735
49	C	0.211035
50	C	-0.359286
51	C	-0.321570
52	C	-0.232270
53	C	-0.402102
54	C	-0.188631
55	C	-0.600123
56	H	0.220378
57	H	0.212517
58	H	0.184616
59	C	-0.625848
60	H	0.193974
61	H	0.216849
62	H	0.209332
63	H	0.275532
64	H	0.278348
65	H	0.505514
66	H	0.300290
67	H	0.225592
68	H	0.317010
69	H	0.269346
70	H	0.351199
71	H	0.308607
72	H	0.202696
73	H	0.276545
74	H	0.303183
75	H	0.265057
76	H	0.311626
77	H	0.179088
78	N	-0.437361
79	N	-0.471568
80	N	-0.482800
81	Tl	0.843670
82	Tl	0.843656
83	C	0.107556
84	C	0.209256
85	C	-0.372062
86	C	-0.306827
87	C	-0.435517
88	C	-0.386861
89	C	-0.251924
90	H	0.250517
91	C	0.216378
92	C	-0.670271
93	H	0.265719
94	H	0.246739
95	H	0.241322
96	C	-0.219981
97	C	-0.594918
98	H	0.206827
99	H	0.207902
100	H	0.194854
101	C	-0.609052
102	H	0.196359
103	H	0.215704
104	H	0.206548

```
 105  C    0.231597
 106  C   -0.679641
 107  H    0.270587
 108  H    0.251188
 109  H    0.241371
 110  C    0.111142
 111  C    0.192365
 112  C   -0.341176
 113  C   -0.265516
 114  C   -0.347540
 115  C   -0.392533
 116  C   -0.218126
 117  C   -0.604925
 118  H    0.196419
 119  H    0.208037
 120  H    0.213894
 121  C   -0.613457
 122  H    0.189680
 123  H    0.211352
 124  H    0.209444
 125  C    0.222759
 126  C   -0.670923
 127  H    0.267528
 128  H    0.247251
 129  H    0.239643
 130  C    0.170366
 131  C    0.209987
 132  C   -0.358604
 133  C   -0.321508
 134  C   -0.232295
 135  C   -0.402321
 136  C   -0.189097
 137  C   -0.600182
 138  H    0.220266
 139  H    0.212347
 140  H    0.184868
 141  C   -0.625824
 142  H    0.193940
 143  H    0.216985
 144  H    0.209350
 145  H    0.275485
 146  H    0.278318
 147  H    0.505515
 148  H    0.300311
 149  H    0.225709
 150  H    0.317645
 151  H    0.269357
 152  H    0.350444
 153  H    0.308662
 154  H    0.202655
 155  H    0.276337
 156  H    0.303414
 157  H    0.265042
 158  H    0.311615
 159  H    0.179342
 160  N   -0.436492
 161  N   -0.471150
 162  N   -0.482849
Sum of Mulliken atomic charges =   2.00000
Mulliken charges with hydrogens summed into heavy atoms:
             1
     1  C   -0.001362
```

3	C	0.216690
4	C	0.084009
8	C	0.107307
9	C	0.209248
10	C	-0.096539
11	C	-0.028482
12	C	0.069983
13	C	-0.086513
14	C	0.006444
15	C	0.014533
19	C	0.009087
23	C	0.231423
24	C	0.084104
28	C	0.111095
29	C	0.192873
30	C	-0.023842
31	C	0.003991
32	C	0.002743
33	C	-0.083856
34	C	-0.015385
35	C	0.013236
39	C	-0.002860
43	C	0.222424
44	C	0.083622
48	C	0.169735
49	C	0.211035
50	C	-0.082741
51	C	-0.018387
52	C	0.032788
53	C	-0.090476
54	C	-0.009543
55	C	0.017389
59	C	-0.005693
78	N	-0.437361
79	N	-0.471568
80	N	-0.482800
81	Tl	0.843670
82	Tl	0.843656
83	C	0.107556
84	C	0.209256
85	C	-0.096577
86	C	-0.028508
87	C	0.069998
88	C	-0.086550
89	C	-0.001407
91	C	0.216378
92	C	0.083509
96	C	0.005728
97	C	0.014664
101	C	0.009558
105	C	0.231597
106	C	0.083506
110	C	0.111142
111	C	0.192365
112	C	-0.023531
113	C	0.003840
114	C	0.002904
115	C	-0.083871
116	C	-0.015471
117	C	0.013425
121	C	-0.002982
125	C	0.222759

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 126  C    0.083499
 130  C    0.170366
 131  C    0.209987
 132  C   -0.082267
 133  C   -0.018094
 134  C    0.032746
 135  C   -0.090707
 136  C   -0.009755
 137  C    0.017299
 141  C   -0.005549
 160  N   -0.436492
 161  N   -0.471150
 162  N   -0.482849
Sum of Mulliken charges with hydrogens summed into heavy atoms =   2.00000
Electronic spatial extent (au):  <R**2>=          55202.9585
Charge=             2.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=           -0.0031    Y=           -0.0015    Z=           -0.0048  Tot=            0.0059
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=         -298.8042   YY=         -390.5274   ZZ=         -383.5218
  XY=           -6.0084   XZ=           31.7039   YZ=           -0.4827
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=           58.8136   YY=          -32.9096   ZZ=          -25.9040
  XY=           -6.0084   XZ=           31.7039   YZ=           -0.4827
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=           -0.0861  YYY=           -0.1594  ZZZ=           -0.0239  XYY=           -0.0297
 XXY=            0.0396  XXZ=           -0.0790  XZZ=           -0.0555  YZZ=           -0.0228
 YYZ=           -0.0745  XYZ=           -0.0551
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=       -31841.8220 YYYY=       -20676.0528 ZZZZ=       -14703.6030 XXXY=         -663.8631
XXXZ=          371.9583 YYYX=          172.2126 YYYZ=          264.2004 ZZZX=          602.2799
ZZZY=         -245.5156 XXYY=        -9057.2627 XXZZ=        -7206.0783 YYZZ=        -5764.0171
XXYZ=          138.3847 YYXZ=         -319.5868 ZZXY=           78.7356
N-N= 1.483812924520D+04 E-N=-3.672155847758D+04  KE= 3.044102641575D+03
******************************Gaussian NBO Version 3.1******************************
         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
******************************Gaussian NBO Version 3.1******************************
     /RESON  / : Allow strongly delocalized NBO set

Analyzing the SCF density

Job title: CSD ENTRY ofm27p-1

Storage needed:   2371396 in NPA (  33481086 available)


NATURAL POPULATIONS:  Natural atomic orbital occupancies

  NAO  Atom  No  lang   Type(AO)    Occupancy      Energy
---------------------------------------------------------
    1    C    1  S      Cor( 1S)     1.99893     -11.27205
    2    C    1  S      Val( 2S)     0.96186      -0.36708
    3    C    1  S      Ryd( 3S)     0.00101       1.58822
    4    C    1  px     Val( 2p)     1.11642      -0.24400
    5    C    1  px     Ryd( 3p)     0.01288       0.55384
    6    C    1  py     Val( 2p)     1.07397      -0.26180
    7    C    1  py     Ryd( 3p)     0.00747       0.50405
    8    C    1  pz     Val( 2p)     1.14276      -0.23518
    9    C    1  pz     Ryd( 3p)     0.01640       0.57488

   10    H    2  S      Val( 1S)     0.79141       0.08711
```

11	H	2	S	Ryd(2S)	0.00188	1.10628
12	C	3	S	Cor(1S)	1.99910	-11.35481
13	C	3	S	Val(2S)	0.86100	-0.30022
14	C	3	S	Ryd(3S)	0.00588	1.14436
15	C	3	px	Val(2p)	0.90866	-0.15295
16	C	3	px	Ryd(3p)	0.00782	0.63484
17	C	3	py	Val(2p)	0.79617	-0.19456
18	C	3	py	Ryd(3p)	0.00875	0.53807
19	C	3	pz	Val(2p)	0.90593	-0.17738
20	C	3	pz	Ryd(3p)	0.00770	0.58516
21	C	4	S	Cor(1S)	1.99921	-11.18998
22	C	4	S	Val(2S)	1.02168	-0.29787
23	C	4	S	Ryd(3S)	0.00048	1.27553
24	C	4	px	Val(2p)	1.24801	-0.19929
25	C	4	px	Ryd(3p)	0.00333	0.28232
26	C	4	py	Val(2p)	1.19165	-0.19665
27	C	4	py	Ryd(3p)	0.00229	0.30510
28	C	4	pz	Val(2p)	1.11551	-0.20203
29	C	4	pz	Ryd(3p)	0.00359	0.28427
30	H	5	S	Val(1S)	0.78906	0.11082
31	H	5	S	Ryd(2S)	0.00177	1.02062
32	H	6	S	Val(1S)	0.78977	0.09810
33	H	6	S	Ryd(2S)	0.00118	0.94870
34	H	7	S	Val(1S)	0.79152	0.09487
35	H	7	S	Ryd(2S)	0.00119	0.95575
36	C	8	S	Cor(1S)	1.99883	-11.29468
37	C	8	S	Val(2S)	0.84033	-0.23918
38	C	8	S	Ryd(3S)	0.00213	1.28228
39	C	8	px	Val(2p)	0.88772	-0.13756
40	C	8	px	Ryd(3p)	0.01529	0.77112
41	C	8	py	Val(2p)	1.06946	-0.19183
42	C	8	py	Ryd(3p)	0.00611	0.60524
43	C	8	pz	Val(2p)	1.02354	-0.22612
44	C	8	pz	Ryd(3p)	0.00968	0.53457
45	C	9	S	Cor(1S)	1.99901	-11.25586
46	C	9	S	Val(2S)	0.89396	-0.26245
47	C	9	S	Ryd(3S)	0.00201	1.34440
48	C	9	px	Val(2p)	1.05920	-0.17506
49	C	9	px	Ryd(3p)	0.00814	0.66532
50	C	9	py	Val(2p)	1.06608	-0.18629
51	C	9	py	Ryd(3p)	0.01044	0.78458
52	C	9	pz	Val(2p)	0.97809	-0.19729
53	C	9	pz	Ryd(3p)	0.00815	0.59846
54	C	10	S	Cor(1S)	1.99917	-11.22975
55	C	10	S	Val(2S)	0.93608	-0.25868
56	C	10	S	Ryd(3S)	0.00123	1.23450
57	C	10	px	Val(2p)	1.10502	-0.14090
58	C	10	px	Ryd(3p)	0.00767	0.53040
59	C	10	py	Val(2p)	1.10607	-0.14228
60	C	10	py	Ryd(3p)	0.00542	0.61848
61	C	10	pz	Val(2p)	0.99658	-0.20457
62	C	10	pz	Ryd(3p)	0.00473	0.44020
63	C	11	S	Cor(1S)	1.99927	-11.22864

64	C	11	S	Val(2S)	0.93766	-0.24601
65	C	11	S	Ryd(3S)	0.00139	1.15270
66	C	11	px	Val(2p)	1.15098	-0.07987
67	C	11	px	Ryd(3p)	0.00767	0.56618
68	C	11	py	Val(2p)	1.04558	-0.15532
69	C	11	py	Ryd(3p)	0.00513	0.49905
70	C	11	pz	Val(2p)	1.00132	-0.20526
71	C	11	pz	Ryd(3p)	0.00544	0.45228
72	C	12	S	Cor(1S)	1.99869	-11.18199
73	C	12	S	Val(2S)	0.87488	-0.08383
74	C	12	S	Ryd(3S)	0.00097	1.16680
75	C	12	px	Val(2p)	1.05697	-0.14698
76	C	12	px	Ryd(3p)	0.00547	0.58273
77	C	12	py	Val(2p)	1.11289	0.02650
78	C	12	py	Ryd(3p)	0.00799	0.45816
79	C	12	pz	Val(2p)	0.99086	-0.19836
80	C	12	pz	Ryd(3p)	0.00622	0.50797
81	C	13	S	Cor(1S)	1.99915	-11.22924
82	C	13	S	Val(2S)	0.92837	-0.24426
83	C	13	S	Ryd(3S)	0.00129	1.29689
84	C	13	px	Val(2p)	1.09602	-0.14647
85	C	13	px	Ryd(3p)	0.00593	0.64182
86	C	13	py	Val(2p)	1.09939	-0.14630
87	C	13	py	Ryd(3p)	0.00857	0.51635
88	C	13	pz	Val(2p)	1.04271	-0.21043
89	C	13	pz	Ryd(3p)	0.00534	0.54299
90	C	14	S	Cor(1S)	1.99908	-11.20315
91	C	14	S	Val(2S)	0.92029	-0.22427
92	C	14	S	Ryd(3S)	0.00056	1.61746
93	C	14	px	Val(2p)	1.12586	-0.10578
94	C	14	px	Ryd(3p)	0.01017	0.50332
95	C	14	py	Val(2p)	1.00669	-0.14877
96	C	14	py	Ryd(3p)	0.00534	0.50625
97	C	14	pz	Val(2p)	1.04396	-0.14629
98	C	14	pz	Ryd(3p)	0.00423	0.57121
99	C	15	S	Cor(1S)	1.99932	-11.14347
100	C	15	S	Val(2S)	1.00955	-0.22887
101	C	15	S	Ryd(3S)	0.00068	1.25091
102	C	15	px	Val(2p)	1.21737	-0.13504
103	C	15	px	Ryd(3p)	0.00289	0.28576
104	C	15	py	Val(2p)	1.21073	-0.13170
105	C	15	py	Ryd(3p)	0.00357	0.32907
106	C	15	pz	Val(2p)	1.06666	-0.14271
107	C	15	pz	Ryd(3p)	0.00339	0.31558
108	H	16	S	Val(1S)	0.81864	0.13188
109	H	16	S	Ryd(2S)	0.00159	0.95180
110	H	17	S	Val(1S)	0.81555	0.13883
111	H	17	S	Ryd(2S)	0.00132	0.94405
112	H	18	S	Val(1S)	0.82517	0.12471
113	H	18	S	Ryd(2S)	0.00153	0.98833
114	C	19	S	Cor(1S)	1.99936	-11.14315
115	C	19	S	Val(2S)	1.00192	-0.21980
116	C	19	S	Ryd(3S)	0.00064	1.29075
117	C	19	px	Val(2p)	1.17466	-0.14137

118	C	19	px	Ryd(3p)	0.00288	0.44358
119	C	19	py	Val(2p)	1.14707	-0.14346
120	C	19	py	Ryd(3p)	0.00406	0.42527
121	C	19	pz	Val(2p)	1.17746	-0.13499
122	C	19	pz	Ryd(3p)	0.00401	0.40581
123	H	20	S	Val(1S)	0.83176	0.11545
124	H	20	S	Ryd(2S)	0.00163	1.13222
125	H	21	S	Val(1S)	0.81431	0.13999
126	H	21	S	Ryd(2S)	0.00130	1.00321
127	H	22	S	Val(1S)	0.82356	0.12103
128	H	22	S	Ryd(2S)	0.00200	1.07722
129	C	23	S	Cor(1S)	1.99910	-11.35409
130	C	23	S	Val(2S)	0.86216	-0.30181
131	C	23	S	Ryd(3S)	0.00599	1.17906
132	C	23	px	Val(2p)	0.94897	-0.16292
133	C	23	px	Ryd(3p)	0.00762	0.61354
134	C	23	py	Val(2p)	0.83456	-0.18183
135	C	23	py	Ryd(3p)	0.00985	0.56420
136	C	23	pz	Val(2p)	0.82173	-0.17730
137	C	23	pz	Ryd(3p)	0.00735	0.56772
138	C	24	S	Cor(1S)	1.99921	-11.18567
139	C	24	S	Val(2S)	1.01945	-0.29248
140	C	24	S	Ryd(3S)	0.00052	1.30306
141	C	24	px	Val(2p)	1.08138	-0.20344
142	C	24	px	Ryd(3p)	0.00417	0.26843
143	C	24	py	Val(2p)	1.23633	-0.19464
144	C	24	py	Ryd(3p)	0.00268	0.28121
145	C	24	pz	Val(2p)	1.24212	-0.19560
146	C	24	pz	Ryd(3p)	0.00273	0.32972
147	H	25	S	Val(1S)	0.78528	0.11765
148	H	25	S	Ryd(2S)	0.00164	1.02729
149	H	26	S	Val(1S)	0.78838	0.10460
150	H	26	S	Ryd(2S)	0.00122	0.95665
151	H	27	S	Val(1S)	0.79309	0.09182
152	H	27	S	Ryd(2S)	0.00141	1.02298
153	C	28	S	Cor(1S)	1.99887	-11.28162
154	C	28	S	Val(2S)	0.84282	-0.22953
155	C	28	S	Ryd(3S)	0.00213	1.25351
156	C	28	px	Val(2p)	1.03844	-0.21037
157	C	28	px	Ryd(3p)	0.00821	0.58847
158	C	28	py	Val(2p)	1.00248	-0.15896
159	C	28	py	Ryd(3p)	0.00740	0.70382
160	C	28	pz	Val(2p)	0.95165	-0.15270
161	C	28	pz	Ryd(3p)	0.01203	0.71391
162	C	29	S	Cor(1S)	1.99909	-11.24637
163	C	29	S	Val(2S)	0.89525	-0.25036
164	C	29	S	Ryd(3S)	0.00166	1.32968
165	C	29	px	Val(2p)	0.98873	-0.17977
166	C	29	px	Ryd(3p)	0.00867	0.61704
167	C	29	py	Val(2p)	1.04083	-0.15566
168	C	29	py	Ryd(3p)	0.00723	0.66828
169	C	29	pz	Val(2p)	1.04026	-0.16926

170	C	29	pz	Ryd(3p)	0.00961	0.71487
171	C	30	S	Cor(1S)	1.99902	-11.18389
172	C	30	S	Val(2S)	0.89533	-0.14333
173	C	30	S	Ryd(3S)	0.00082	1.17866
174	C	30	px	Val(2p)	1.01966	-0.15725
175	C	30	px	Ryd(3p)	0.00358	0.48237
176	C	30	py	Val(2p)	1.13809	-0.05310
177	C	30	py	Ryd(3p)	0.00844	0.38633
178	C	30	pz	Val(2p)	1.06352	-0.15371
179	C	30	pz	Ryd(3p)	0.00401	0.60754
180	C	31	S	Cor(1S)	1.99930	-11.21043
181	C	31	S	Val(2S)	0.93314	-0.21601
182	C	31	S	Ryd(3S)	0.00092	1.09451
183	C	31	px	Val(2p)	1.00363	-0.17061
184	C	31	px	Ryd(3p)	0.00445	0.43618
185	C	31	py	Val(2p)	1.07636	-0.12849
186	C	31	py	Ryd(3p)	0.00569	0.45170
187	C	31	pz	Val(2p)	1.11755	-0.07846
188	C	31	pz	Ryd(3p)	0.00613	0.47506
189	C	32	S	Cor(1S)	1.99915	-11.19673
190	C	32	S	Val(2S)	0.91255	-0.16364
191	C	32	S	Ryd(3S)	0.00067	1.09116
192	C	32	px	Val(2p)	1.01505	-0.15677
193	C	32	px	Ryd(3p)	0.00597	0.41362
194	C	32	py	Val(2p)	1.05668	-0.12009
195	C	32	py	Ryd(3p)	0.00459	0.49367
196	C	32	pz	Val(2p)	1.08833	-0.06421
197	C	32	pz	Ryd(3p)	0.00686	0.41796
198	C	33	S	Cor(1S)	1.99918	-11.21233
199	C	33	S	Val(2S)	0.92214	-0.22080
200	C	33	S	Ryd(3S)	0.00108	1.22010
201	C	33	px	Val(2p)	1.03973	-0.20267
202	C	33	px	Ryd(3p)	0.00596	0.48339
203	C	33	py	Val(2p)	1.15018	-0.08704
204	C	33	py	Ryd(3p)	0.00758	0.65136
205	C	33	pz	Val(2p)	1.06724	-0.18083
206	C	33	pz	Ryd(3p)	0.00603	0.60472
207	C	34	S	Cor(1S)	1.99922	-11.21822
208	C	34	S	Val(2S)	0.94685	-0.27348
209	C	34	S	Ryd(3S)	0.00058	1.60318
210	C	34	px	Val(2p)	1.00594	-0.15481
211	C	34	px	Ryd(3p)	0.00377	0.48577
212	C	34	py	Val(2p)	1.08159	-0.14814
213	C	34	py	Ryd(3p)	0.00895	0.63338
214	C	34	pz	Val(2p)	1.08489	-0.12302
215	C	34	pz	Ryd(3p)	0.00665	0.42957
216	C	35	S	Cor(1S)	1.99931	-11.13756
217	C	35	S	Val(2S)	1.01098	-0.22442
218	C	35	S	Ryd(3S)	0.00059	1.23917
219	C	35	px	Val(2p)	1.20587	-0.12728
220	C	35	px	Ryd(3p)	0.00357	0.32649
221	C	35	py	Val(2p)	1.08910	-0.13169
222	C	35	py	Ryd(3p)	0.00312	0.31026
223	C	35	pz	Val(2p)	1.19755	-0.12897
224	C	35	pz	Ryd(3p)	0.00315	0.30823

225	H	36	S	Val(1S)	0.82602	0.12908
226	H	36	S	Ryd(2S)	0.00159	0.97989
227	H	37	S	Val(1S)	0.81581	0.14498
228	H	37	S	Ryd(2S)	0.00133	0.95319
229	H	38	S	Val(1S)	0.81484	0.14803
230	H	38	S	Ryd(2S)	0.00140	0.94508
231	C	39	S	Cor(1S)	1.99933	-11.15296
232	C	39	S	Val(2S)	1.00867	-0.23427
233	C	39	S	Ryd(3S)	0.00076	1.24935
234	C	39	px	Val(2p)	1.08397	-0.15863
235	C	39	px	Ryd(3p)	0.00496	0.53590
236	C	39	py	Val(2p)	1.20378	-0.13693
237	C	39	py	Ryd(3p)	0.00374	0.36585
238	C	39	pz	Val(2p)	1.21023	-0.14001
239	C	39	pz	Ryd(3p)	0.00295	0.46601
240	H	40	S	Val(1S)	0.83655	0.10713
241	H	40	S	Ryd(2S)	0.00170	1.10801
242	H	41	S	Val(1S)	0.81644	0.13023
243	H	41	S	Ryd(2S)	0.00148	0.98739
244	H	42	S	Val(1S)	0.82081	0.12650
245	H	42	S	Ryd(2S)	0.00161	1.00927
246	C	43	S	Cor(1S)	1.99909	-11.35547
247	C	43	S	Val(2S)	0.86016	-0.30019
248	C	43	S	Ryd(3S)	0.00600	1.14807
249	C	43	px	Val(2p)	0.74324	-0.19945
250	C	43	px	Ryd(3p)	0.00859	0.52761
251	C	43	py	Val(2p)	0.98410	-0.20557
252	C	43	py	Ryd(3p)	0.00755	0.67900
253	C	43	pz	Val(2p)	0.87663	-0.12188
254	C	43	pz	Ryd(3p)	0.00848	0.59986
255	C	44	S	Cor(1S)	1.99921	-11.19041
256	C	44	S	Val(2S)	1.02112	-0.29796
257	C	44	S	Ryd(3S)	0.00051	1.28171
258	C	44	px	Val(2p)	1.22623	-0.19376
259	C	44	px	Ryd(3p)	0.00179	0.34341
260	C	44	py	Val(2p)	1.14573	-0.20379
261	C	44	py	Ryd(3p)	0.00426	0.30051
262	C	44	pz	Val(2p)	1.18567	-0.20297
263	C	44	pz	Ryd(3p)	0.00312	0.25621
264	H	45	S	Val(1S)	0.78619	0.11333
265	H	45	S	Ryd(2S)	0.00161	1.01208
266	H	46	S	Val(1S)	0.79046	0.10100
267	H	46	S	Ryd(2S)	0.00114	0.95458
268	H	47	S	Val(1S)	0.79155	0.09297
269	H	47	S	Ryd(2S)	0.00122	0.98862
270	C	48	S	Cor(1S)	1.99888	-11.29133
271	C	48	S	Val(2S)	0.84005	-0.23402
272	C	48	S	Ryd(3S)	0.00221	1.27263
273	C	48	px	Val(2p)	1.07657	-0.19916
274	C	48	px	Ryd(3p)	0.00627	0.60824

275	C	48	py	Val(2p)	0.89827	-0.13605
276	C	48	py	Ryd(3p)	0.00816	0.66725
277	C	48	pz	Val(2p)	1.00999	-0.19723
278	C	48	pz	Ryd(3p)	0.01303	0.75660
279	C	49	S	Cor(1S)	1.99907	-11.24745
280	C	49	S	Val(2S)	0.89313	-0.25013
281	C	49	S	Ryd(3S)	0.00171	1.32706
282	C	49	px	Val(2p)	1.04443	-0.17918
283	C	49	px	Ryd(3p)	0.00929	0.77333
284	C	49	py	Val(2p)	1.04011	-0.17592
285	C	49	py	Ryd(3p)	0.00771	0.62753
286	C	49	pz	Val(2p)	1.01875	-0.17475
287	C	49	pz	Ryd(3p)	0.00801	0.61591
288	C	50	S	Cor(1S)	1.99918	-11.21129
289	C	50	S	Val(2S)	0.93155	-0.22962
290	C	50	S	Ryd(3S)	0.00095	1.18040
291	C	50	px	Val(2p)	1.08404	-0.14323
292	C	50	px	Ryd(3p)	0.00532	0.51336
293	C	50	py	Val(2p)	1.04000	-0.15714
294	C	50	py	Ryd(3p)	0.00481	0.49488
295	C	50	pz	Val(2p)	1.08180	-0.13480
296	C	50	pz	Ryd(3p)	0.00644	0.42841
297	C	51	S	Cor(1S)	1.99924	-11.20373
298	C	51	S	Val(2S)	0.92674	-0.20259
299	C	51	S	Ryd(3S)	0.00073	1.07607
300	C	51	px	Val(2p)	1.03213	-0.15114
301	C	51	px	Ryd(3p)	0.00441	0.46321
302	C	51	py	Val(2p)	1.08880	-0.11276
303	C	51	py	Ryd(3p)	0.00677	0.39913
304	C	51	pz	Val(2p)	1.06578	-0.11621
305	C	51	pz	Ryd(3p)	0.00537	0.42501
306	C	52	S	Cor(1S)	1.99931	-11.22261
307	C	52	S	Val(2S)	0.93789	-0.23607
308	C	52	S	Ryd(3S)	0.00080	1.09222
309	C	52	px	Val(2p)	1.10719	-0.12363
310	C	52	px	Ryd(3p)	0.00753	0.56947
311	C	52	py	Val(2p)	1.06525	-0.13207
312	C	52	py	Ryd(3p)	0.00572	0.44094
313	C	52	pz	Val(2p)	1.02510	-0.16868
314	C	52	pz	Ryd(3p)	0.00495	0.45743
315	C	53	S	Cor(1S)	1.99917	-11.22051
316	C	53	S	Val(2S)	0.92171	-0.22801
317	C	53	S	Ryd(3S)	0.00119	1.22741
318	C	53	px	Val(2p)	1.10495	-0.14244
319	C	53	px	Ryd(3p)	0.00781	0.55883
320	C	53	py	Val(2p)	1.05827	-0.19058
321	C	53	py	Ryd(3p)	0.00536	0.55804
322	C	53	pz	Val(2p)	1.09553	-0.15512
323	C	53	pz	Ryd(3p)	0.00615	0.54939
324	C	54	S	Cor(1S)	1.99926	-11.22233
325	C	54	S	Val(2S)	0.95163	-0.28527
326	C	54	S	Ryd(3S)	0.00053	1.62833
327	C	54	px	Val(2p)	1.01768	-0.15426
328	C	54	px	Ryd(3p)	0.00480	0.53404
329	C	54	py	Val(2p)	1.12147	-0.12629
330	C	54	py	Ryd(3p)	0.00780	0.45924

331	C	54	pz	Val(2p)	1.02786	-0.15897
332	C	54	pz	Ryd(3p)	0.00615	0.61665
333	C	55	S	Cor(1S)	1.99931	-11.14166
334	C	55	S	Val(2S)	1.00925	-0.22704
335	C	55	S	Ryd(3S)	0.00071	1.26559
336	C	55	px	Val(2p)	1.14386	-0.13778
337	C	55	px	Ryd(3p)	0.00375	0.32307
338	C	55	py	Val(2p)	1.21456	-0.13406
339	C	55	py	Ryd(3p)	0.00254	0.34287
340	C	55	pz	Val(2p)	1.13381	-0.13154
341	C	55	pz	Ryd(3p)	0.00380	0.34172
342	H	56	S	Val(1S)	0.81336	0.14778
343	H	56	S	Ryd(2S)	0.00168	0.96431
344	H	57	S	Val(1S)	0.81524	0.14048
345	H	57	S	Ryd(2S)	0.00138	0.94484
346	H	58	S	Val(1S)	0.83798	0.11261
347	H	58	S	Ryd(2S)	0.00199	1.09642
348	C	59	S	Cor(1S)	1.99932	-11.14035
349	C	59	S	Val(2S)	1.01030	-0.22745
350	C	59	S	Ryd(3S)	0.00062	1.25896
351	C	59	px	Val(2p)	1.19358	-0.12950
352	C	59	px	Ryd(3p)	0.00370	0.34019
353	C	59	py	Val(2p)	1.22378	-0.12999
354	C	59	py	Ryd(3p)	0.00266	0.32920
355	C	59	pz	Val(2p)	1.08689	-0.13840
356	C	59	pz	Ryd(3p)	0.00364	0.31959
357	H	60	S	Val(1S)	0.82474	0.12813
358	H	60	S	Ryd(2S)	0.00151	1.00355
359	H	61	S	Val(1S)	0.81045	0.14938
360	H	61	S	Ryd(2S)	0.00124	0.98023
361	H	62	S	Val(1S)	0.81770	0.13986
362	H	62	S	Ryd(2S)	0.00177	0.94219
363	H	63	S	Val(1S)	0.81638	0.16565
364	H	63	S	Ryd(2S)	0.00161	1.09128
365	H	64	S	Val(1S)	0.82582	0.18861
366	H	64	S	Ryd(2S)	0.00184	1.03693
367	H	65	S	Val(1S)	0.91394	0.31883
368	H	65	S	Ryd(2S)	0.00253	0.94337
369	H	66	S	Val(1S)	0.82798	0.16987
370	H	66	S	Ryd(2S)	0.00223	1.13794
371	H	67	S	Val(1S)	0.84958	0.19413
372	H	67	S	Ryd(2S)	0.00349	1.04760
373	H	68	S	Val(1S)	0.86108	0.26314
374	H	68	S	Ryd(2S)	0.00244	1.02363
375	H	69	S	Val(1S)	0.81684	0.20103
376	H	69	S	Ryd(2S)	0.00185	1.00919

377	H	70	S	Val(1S)	0.87358	0.26751
378	H	70	S	Ryd(2S)	0.00166	0.95212
379	H	71	S	Val(1S)	0.84246	0.18418
380	H	71	S	Ryd(2S)	0.00196	1.17034
381	H	72	S	Val(1S)	0.82959	0.15266
382	H	72	S	Ryd(2S)	0.00297	1.04587
383	H	73	S	Val(1S)	0.82115	0.18636
384	H	73	S	Ryd(2S)	0.00177	1.03754
385	H	74	S	Val(1S)	0.83755	0.23446
386	H	74	S	Ryd(2S)	0.00193	0.97402
387	H	75	S	Val(1S)	0.82226	0.17974
388	H	75	S	Ryd(2S)	0.00167	1.03300
389	H	76	S	Val(1S)	0.83390	0.18064
390	H	76	S	Ryd(2S)	0.00185	1.10447
391	H	77	S	Val(1S)	0.83288	0.11470
392	H	77	S	Ryd(2S)	0.00288	1.13127
393	N	78	S	Cor(1S)	1.99942	-15.54873
394	N	78	S	Val(2S)	1.35763	-0.82856
395	N	78	S	Ryd(3S)	0.00224	1.87193
396	N	78	px	Val(2p)	1.27956	-0.41181
397	N	78	px	Ryd(3p)	0.00618	1.05621
398	N	78	py	Val(2p)	1.39925	-0.43528
399	N	78	py	Ryd(3p)	0.00648	0.86972
400	N	78	pz	Val(2p)	1.60873	-0.51914
401	N	78	pz	Ryd(3p)	0.01133	0.83397
402	N	79	S	Cor(1S)	1.99943	-15.54541
403	N	79	S	Val(2S)	1.36584	-0.83321
404	N	79	S	Ryd(3S)	0.00235	1.87886
405	N	79	px	Val(2p)	1.71077	-0.55281
406	N	79	px	Ryd(3p)	0.01103	0.81731
407	N	79	py	Val(2p)	1.30273	-0.40644
408	N	79	py	Ryd(3p)	0.00815	1.01902
409	N	79	pz	Val(2p)	1.29188	-0.40687
410	N	79	pz	Ryd(3p)	0.00462	0.94962
411	N	80	S	Cor(1S)	1.99940	-15.54890
412	N	80	S	Val(2S)	1.35513	-0.83043
413	N	80	S	Ryd(3S)	0.00248	1.86850
414	N	80	px	Val(2p)	1.31360	-0.41128
415	N	80	px	Ryd(3p)	0.00635	0.90966
416	N	80	py	Val(2p)	1.58469	-0.49613
417	N	80	py	Ryd(3p)	0.01192	1.03300
418	N	80	pz	Val(2p)	1.41789	-0.47985
419	N	80	pz	Ryd(3p)	0.00703	0.86495
420	Tl	81	S	Val(6S)	1.86031	-0.50950
421	Tl	81	S	Ryd(7S)	0.00026	10.43803
422	Tl	81	px	Val(6p)	0.14815	0.29681
423	Tl	81	px	Ryd(7p)	0.00689	0.74371
424	Tl	81	py	Val(6p)	0.04989	0.08526
425	Tl	81	py	Ryd(7p)	0.00252	0.39611
426	Tl	81	pz	Val(6p)	0.07609	0.14829
427	Tl	81	pz	Ryd(7p)	0.00571	0.53874

428	Tl	81	dxy	Cor(5d)	1.99543	-0.98571
429	Tl	81	dxy	Ryd(6d)	0.00005	1.79162
430	Tl	81	dxz	Cor(5d)	1.99594	-0.98407
431	Tl	81	dxz	Ryd(6d)	0.00005	1.78469
432	Tl	81	dyz	Cor(5d)	1.99760	-0.98521
433	Tl	81	dyz	Ryd(6d)	0.00004	1.73441
434	Tl	81	dx2y2	Cor(5d)	1.99727	-0.98780
435	Tl	81	dx2y2	Ryd(6d)	0.00003	1.67956
436	Tl	81	dz2	Cor(5d)	1.99654	-0.98333
437	Tl	81	dz2	Ryd(6d)	0.00007	1.80301
438	Tl	82	S	Val(6S)	1.86039	-0.50954
439	Tl	82	S	Ryd(7S)	0.00026	10.43798
440	Tl	82	px	Val(6p)	0.14816	0.29684
441	Tl	82	px	Ryd(7p)	0.00688	0.74394
442	Tl	82	py	Val(6p)	0.04989	0.08527
443	Tl	82	py	Ryd(7p)	0.00252	0.39612
444	Tl	82	pz	Val(6p)	0.07610	0.14835
445	Tl	82	pz	Ryd(7p)	0.00571	0.53868
446	Tl	82	dxy	Cor(5d)	1.99543	-0.98573
447	Tl	82	dxy	Ryd(6d)	0.00005	1.79162
448	Tl	82	dxz	Cor(5d)	1.99594	-0.98408
449	Tl	82	dxz	Ryd(6d)	0.00005	1.78463
450	Tl	82	dyz	Cor(5d)	1.99760	-0.98523
451	Tl	82	dyz	Ryd(6d)	0.00004	1.73438
452	Tl	82	dx2y2	Cor(5d)	1.99727	-0.98781
453	Tl	82	dx2y2	Ryd(6d)	0.00003	1.67961
454	Tl	82	dz2	Cor(5d)	1.99654	-0.98335
455	Tl	82	dz2	Ryd(6d)	0.00007	1.80303
456	C	83	S	Cor(1S)	1.99883	-11.29468
457	C	83	S	Val(2S)	0.84034	-0.23916
458	C	83	S	Ryd(3S)	0.00213	1.28231
459	C	83	px	Val(2p)	0.88768	-0.13748
460	C	83	px	Ryd(3p)	0.01529	0.77123
461	C	83	py	Val(2p)	1.06946	-0.19181
462	C	83	py	Ryd(3p)	0.00611	0.60529
463	C	83	pz	Val(2p)	1.02356	-0.22609
464	C	83	pz	Ryd(3p)	0.00968	0.53457
465	C	84	S	Cor(1S)	1.99901	-11.25583
466	C	84	S	Val(2S)	0.89397	-0.26245
467	C	84	S	Ryd(3S)	0.00201	1.34441
468	C	84	px	Val(2p)	1.05922	-0.17505
469	C	84	px	Ryd(3p)	0.00813	0.66533
470	C	84	py	Val(2p)	1.06614	-0.18630
471	C	84	py	Ryd(3p)	0.01043	0.78452
472	C	84	pz	Val(2p)	0.97812	-0.19727
473	C	84	pz	Ryd(3p)	0.00815	0.59847
474	C	85	S	Cor(1S)	1.99917	-11.22972
475	C	85	S	Val(2S)	0.93607	-0.25865
476	C	85	S	Ryd(3S)	0.00123	1.23445
477	C	85	px	Val(2p)	1.10500	-0.14087
478	C	85	px	Ryd(3p)	0.00767	0.53039
479	C	85	py	Val(2p)	1.10607	-0.14225
480	C	85	py	Ryd(3p)	0.00542	0.61848
481	C	85	pz	Val(2p)	0.99662	-0.20455
482	C	85	pz	Ryd(3p)	0.00473	0.44022
483	C	86	S	Cor(1S)	1.99927	-11.22861
484	C	86	S	Val(2S)	0.93766	-0.24597

485	C	86	S	Ryd(3S)	0.00139	1.15275
486	C	86	px	Val(2p)	1.15098	-0.07984
487	C	86	px	Ryd(3p)	0.00767	0.56616
488	C	86	py	Val(2p)	1.04559	-0.15529
489	C	86	py	Ryd(3p)	0.00513	0.49903
490	C	86	pz	Val(2p)	1.00133	-0.20523
491	C	86	pz	Ryd(3p)	0.00544	0.45231
492	C	87	S	Cor(1S)	1.99869	-11.18196
493	C	87	S	Val(2S)	0.87488	-0.08380
494	C	87	S	Ryd(3S)	0.00097	1.16683
495	C	87	px	Val(2p)	1.05696	-0.14693
496	C	87	px	Ryd(3p)	0.00547	0.58273
497	C	87	py	Val(2p)	1.11289	0.02654
498	C	87	py	Ryd(3p)	0.00799	0.45816
499	C	87	pz	Val(2p)	0.99084	-0.19831
500	C	87	pz	Ryd(3p)	0.00621	0.50800
501	C	88	S	Cor(1S)	1.99915	-11.22921
502	C	88	S	Val(2S)	0.92837	-0.24422
503	C	88	S	Ryd(3S)	0.00129	1.29694
504	C	88	px	Val(2p)	1.09602	-0.14643
505	C	88	px	Ryd(3p)	0.00593	0.64185
506	C	88	py	Val(2p)	1.09938	-0.14626
507	C	88	py	Ryd(3p)	0.00857	0.51636
508	C	88	pz	Val(2p)	1.04269	-0.21038
509	C	88	pz	Ryd(3p)	0.00534	0.54306
510	C	89	S	Cor(1S)	1.99893	-11.27202
511	C	89	S	Val(2S)	0.96185	-0.36717
512	C	89	S	Ryd(3S)	0.00101	1.58842
513	C	89	px	Val(2p)	1.11642	-0.24406
514	C	89	px	Ryd(3p)	0.01289	0.55418
515	C	89	py	Val(2p)	1.07403	-0.26174
516	C	89	py	Ryd(3p)	0.00747	0.50413
517	C	89	pz	Val(2p)	1.14282	-0.23530
518	C	89	pz	Ryd(3p)	0.01641	0.57556
519	H	90	S	Val(1S)	0.79125	0.08655
520	H	90	S	Ryd(2S)	0.00188	1.10619
521	C	91	S	Cor(1S)	1.99910	-11.35455
522	C	91	S	Val(2S)	0.86065	-0.29960
523	C	91	S	Ryd(3S)	0.00589	1.14423
524	C	91	px	Val(2p)	0.90879	-0.15275
525	C	91	px	Ryd(3p)	0.00783	0.63511
526	C	91	py	Val(2p)	0.79640	-0.19449
527	C	91	py	Ryd(3p)	0.00876	0.53820
528	C	91	pz	Val(2p)	0.90615	-0.17730
529	C	91	pz	Ryd(3p)	0.00770	0.58503
530	C	92	S	Cor(1S)	1.99921	-11.19006
531	C	92	S	Val(2S)	1.02181	-0.29809
532	C	92	S	Ryd(3S)	0.00048	1.27597
533	C	92	px	Val(2p)	1.24802	-0.19928
534	C	92	px	Ryd(3p)	0.00333	0.28255
535	C	92	py	Val(2p)	1.19169	-0.19683
536	C	92	py	Ryd(3p)	0.00229	0.30523
537	C	92	pz	Val(2p)	1.11562	-0.20189
538	C	92	pz	Ryd(3p)	0.00359	0.28427
539	H	93	S	Val(1S)	0.78904	0.11101

540	H	93	S	Ryd(2S)	0.00177	1.02048
541	H	94	S	Val(1S)	0.78975	0.09822
542	H	94	S	Ryd(2S)	0.00118	0.94872
543	H	95	S	Val(1S)	0.79136	0.09422
544	H	95	S	Ryd(2S)	0.00118	0.95616
545	C	96	S	Cor(1S)	1.99908	-11.20329
546	C	96	S	Val(2S)	0.92052	-0.22450
547	C	96	S	Ryd(3S)	0.00056	1.61743
548	C	96	px	Val(2p)	1.12566	-0.10567
549	C	96	px	Ryd(3p)	0.01018	0.50347
550	C	96	py	Val(2p)	1.00654	-0.14877
551	C	96	py	Ryd(3p)	0.00534	0.50629
552	C	96	pz	Val(2p)	1.04388	-0.14624
553	C	96	pz	Ryd(3p)	0.00423	0.57119
554	C	97	S	Cor(1S)	1.99932	-11.14324
555	C	97	S	Val(2S)	1.00935	-0.22840
556	C	97	S	Ryd(3S)	0.00068	1.25086
557	C	97	px	Val(2p)	1.21739	-0.13490
558	C	97	px	Ryd(3p)	0.00289	0.28575
559	C	97	py	Val(2p)	1.21078	-0.13156
560	C	97	py	Ryd(3p)	0.00357	0.32908
561	C	97	pz	Val(2p)	1.06673	-0.14265
562	C	97	pz	Ryd(3p)	0.00339	0.31561
563	H	98	S	Val(1S)	0.81865	0.13182
564	H	98	S	Ryd(2S)	0.00159	0.95202
565	H	99	S	Val(1S)	0.81555	0.13876
566	H	99	S	Ryd(2S)	0.00132	0.94424
567	H	100	S	Val(1S)	0.82526	0.12570
568	H	100	S	Ryd(2S)	0.00153	0.98777
569	C	101	S	Cor(1S)	1.99936	-11.14319
570	C	101	S	Val(2S)	1.00207	-0.21988
571	C	101	S	Ryd(3S)	0.00064	1.29054
572	C	101	px	Val(2p)	1.17457	-0.14100
573	C	101	px	Ryd(3p)	0.00288	0.44386
574	C	101	py	Val(2p)	1.14685	-0.14379
575	C	101	py	Ryd(3p)	0.00406	0.42544
576	C	101	pz	Val(2p)	1.17738	-0.13475
577	C	101	pz	Ryd(3p)	0.00401	0.40590
578	H	102	S	Val(1S)	0.83185	0.11561
579	H	102	S	Ryd(2S)	0.00163	1.13193
580	H	103	S	Val(1S)	0.81428	0.13908
581	H	103	S	Ryd(2S)	0.00131	1.00349
582	H	104	S	Val(1S)	0.82369	0.12207
583	H	104	S	Ryd(2S)	0.00200	1.07621
584	C	105	S	Cor(1S)	1.99910	-11.35397
585	C	105	S	Val(2S)	0.86193	-0.30149
586	C	105	S	Ryd(3S)	0.00598	1.17885
587	C	105	px	Val(2p)	0.94892	-0.16277
588	C	105	px	Ryd(3p)	0.00761	0.61342
589	C	105	py	Val(2p)	0.83481	-0.18182

590	C	105	py	Ryd(3p)	0.00985	0.56421
591	C	105	pz	Val(2p)	0.82168	-0.17726
592	C	105	pz	Ryd(3p)	0.00735	0.56770
593	C	106	S	Cor(1S)	1.99921	-11.18582
594	C	106	S	Val(2S)	1.01962	-0.29308
595	C	106	S	Ryd(3S)	0.00052	1.30329
596	C	106	px	Val(2p)	1.08186	-0.20365
597	C	106	px	Ryd(3p)	0.00417	0.26828
598	C	106	py	Val(2p)	1.23632	-0.19512
599	C	106	py	Ryd(3p)	0.00269	0.28123
600	C	106	pz	Val(2p)	1.24214	-0.19561
601	C	106	pz	Ryd(3p)	0.00273	0.32962
602	H	107	S	Val(1S)	0.78517	0.11761
603	H	107	S	Ryd(2S)	0.00164	1.02730
604	H	108	S	Val(1S)	0.78830	0.10473
605	H	108	S	Ryd(2S)	0.00122	0.95662
606	H	109	S	Val(1S)	0.79279	0.09048
607	H	109	S	Ryd(2S)	0.00141	1.02411
608	C	110	S	Cor(1S)	1.99887	-11.28149
609	C	110	S	Val(2S)	0.84263	-0.22916
610	C	110	S	Ryd(3S)	0.00213	1.25351
611	C	110	px	Val(2p)	1.03840	-0.21033
612	C	110	px	Ryd(3p)	0.00821	0.58846
613	C	110	py	Val(2p)	1.00279	-0.15896
614	C	110	py	Ryd(3p)	0.00739	0.70363
615	C	110	pz	Val(2p)	0.95167	-0.15270
616	C	110	pz	Ryd(3p)	0.01203	0.71385
617	C	111	S	Cor(1S)	1.99908	-11.24616
618	C	111	S	Val(2S)	0.89514	-0.25003
619	C	111	S	Ryd(3S)	0.00167	1.32999
620	C	111	px	Val(2p)	0.98888	-0.17974
621	C	111	px	Ryd(3p)	0.00868	0.61727
622	C	111	py	Val(2p)	1.04115	-0.15562
623	C	111	py	Ryd(3p)	0.00723	0.66809
624	C	111	pz	Val(2p)	1.04033	-0.16924
625	C	111	pz	Ryd(3p)	0.00962	0.71511
626	C	112	S	Cor(1S)	1.99902	-11.18373
627	C	112	S	Val(2S)	0.89516	-0.14274
628	C	112	S	Ryd(3S)	0.00081	1.17885
629	C	112	px	Val(2p)	1.01954	-0.15701
630	C	112	px	Ryd(3p)	0.00358	0.48234
631	C	112	py	Val(2p)	1.13783	-0.05264
632	C	112	py	Ryd(3p)	0.00844	0.38605
633	C	112	pz	Val(2p)	1.06339	-0.15366
634	C	112	pz	Ryd(3p)	0.00402	0.60764
635	C	113	S	Cor(1S)	1.99930	-11.21030
636	C	113	S	Val(2S)	0.93307	-0.21585
637	C	113	S	Ryd(3S)	0.00092	1.09449
638	C	113	px	Val(2p)	1.00370	-0.17062
639	C	113	px	Ryd(3p)	0.00445	0.43604
640	C	113	py	Val(2p)	1.07645	-0.12845
641	C	113	py	Ryd(3p)	0.00569	0.45157
642	C	113	pz	Val(2p)	1.11755	-0.07845
643	C	113	pz	Ryd(3p)	0.00613	0.47490

644	C	114	S	Cor(1S)	1.99915	-11.19675
645	C	114	S	Val(2S)	0.91269	-0.16405
646	C	114	S	Ryd(3S)	0.00067	1.09091
647	C	114	px	Val(2p)	1.01510	-0.15671
648	C	114	px	Ryd(3p)	0.00596	0.41394
649	C	114	py	Val(2p)	1.05685	-0.12015
650	C	114	py	Ryd(3p)	0.00459	0.49401
651	C	114	pz	Val(2p)	1.08854	-0.06471
652	C	114	pz	Ryd(3p)	0.00686	0.41810
653	C	115	S	Cor(1S)	1.99918	-11.21239
654	C	115	S	Val(2S)	0.92220	-0.22089
655	C	115	S	Ryd(3S)	0.00108	1.22015
656	C	115	px	Val(2p)	1.03967	-0.20264
657	C	115	px	Ryd(3p)	0.00597	0.48330
658	C	115	py	Val(2p)	1.15010	-0.08697
659	C	115	py	Ryd(3p)	0.00757	0.65134
660	C	115	pz	Val(2p)	1.06702	-0.18070
661	C	115	pz	Ryd(3p)	0.00604	0.60482
662	C	116	S	Cor(1S)	1.99922	-11.21823
663	C	116	S	Val(2S)	0.94693	-0.27350
664	C	116	S	Ryd(3S)	0.00058	1.60309
665	C	116	px	Val(2p)	1.00581	-0.15472
666	C	116	px	Ryd(3p)	0.00377	0.48577
667	C	116	py	Val(2p)	1.08150	-0.14803
668	C	116	py	Ryd(3p)	0.00895	0.63346
669	C	116	pz	Val(2p)	1.08471	-0.12287
670	C	116	pz	Ryd(3p)	0.00665	0.42958
671	C	117	S	Cor(1S)	1.99931	-11.13742
672	C	117	S	Val(2S)	1.01089	-0.22419
673	C	117	S	Ryd(3S)	0.00059	1.23901
674	C	117	px	Val(2p)	1.20583	-0.12711
675	C	117	px	Ryd(3p)	0.00357	0.32647
676	C	117	py	Val(2p)	1.08912	-0.13173
677	C	117	py	Ryd(3p)	0.00312	0.31038
678	C	117	pz	Val(2p)	1.19754	-0.12883
679	C	117	pz	Ryd(3p)	0.00314	0.30817
680	H	118	S	Val(1S)	0.82608	0.12912
681	H	118	S	Ryd(2S)	0.00159	0.97998
682	H	119	S	Val(1S)	0.81581	0.14495
683	H	119	S	Ryd(2S)	0.00133	0.95332
684	H	120	S	Val(1S)	0.81492	0.14837
685	H	120	S	Ryd(2S)	0.00141	0.94496
686	C	121	S	Cor(1S)	1.99933	-11.15289
687	C	121	S	Val(2S)	1.00867	-0.23423
688	C	121	S	Ryd(3S)	0.00076	1.24944
689	C	121	px	Val(2p)	1.08409	-0.15863
690	C	121	px	Ryd(3p)	0.00496	0.53596
691	C	121	py	Val(2p)	1.20376	-0.13688
692	C	121	py	Ryd(3p)	0.00374	0.36587
693	C	121	pz	Val(2p)	1.21021	-0.13996
694	C	121	pz	Ryd(3p)	0.00295	0.46597
695	H	122	S	Val(1S)	0.83655	0.10716
696	H	122	S	Ryd(2S)	0.00170	1.10802

697	H	123	S	Val(1S)	0.81645	0.13028
698	H	123	S	Ryd(2S)	0.00148	0.98744
699	H	124	S	Val(1S)	0.82084	0.12649
700	H	124	S	Ryd(2S)	0.00161	1.00931
701	C	125	S	Cor(1S)	1.99909	-11.35531
702	C	125	S	Val(2S)	0.85993	-0.29986
703	C	125	S	Ryd(3S)	0.00600	1.14817
704	C	125	px	Val(2p)	0.74326	-0.19940
705	C	125	px	Ryd(3p)	0.00859	0.52768
706	C	125	py	Val(2p)	0.98437	-0.20561
707	C	125	py	Ryd(3p)	0.00754	0.67895
708	C	125	pz	Val(2p)	0.87677	-0.12190
709	C	125	pz	Ryd(3p)	0.00847	0.59996
710	C	126	S	Cor(1S)	1.99921	-11.19050
711	C	126	S	Val(2S)	1.02120	-0.29815
712	C	126	S	Ryd(3S)	0.00051	1.28191
713	C	126	px	Val(2p)	1.22624	-0.19391
714	C	126	px	Ryd(3p)	0.00180	0.34355
715	C	126	py	Val(2p)	1.14572	-0.20374
716	C	126	py	Ryd(3p)	0.00426	0.30048
717	C	126	pz	Val(2p)	1.18569	-0.20299
718	C	126	pz	Ryd(3p)	0.00312	0.25620
719	H	127	S	Val(1S)	0.78621	0.11337
720	H	127	S	Ryd(2S)	0.00161	1.01202
721	H	128	S	Val(1S)	0.79044	0.10108
722	H	128	S	Ryd(2S)	0.00114	0.95450
723	H	129	S	Val(1S)	0.79143	0.09249
724	H	129	S	Ryd(2S)	0.00122	0.98891
725	C	130	S	Cor(1S)	1.99888	-11.29111
726	C	130	S	Val(2S)	0.83986	-0.23365
727	C	130	S	Ryd(3S)	0.00221	1.27262
728	C	130	px	Val(2p)	1.07673	-0.19922
729	C	130	px	Ryd(3p)	0.00627	0.60824
730	C	130	py	Val(2p)	0.89842	-0.13606
731	C	130	py	Ryd(3p)	0.00816	0.66729
732	C	130	pz	Val(2p)	1.01022	-0.19726
733	C	130	pz	Ryd(3p)	0.01302	0.75667
734	C	131	S	Cor(1S)	1.99907	-11.24747
735	C	131	S	Val(2S)	0.89318	-0.25020
736	C	131	S	Ryd(3S)	0.00171	1.32752
737	C	131	px	Val(2p)	1.04439	-0.17915
738	C	131	px	Ryd(3p)	0.00930	0.77326
739	C	131	py	Val(2p)	1.04001	-0.17593
740	C	131	py	Ryd(3p)	0.00772	0.62793
741	C	131	pz	Val(2p)	1.01873	-0.17473
742	C	131	pz	Ryd(3p)	0.00801	0.61589
743	C	132	S	Cor(1S)	1.99918	-11.21134
744	C	132	S	Val(2S)	0.93155	-0.22969
745	C	132	S	Ryd(3S)	0.00095	1.18026
746	C	132	px	Val(2p)	1.08425	-0.14314
747	C	132	px	Ryd(3p)	0.00531	0.51344
748	C	132	py	Val(2p)	1.03979	-0.15705

749	C	132	py	Ryd(3p)	0.00482	0.49495
750	C	132	pz	Val(2p)	1.08166	-0.13502
751	C	132	pz	Ryd(3p)	0.00645	0.42831
752	C	133	S	Cor(1S)	1.99924	-11.20339
753	C	133	S	Val(2S)	0.92643	-0.20196
754	C	133	S	Ryd(3S)	0.00073	1.07605
755	C	133	px	Val(2p)	1.03246	-0.15120
756	C	133	px	Ryd(3p)	0.00441	0.46319
757	C	133	py	Val(2p)	1.08900	-0.11273
758	C	133	py	Ryd(3p)	0.00676	0.39878
759	C	133	pz	Val(2p)	1.06585	-0.11615
760	C	133	pz	Ryd(3p)	0.00537	0.42497
761	C	134	S	Cor(1S)	1.99931	-11.22262
762	C	134	S	Val(2S)	0.93790	-0.23607
763	C	134	S	Ryd(3S)	0.00080	1.09229
764	C	134	px	Val(2p)	1.10707	-0.12358
765	C	134	px	Ryd(3p)	0.00753	0.56952
766	C	134	py	Val(2p)	1.06520	-0.13205
767	C	134	py	Ryd(3p)	0.00573	0.44097
768	C	134	pz	Val(2p)	1.02500	-0.16863
769	C	134	pz	Ryd(3p)	0.00495	0.45747
770	C	135	S	Cor(1S)	1.99917	-11.22050
771	C	135	S	Val(2S)	0.92170	-0.22799
772	C	135	S	Ryd(3S)	0.00119	1.22757
773	C	135	px	Val(2p)	1.10490	-0.14239
774	C	135	px	Ryd(3p)	0.00781	0.55885
775	C	135	py	Val(2p)	1.05829	-0.19057
776	C	135	py	Ryd(3p)	0.00536	0.55803
777	C	135	pz	Val(2p)	1.09554	-0.15512
778	C	135	pz	Ryd(3p)	0.00616	0.54943
779	C	136	S	Cor(1S)	1.99926	-11.22230
780	C	136	S	Val(2S)	0.95162	-0.28514
781	C	136	S	Ryd(3S)	0.00053	1.62843
782	C	136	px	Val(2p)	1.01768	-0.15429
783	C	136	px	Ryd(3p)	0.00480	0.53403
784	C	136	py	Val(2p)	1.12150	-0.12603
785	C	136	py	Ryd(3p)	0.00780	0.45924
786	C	136	pz	Val(2p)	1.02783	-0.15899
787	C	136	pz	Ryd(3p)	0.00615	0.61696
788	C	137	S	Cor(1S)	1.99931	-11.14179
789	C	137	S	Val(2S)	1.00940	-0.22738
790	C	137	S	Ryd(3S)	0.00071	1.26574
791	C	137	px	Val(2p)	1.14385	-0.13775
792	C	137	px	Ryd(3p)	0.00374	0.32298
793	C	137	py	Val(2p)	1.21458	-0.13447
794	C	137	py	Ryd(3p)	0.00254	0.34312
795	C	137	pz	Val(2p)	1.13381	-0.13140
796	C	137	pz	Ryd(3p)	0.00381	0.34193
797	H	138	S	Val(1S)	0.81327	0.14732
798	H	138	S	Ryd(2S)	0.00168	0.96454
799	H	139	S	Val(1S)	0.81514	0.13989
800	H	139	S	Ryd(2S)	0.00137	0.94512
801	H	140	S	Val(1S)	0.83804	0.11309
802	H	140	S	Ryd(2S)	0.00200	1.09620

803	C	141	S	Cor(1S)	1.99931	-11.14032
804	C	141	S	Val(2S)	1.01028	-0.22726
805	C	141	S	Ryd(3S)	0.00062	1.25882
806	C	141	px	Val(2p)	1.19351	-0.12944
807	C	141	px	Ryd(3p)	0.00370	0.34021
808	C	141	py	Val(2p)	1.22378	-0.12977
809	C	141	py	Ryd(3p)	0.00266	0.32923
810	C	141	pz	Val(2p)	1.08679	-0.13839
811	C	141	pz	Ryd(3p)	0.00364	0.31967
812	H	142	S	Val(1S)	0.82478	0.12808
813	H	142	S	Ryd(2S)	0.00151	1.00358
814	H	143	S	Val(1S)	0.81056	0.14990
815	H	143	S	Ryd(2S)	0.00124	0.97989
816	H	144	S	Val(1S)	0.81772	0.13987
817	H	144	S	Ryd(2S)	0.00177	0.94216
818	H	145	S	Val(1S)	0.81640	0.16564
819	H	145	S	Ryd(2S)	0.00161	1.09128
820	H	146	S	Val(1S)	0.82583	0.18862
821	H	146	S	Ryd(2S)	0.00184	1.03696
822	H	147	S	Val(1S)	0.91394	0.31887
823	H	147	S	Ryd(2S)	0.00253	0.94340
824	H	148	S	Val(1S)	0.82797	0.16991
825	H	148	S	Ryd(2S)	0.00223	1.13799
826	H	149	S	Val(1S)	0.84971	0.19415
827	H	149	S	Ryd(2S)	0.00348	1.04746
828	H	150	S	Val(1S)	0.86148	0.26369
829	H	150	S	Ryd(2S)	0.00244	1.02296
830	H	151	S	Val(1S)	0.81683	0.20100
831	H	151	S	Ryd(2S)	0.00185	1.00930
832	H	152	S	Val(1S)	0.87314	0.26710
833	H	152	S	Ryd(2S)	0.00167	0.95303
834	H	153	S	Val(1S)	0.84252	0.18418
835	H	153	S	Ryd(2S)	0.00196	1.17020
836	H	154	S	Val(1S)	0.82968	0.15270
837	H	154	S	Ryd(2S)	0.00297	1.04581
838	H	155	S	Val(1S)	0.82101	0.18600
839	H	155	S	Ryd(2S)	0.00177	1.03790
840	H	156	S	Val(1S)	0.83755	0.23471
841	H	156	S	Ryd(2S)	0.00193	0.97432
842	H	157	S	Val(1S)	0.82229	0.17970
843	H	157	S	Ryd(2S)	0.00166	1.03297
844	H	158	S	Val(1S)	0.83391	0.18066
845	H	158	S	Ryd(2S)	0.00185	1.10447

846	H	159	S	Val(1S)	0.83294	0.11519
847	H	159	S	Ryd(2S)	0.00288	1.13083
848	N	160	S	Cor(1S)	1.99942	-15.54851
849	N	160	S	Val(2S)	1.35721	-0.82817
850	N	160	S	Ryd(3S)	0.00225	1.87186
851	N	160	px	Val(2p)	1.27968	-0.41187
852	N	160	px	Ryd(3p)	0.00618	1.05618
853	N	160	py	Val(2p)	1.39898	-0.43518
854	N	160	py	Ryd(3p)	0.00648	0.86973
855	N	160	pz	Val(2p)	1.60890	-0.51920
856	N	160	pz	Ryd(3p)	0.01135	0.83387
857	N	161	S	Cor(1S)	1.99943	-15.54535
858	N	161	S	Val(2S)	1.36558	-0.83292
859	N	161	S	Ryd(3S)	0.00235	1.87891
860	N	161	px	Val(2p)	1.71081	-0.55270
861	N	161	px	Ryd(3p)	0.01103	0.81737
862	N	161	py	Val(2p)	1.30279	-0.40637
863	N	161	py	Ryd(3p)	0.00815	1.01922
864	N	161	pz	Val(2p)	1.29177	-0.40673
865	N	161	pz	Ryd(3p)	0.00462	0.94985
866	N	162	S	Cor(1S)	1.99940	-15.54887
867	N	162	S	Val(2S)	1.35514	-0.83035
868	N	162	S	Ryd(3S)	0.00248	1.86869
869	N	162	px	Val(2p)	1.31359	-0.41126
870	N	162	px	Ryd(3p)	0.00635	0.90977
871	N	162	py	Val(2p)	1.58465	-0.49606
872	N	162	py	Ryd(3p)	0.01192	1.03311
873	N	162	pz	Val(2p)	1.41781	-0.47975
874	N	162	pz	Ryd(3p)	0.00703	0.86500

[136 electrons found in the effective core potential]

WARNING: 1 low occupancy (<1.9990e) core orbital found on C 1
1 low occupancy (<1.9990e) core orbital found on C 8
1 low occupancy (<1.9990e) core orbital found on C 12
1 low occupancy (<1.9990e) core orbital found on C 28
1 low occupancy (<1.9990e) core orbital found on C 48
5 low occupancy (<1.9990e) core orbitals found on Tl 81
5 low occupancy (<1.9990e) core orbitals found on Tl 82
1 low occupancy (<1.9990e) core orbital found on C 83
1 low occupancy (<1.9990e) core orbital found on C 87
1 low occupancy (<1.9990e) core orbital found on C 89
1 low occupancy (<1.9990e) core orbital found on C 110
1 low occupancy (<1.9990e) core orbital found on C 130

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.33170	1.99893	4.29501	0.03776	6.33170
H	2	0.20671	0.00000	0.79141	0.00188	0.79329
C	3	0.49899	1.99910	3.47176	0.03016	5.50101
C	4	-0.58574	1.99921	4.57684	0.00969	6.58574
H	5	0.20917	0.00000	0.78906	0.00177	0.79083
H	6	0.20905	0.00000	0.78977	0.00118	0.79095
H	7	0.20729	0.00000	0.79152	0.00119	0.79271

C	8	0.14692	1.99883	3.82105	0.03320	5.85308
C	9	-0.02507	1.99901	3.99733	0.02873	6.02507
C	10	-0.16196	1.99917	4.14374	0.01905	6.16196
C	11	-0.15445	1.99927	4.13555	0.01964	6.15445
C	12	-0.05493	1.99869	4.03560	0.02065	6.05493
C	13	-0.18677	1.99915	4.16649	0.02113	6.18677
C	14	-0.11619	1.99908	4.09680	0.02031	6.11619
C	15	-0.51416	1.99932	4.50431	0.01053	6.51416
H	16	0.17977	0.00000	0.81864	0.00159	0.82023
H	17	0.18313	0.00000	0.81555	0.00132	0.81687
H	18	0.17331	0.00000	0.82517	0.00153	0.82669
C	19	-0.51206	1.99936	4.50111	0.01159	6.51206
H	20	0.16661	0.00000	0.83176	0.00163	0.83339
H	21	0.18439	0.00000	0.81431	0.00130	0.81561
H	22	0.17443	0.00000	0.82356	0.00200	0.82557
C	23	0.50268	1.99910	3.46742	0.03080	5.49732
C	24	-0.58859	1.99921	4.57927	0.01010	6.58859
H	25	0.21308	0.00000	0.78528	0.00164	0.78692
H	26	0.21040	0.00000	0.78838	0.00122	0.78960
H	27	0.20550	0.00000	0.79309	0.00141	0.79450
C	28	0.13597	1.99887	3.83539	0.02977	5.86403
C	29	0.00865	1.99909	3.96508	0.02719	5.99135
C	30	-0.13247	1.99902	4.11660	0.01685	6.13247
C	31	-0.14719	1.99930	4.13069	0.01719	6.14719
C	32	-0.08984	1.99915	4.07261	0.01809	6.08984
C	33	-0.19912	1.99918	4.17929	0.02065	6.19912
C	34	-0.13845	1.99922	4.11927	0.01996	6.13845
C	35	-0.51323	1.99931	4.50350	0.01043	6.51323
H	36	0.17239	0.00000	0.82602	0.00159	0.82761
H	37	0.18286	0.00000	0.81581	0.00133	0.81714
H	38	0.18376	0.00000	0.81484	0.00140	0.81624
C	39	-0.51840	1.99933	4.50665	0.01242	6.51840
H	40	0.16176	0.00000	0.83655	0.00170	0.83824
H	41	0.18208	0.00000	0.81644	0.00148	0.81792
H	42	0.17759	0.00000	0.82081	0.00161	0.82241
C	43	0.50615	1.99909	3.46414	0.03062	5.49385
C	44	-0.58765	1.99921	4.57875	0.00969	6.58765
H	45	0.21220	0.00000	0.78619	0.00161	0.78780
H	46	0.20840	0.00000	0.79046	0.00114	0.79160
H	47	0.20723	0.00000	0.79155	0.00122	0.79277
C	48	0.14657	1.99888	3.82488	0.02968	5.85343
C	49	-0.02221	1.99907	3.99642	0.02672	6.02221
C	50	-0.15409	1.99918	4.13739	0.01752	6.15409
C	51	-0.12997	1.99924	4.11345	0.01727	6.12997
C	52	-0.15375	1.99931	4.13543	0.01901	6.15375
C	53	-0.20014	1.99917	4.18046	0.02051	6.20014
C	54	-0.13718	1.99926	4.11864	0.01928	6.13718
C	55	-0.51158	1.99931	4.50148	0.01080	6.51158
H	56	0.18496	0.00000	0.81336	0.00168	0.81504
H	57	0.18339	0.00000	0.81524	0.00138	0.81661
H	58	0.16002	0.00000	0.83798	0.00199	0.83998
C	59	-0.52448	1.99932	4.51455	0.01062	6.52448
H	60	0.17375	0.00000	0.82474	0.00151	0.82625
H	61	0.18831	0.00000	0.81045	0.00124	0.81169
H	62	0.18052	0.00000	0.81770	0.00177	0.81948
H	63	0.18201	0.00000	0.81638	0.00161	0.81799
H	64	0.17234	0.00000	0.82582	0.00184	0.82766
H	65	0.08353	0.00000	0.91394	0.00253	0.91647
H	66	0.16979	0.00000	0.82798	0.00223	0.83021
H	67	0.14693	0.00000	0.84958	0.00349	0.85307
H	68	0.13648	0.00000	0.86108	0.00244	0.86352
H	69	0.18131	0.00000	0.81684	0.00185	0.81869

H	70	0.12476	0.00000	0.87358	0.00166	0.87524
H	71	0.15557	0.00000	0.84246	0.00196	0.84443
H	72	0.16745	0.00000	0.82959	0.00297	0.83255
H	73	0.17708	0.00000	0.82115	0.00177	0.82292
H	74	0.16053	0.00000	0.83755	0.00193	0.83947
H	75	0.17607	0.00000	0.82226	0.00167	0.82393
H	76	0.16426	0.00000	0.83390	0.00185	0.83574
H	77	0.16424	0.00000	0.83288	0.00288	0.83576
N	78	-0.67081	1.99942	5.64517	0.02622	7.67081
N	79	-0.69679	1.99943	5.67122	0.02614	7.69679
N	80	-0.69850	1.99940	5.67131	0.02779	7.69850
Tl	81	0.86717	77.98277	2.13444	0.01562	80.13283
Tl	82	0.86705	77.98278	2.13455	0.01562	80.13295
C	83	0.14694	1.99883	3.82104	0.03320	5.85306
C	84	-0.02517	1.99901	3.99745	0.02872	6.02517
C	85	-0.16197	1.99917	4.14376	0.01905	6.16197
C	86	-0.15446	1.99927	4.13555	0.01963	6.15446
C	87	-0.05491	1.99869	4.03557	0.02064	6.05491
C	88	-0.18673	1.99915	4.16646	0.02113	6.18673
C	89	-0.33183	1.99893	4.29512	0.03778	6.33183
H	90	0.20688	0.00000	0.79125	0.00188	0.79312
C	91	0.49873	1.99910	3.47198	0.03018	5.50127
C	92	-0.58605	1.99921	4.57714	0.00970	6.58605
H	93	0.20919	0.00000	0.78904	0.00177	0.79081
H	94	0.20907	0.00000	0.78975	0.00118	0.79093
H	95	0.20746	0.00000	0.79136	0.00118	0.79254
C	96	-0.11599	1.99908	4.09660	0.02031	6.11599
C	97	-0.51410	1.99932	4.50425	0.01053	6.51410
H	98	0.17977	0.00000	0.81865	0.00159	0.82023
H	99	0.18312	0.00000	0.81555	0.00132	0.81688
H	100	0.17321	0.00000	0.82526	0.00153	0.82679
C	101	-0.51181	1.99936	4.50087	0.01158	6.51181
H	102	0.16652	0.00000	0.83185	0.00163	0.83348
H	103	0.18441	0.00000	0.81428	0.00131	0.81559
H	104	0.17431	0.00000	0.82369	0.00200	0.82569
C	105	0.50277	1.99910	3.46734	0.03079	5.49723
C	106	-0.58926	1.99921	4.57994	0.01011	6.58926
H	107	0.21319	0.00000	0.78517	0.00164	0.78681
H	108	0.21048	0.00000	0.78830	0.00122	0.78952
H	109	0.20580	0.00000	0.79279	0.00141	0.79420
C	110	0.13588	1.99887	3.83549	0.02976	5.86412
C	111	0.00820	1.99908	3.96550	0.02721	5.99180
C	112	-0.13178	1.99902	4.11591	0.01685	6.13178
C	113	-0.14726	1.99930	4.13077	0.01719	6.14726
C	114	-0.09041	1.99915	4.07318	0.01808	6.09041
C	115	-0.19882	1.99918	4.17899	0.02065	6.19882
C	116	-0.13812	1.99922	4.11895	0.01995	6.13812
C	117	-0.51311	1.99931	4.50338	0.01042	6.51311
H	118	0.17233	0.00000	0.82608	0.00159	0.82767
H	119	0.18286	0.00000	0.81581	0.00133	0.81714
H	120	0.18367	0.00000	0.81492	0.00141	0.81633
C	121	-0.51849	1.99933	4.50674	0.01242	6.51849
H	122	0.16175	0.00000	0.83655	0.00170	0.83825
H	123	0.18207	0.00000	0.81645	0.00148	0.81793
H	124	0.17755	0.00000	0.82084	0.00161	0.82245
C	125	0.50598	1.99909	3.46433	0.03060	5.49402
C	126	-0.58774	1.99921	4.57884	0.00969	6.58774
H	127	0.21218	0.00000	0.78621	0.00161	0.78782
H	128	0.20842	0.00000	0.79044	0.00114	0.79158
H	129	0.20735	0.00000	0.79143	0.00122	0.79265
C	130	0.14623	1.99888	3.82523	0.02966	5.85377
C	131	-0.02211	1.99907	3.99631	0.02673	6.02211

C	132	-0.15395	1.99918	4.13725	0.01752	6.15395
C	133	-0.13025	1.99924	4.11375	0.01727	6.13025
C	134	-0.15348	1.99931	4.13516	0.01901	6.15348
C	135	-0.20012	1.99917	4.18044	0.02052	6.20012
C	136	-0.13718	1.99926	4.11863	0.01929	6.13718
C	137	-0.51175	1.99931	4.50164	0.01080	6.51175
H	138	0.18505	0.00000	0.81327	0.00168	0.81495
H	139	0.18349	0.00000	0.81514	0.00137	0.81651
H	140	0.15996	0.00000	0.83804	0.00200	0.84004
C	141	-0.52429	1.99931	4.51436	0.01061	6.52429
H	142	0.17372	0.00000	0.82478	0.00151	0.82628
H	143	0.18820	0.00000	0.81056	0.00124	0.81180
H	144	0.18052	0.00000	0.81772	0.00177	0.81948
H	145	0.18199	0.00000	0.81640	0.00161	0.81801
H	146	0.17233	0.00000	0.82583	0.00184	0.82767
H	147	0.08353	0.00000	0.91394	0.00253	0.91647
H	148	0.16980	0.00000	0.82797	0.00223	0.83020
H	149	0.14681	0.00000	0.84971	0.00348	0.85319
H	150	0.13608	0.00000	0.86148	0.00244	0.86392
H	151	0.18132	0.00000	0.81683	0.00185	0.81868
H	152	0.12520	0.00000	0.87314	0.00167	0.87480
H	153	0.15552	0.00000	0.84252	0.00196	0.84448
H	154	0.16735	0.00000	0.82968	0.00297	0.83265
H	155	0.17722	0.00000	0.82101	0.00177	0.82278
H	156	0.16052	0.00000	0.83755	0.00193	0.83948
H	157	0.17605	0.00000	0.82229	0.00166	0.82395
H	158	0.16424	0.00000	0.83391	0.00185	0.83576
H	159	0.16418	0.00000	0.83294	0.00288	0.83582
N	160	-0.67044	1.99942	5.64477	0.02626	7.67044
N	161	-0.69654	1.99943	5.67096	0.02614	7.69654
N	162	-0.69839	1.99940	5.67120	0.02779	7.69839
* Total *		2.00000	303.90385	390.37947	1.71668	696.00000

Natural Population

Effective Core	136.00000
Core	167.90385 (99.9428% of 168)
Valence	390.37947 (99.5866% of 392)
Natural Minimal Basis	694.28332 (99.7534% of 696)
Natural Rydberg Basis	1.71668 (0.2466% of 696)

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.96)2p(3.33)3p(0.04)
H	2	1S(0.79)
C	3	[core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C	4	[core]2S(1.02)2p(3.56)3p(0.01)
H	5	1S(0.79)
H	6	1S(0.79)
H	7	1S(0.79)
C	8	[core]2S(0.84)2p(2.98)3p(0.03)
C	9	[core]2S(0.89)2p(3.10)3p(0.03)
C	10	[core]2S(0.94)2p(3.21)3p(0.02)
C	11	[core]2S(0.94)2p(3.20)3p(0.02)
C	12	[core]2S(0.87)2p(3.16)3p(0.02)
C	13	[core]2S(0.93)2p(3.24)3p(0.02)
C	14	[core]2S(0.92)2p(3.18)3p(0.02)
C	15	[core]2S(1.01)2p(3.49)3p(0.01)
H	16	1S(0.82)
H	17	1S(0.82)

H	18	1S(0.83)
C	19	[core]2S(1.00)2p(3.50)3p(0.01)
H	20	1S(0.83)
H	21	1S(0.81)
H	22	1S(0.82)
C	23	[core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C	24	[core]2S(1.02)2p(3.56)3p(0.01)
H	25	1S(0.79)
H	26	1S(0.79)
H	27	1S(0.79)
C	28	[core]2S(0.84)2p(2.99)3p(0.03)
C	29	[core]2S(0.90)2p(3.07)3p(0.03)
C	30	[core]2S(0.90)2p(3.22)3p(0.02)
C	31	[core]2S(0.93)2p(3.20)3p(0.02)
C	32	[core]2S(0.91)2p(3.16)3p(0.02)
C	33	[core]2S(0.92)2p(3.26)3p(0.02)
C	34	[core]2S(0.95)2p(3.17)3p(0.02)
C	35	[core]2S(1.01)2p(3.49)3p(0.01)
H	36	1S(0.83)
H	37	1S(0.82)
H	38	1S(0.81)
C	39	[core]2S(1.01)2p(3.50)3p(0.01)
H	40	1S(0.84)
H	41	1S(0.82)
H	42	1S(0.82)
C	43	[core]2S(0.86)2p(2.60)3S(0.01)3p(0.02)
C	44	[core]2S(1.02)2p(3.56)3p(0.01)
H	45	1S(0.79)
H	46	1S(0.79)
H	47	1S(0.79)
C	48	[core]2S(0.84)2p(2.98)3p(0.03)
C	49	[core]2S(0.89)2p(3.10)3p(0.03)
C	50	[core]2S(0.93)2p(3.21)3p(0.02)
C	51	[core]2S(0.93)2p(3.19)3p(0.02)
C	52	[core]2S(0.94)2p(3.20)3p(0.02)
C	53	[core]2S(0.92)2p(3.26)3p(0.02)
C	54	[core]2S(0.95)2p(3.17)3p(0.02)
C	55	[core]2S(1.01)2p(3.49)3p(0.01)
H	56	1S(0.81)
H	57	1S(0.82)
H	58	1S(0.84)
C	59	[core]2S(1.01)2p(3.50)3p(0.01)
H	60	1S(0.82)
H	61	1S(0.81)
H	62	1S(0.82)
H	63	1S(0.82)
H	64	1S(0.83)
H	65	1S(0.91)
H	66	1S(0.83)
H	67	1S(0.85)
H	68	1S(0.86)
H	69	1S(0.82)
H	70	1S(0.87)
H	71	1S(0.84)
H	72	1S(0.83)
H	73	1S(0.82)
H	74	1S(0.84)
H	75	1S(0.82)
H	76	1S(0.83)
H	77	1S(0.83)
N	78	[core]2S(1.36)2p(4.29)3p(0.02)
N	79	[core]2S(1.37)2p(4.31)3p(0.02)

N	80	[core]2S(1.36)2p(4.32)3p(0.03)
Tl	81	[core]6S(1.86)6p(0.27)7p(0.02)
Tl	82	[core]6S(1.86)6p(0.27)7p(0.02)
C	83	[core]2S(0.84)2p(2.98)3p(0.03)
C	84	[core]2S(0.89)2p(3.10)3p(0.03)
C	85	[core]2S(0.94)2p(3.21)3p(0.02)
C	86	[core]2S(0.94)2p(3.20)3p(0.02)
C	87	[core]2S(0.87)2p(3.16)3p(0.02)
C	88	[core]2S(0.93)2p(3.24)3p(0.02)
C	89	[core]2S(0.96)2p(3.33)3p(0.04)
H	90	1S(0.79)
C	91	[core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C	92	[core]2S(1.02)2p(3.56)3p(0.01)
H	93	1S(0.79)
H	94	1S(0.79)
H	95	1S(0.79)
C	96	[core]2S(0.92)2p(3.18)3p(0.02)
C	97	[core]2S(1.01)2p(3.49)3p(0.01)
H	98	1S(0.82)
H	99	1S(0.82)
H	100	1S(0.83)
C	101	[core]2S(1.00)2p(3.50)3p(0.01)
H	102	1S(0.83)
H	103	1S(0.81)
H	104	1S(0.82)
C	105	[core]2S(0.86)2p(2.61)3S(0.01)3p(0.02)
C	106	[core]2S(1.02)2p(3.56)3p(0.01)
H	107	1S(0.79)
H	108	1S(0.79)
H	109	1S(0.79)
C	110	[core]2S(0.84)2p(2.99)3p(0.03)
C	111	[core]2S(0.90)2p(3.07)3p(0.03)
C	112	[core]2S(0.90)2p(3.22)3p(0.02)
C	113	[core]2S(0.93)2p(3.20)3p(0.02)
C	114	[core]2S(0.91)2p(3.16)3p(0.02)
C	115	[core]2S(0.92)2p(3.26)3p(0.02)
C	116	[core]2S(0.95)2p(3.17)3p(0.02)
C	117	[core]2S(1.01)2p(3.49)3p(0.01)
H	118	1S(0.83)
H	119	1S(0.82)
H	120	1S(0.81)
C	121	[core]2S(1.01)2p(3.50)3p(0.01)
H	122	1S(0.84)
H	123	1S(0.82)
H	124	1S(0.82)
C	125	[core]2S(0.86)2p(2.60)3S(0.01)3p(0.02)
C	126	[core]2S(1.02)2p(3.56)3p(0.01)
H	127	1S(0.79)
H	128	1S(0.79)
H	129	1S(0.79)
C	130	[core]2S(0.84)2p(2.99)3p(0.03)
C	131	[core]2S(0.89)2p(3.10)3p(0.03)
C	132	[core]2S(0.93)2p(3.21)3p(0.02)
C	133	[core]2S(0.93)2p(3.19)3p(0.02)
C	134	[core]2S(0.94)2p(3.20)3p(0.02)
C	135	[core]2S(0.92)2p(3.26)3p(0.02)
C	136	[core]2S(0.95)2p(3.17)3p(0.02)
C	137	[core]2S(1.01)2p(3.49)3p(0.01)
H	138	1S(0.81)
H	139	1S(0.82)
H	140	1S(0.84)
C	141	[core]2S(1.01)2p(3.50)3p(0.01)

H 142 1S(0.82)
H 143 1S(0.81)
H 144 1S(0.82)
H 145 1S(0.82)
H 146 1S(0.83)
H 147 1S(0.91)
H 148 1S(0.83)
H 149 1S(0.85)
H 150 1S(0.86)
H 151 1S(0.82)
H 152 1S(0.87)
H 153 1S(0.84)
H 154 1S(0.83)
H 155 1S(0.82)
H 156 1S(0.84)
H 157 1S(0.82)
H 158 1S(0.83)
H 159 1S(0.83)
N 160 [core]2S(1.36)2p(4.29)3p(0.02)
N 161 [core]2S(1.37)2p(4.31)3p(0.02)
N 162 [core]2S(1.36)2p(4.32)3p(0.03)

NBO analysis skipped by request.
1|1|UNPC-E-C07CYG43054|SP|RHF|LANL2DZ|C68H86N6Tl2(2+)|MCDSTFM|28-Mar-2
013|0||# hf/lanl2dz guess=local pop=npa geom=connectivity||CSD ENTRY o
fm27p-1||2,1|C,0,-0.621,11.017,13.349|H,0,-1.177,10.346,12.9|C,0,-0.73
9,10.785,14.852|C,0,-2.015,10.148,15.295|H,0,-2.016,10.067,16.252|H,0,
-2.09,9.275,14.9|H,0,-2.757,10.69,15.018|C,0,0.148,11.089,17.013|C,0,0
.985,10.208,17.693|C,0,0.971,10.268,19.087|C,0,0.176,11.185,19.77|C,0,
-0.627,12.047,19.077|C,0,-0.643,11.998,17.693|C,0,1.819,9.184,16.967|C
,0,1.205,7.812,17.086|H,0,1.219,7.534,18.005|H,0,1.706,7.189,16.556|H,
0,0.296,7.84,16.775|C,0,3.252,9.155,17.411|H,0,3.644,10.023,17.287|H,0
,3.736,8.508,16.894|H,0,3.294,8.916,18.342|C,0,-1.123,12.389,12.928|C,
0,-1.683,12.464,11.553|H,0,-1.952,13.366,11.366|H,0,-2.443,11.882,11.4
85|H,0,-1.013,12.193,10.92|C,0,-1.289,14.701,13.374|C,0,-2.299,15.389,
14.053|C,0,-2.443,16.734,13.698|C,0,-1.672,17.353,12.804|C,0,-0.656,16
.666,12.16|C,0,-0.475,15.328,12.454|C,0,-3.102,14.741,15.141|C,0,-4.59
7,15.06,15.071|H,0,-4.721,16.012,15.051|H,0,-5.038,14.696,15.841|H,0,-
4.969,14.672,14.275|C,0,-2.556,15.167,16.506|H,0,-1.629,14.924,16.571|
H,0,-3.051,14.724,17.201|H,0,-2.647,16.117,16.605|C,0,0.815,10.804,12.
893|C,0,1.185,9.393,12.567|H,0,2.083,9.368,12.227|H,0,0.582,9.048,11.9
05|H,0,1.129,8.856,13.361|C,0,2.969,11.72,12.532|C,0,3.431,12.293,11.3
44|C,0,4.804,12.3,11.145|C,0,5.677,11.78,12.074|C,0,5.203,11.206,13.22
4|C,0,3.845,11.176,13.461|C,0,2.448,12.825,10.329|C,0,1.935,11.697,9.4
45|H,0,2.663,11.335,8.935|H,0,1.264,12.038,8.848|H,0,1.555,11.008,9.99
4|C,0,3.008,13.957,9.46|H,0,3.415,14.62,10.024|H,0,2.294,14.36,8.959|H
,0,3.663,13.603,8.857|H,0,1.538,9.696,19.606|H,0,0.278,11.174,20.699|H
,0,-1.078,12.575,19.405|H,0,-1.108,12.636,17.199|H,0,1.915,9.405,16.08
8|H,0,-3.034,17.078,14.214|H,0,-1.668,18.26,12.539|H,0,-0.128,17.012,1
1.593|H,0,0.176,14.842,12.038|H,0,-3.047,13.778,15.075|H,0,5.205,12.70
8,10.391|H,0,6.536,11.897,11.825|H,0,5.812,10.806,13.832|H,0,3.561,10.
76,14.23|H,0,1.65,13.154,10.819|N,0,0.214,11.175,15.584|N,0,-0.994,13.
352,13.751|N,0,1.576,11.81,12.849|Tl,0,1.393,13.539,14.838|Tl,0,2.419,
13.341,18.333|C,0,3.665,15.791,16.158|C,0,2.828,16.672,15.478|C,0,2.84
2,16.612,14.084|C,0,3.637,15.695,13.401|C,0,4.44,14.833,14.094|C,0,4.4
56,14.882,15.478|C,0,4.433,15.863,19.822|H,0,4.99,16.534,20.271|C,0,4.
551,16.095,18.319|C,0,5.827,16.732,17.876|H,0,5.829,16.813,16.919|H,0,
5.903,17.605,18.271|H,0,6.57,16.19,18.153|C,0,1.994,17.696,16.204|C,0,
2.608,19.068,16.085|H,0,2.594,19.346,15.166|H,0,2.107,19.691,16.615|H,
0,3.516,19.04,16.396|C,0,0.56,17.725,15.759|H,0,0.169,16.857,15.884|H,
0,0.077,18.373,16.277|H,0,0.519,17.964,14.829|C,0,4.936,14.491,20.243|

C,0,5.496,14.416,21.617|H,0,5.765,13.514,21.805|H,0,6.256,14.998,21.68
5|H,0,4.825,14.687,22.251|C,0,5.102,12.179,19.796|C,0,6.111,11.491,19.
118|C,0,6.256,10.146,19.473|C,0,5.485,9.527,20.367|C,0,4.469,10.214,21
.01|C,0,4.288,11.552,20.717|C,0,6.915,12.139,18.03|C,0,8.41,11.82,18.1
|H,0,8.533,10.868,18.12|H,0,8.851,12.184,17.33|H,0,8.781,12.208,18.896
|C,0,6.369,11.713,16.665|H,0,5.442,11.956,16.6|H,0,6.864,12.156,15.97|
H,0,6.46,10.763,16.566|C,0,2.998,16.076,20.278|C,0,2.628,17.487,20.604
|H,0,1.73,17.512,20.944|H,0,3.231,17.832,21.266|H,0,2.684,18.025,19.81
|C,0,0.844,15.16,20.639|C,0,0.382,14.587,21.826|C,0,-0.992,14.58,22.02
5|C,0,-1.864,15.1,21.097|C,0,-1.39,15.674,19.947|C,0,-0.032,15.704,19.
71|C,0,1.365,14.055,22.841|C,0,1.878,15.183,23.725|H,0,1.15,15.545,24.
236|H,0,2.549,14.842,24.323|H,0,2.257,15.872,23.176|C,0,0.805,12.923,2
3.711|H,0,0.398,12.26,23.147|H,0,1.519,12.52,24.211|H,0,0.15,13.277,24
.314|H,0,2.275,17.184,13.565|H,0,3.535,15.706,12.472|H,0,4.891,14.305,
13.766|H,0,4.921,14.244,15.972|H,0,1.898,17.475,17.083|H,0,6.846,9.802
,18.957|H,0,5.481,8.62,20.632|H,0,3.941,9.868,21.578|H,0,3.637,12.038,
21.133|H,0,6.86,13.102,18.096|H,0,-1.392,14.172,22.78|H,0,-2.723,14.98
3,21.345|H,0,-1.999,16.074,19.339|H,0,0.252,16.12,18.941|H,0,2.163,13.
726,22.352|N,0,3.599,15.705,17.587|N,0,4.807,13.528,19.42|N,0,2.237,15
.07,20.322||Version=IA32W-G09RevB.01|State=1-A|HF=-3049.1821674|RMSD=8
.302e-009|Dipole=-0.001815,-0.0012772,-0.0006786|Quadrupole=-12.769624
6,-18.9043313,31.6739558,9.3717472,25.6909605,22.5116277|PG=C01 [X(C68
H86N6Tl2)]||@

IT IS THE BEHAVIOR AND DISTRIBUTION OF THE ELECTRONS
AROUND THE NUCLEUS THAT GIVES THE FUNDAMENTAL
CHARACTER OF AN ATOM: IT MUST BE THE SAME FOR MOLECULES.

-- C. A. COULSON, 1951

Job cpu time: 0 days 8 hours 52 minutes 45.0 seconds.
File lengths (MBytes): RWF= 410 Int= 0 D2E= 0 Chk= 28 Scr= 1
Normal termination of Gaussian 09 at Thu Mar 28 20:58:12 2013.

Appendix 4. Gaussian output for dication dimer, LANL2-DZ, DF-B3LYP.

```
 *******************************************
 Gaussian 09:  IA32W-G09RevB.01 12-Aug-2010
              03-Apr-2013
 *******************************************
 %chk=\\vdm09-g1.ds.man.ac.uk\HOME\Desktop\cation_only_edited.chk
 ----------------------------------------------------
 # b3lyp/lanl2dz guess=local pop=npa geom=connectivity
 ----------------------------------------------------
 1/38=1,57=2/1;
 2/12=2,17=6,18=5,40=1/2;
 3/5=6,6=3,11=2,16=1,25=1,30=1,74=-5/1,2,3;
 4/9=10/1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1,40=-1/1,7;
 99/5=1,9=1/99;
 ------------------
 CSD ENTRY ofm27p-1
 ------------------
 Symbolic Z-matrix:
 Charge =  2 Multiplicity = 1
 C(PDBName=C1,ResName=UNK,ResNum=1) -3.90302   0.0513   -2.73798
 H(PDBName=H1,ResName=UNK,ResNum=1) -4.51453   0.0856   -3.50339
 C(PDBName=C2,ResName=UNK,ResNum=1) -2.50325  -0.22743  -3.27621
 C(PDBName=C3,ResName=UNK,ResNum=1) -2.46016  -0.97293  -4.56949
```

H(PDBName=H3A,ResName=UNK,ResNum=1) -1.54561 -1.12942 -4.81752
H(PDBName=H3B,ResName=UNK,ResNum=1) -2.8923 -0.45272 -5.25244
H(PDBName=H3C,ResName=UNK,ResNum=1) -2.91413 -1.81271 -4.47078
C(PDBName=C4,ResName=UNK,ResNum=1) -0.17044 -0.15078 -2.95803
C(PDBName=C5,ResName=UNK,ResNum=1) 0.68419 0.87238 -3.3604
C(PDBName=C6,ResName=UNK,ResNum=1) 2.01941 0.53322 -3.58217
C(PDBName=C7,ResName=UNK,ResNum=1) 2.48511 -0.76438 -3.38534
C(PDBName=C8,ResName=UNK,ResNum=1) 1.62687 -1.74696 -2.97785
C(PDBName=C9,ResName=UNK,ResNum=1) 0.29322 -1.44002 -2.76505
C(PDBName=C10,ResName=UNK,ResNum=1) 0.18424 2.27091 -3.61605
C(PDBName=C11,ResName=UNK,ResNum=1) 0.0753 2.53808 -5.09601
H(PDBName=H11A,ResName=UNK,ResNum=1) 0.95035 2.51358 -5.49065
H(PDBName=H11B,ResName=UNK,ResNum=1) -0.31535 3.40247 -5.2383
H(PDBName=H11C,ResName=UNK,ResNum=1) -0.47715 1.86506 -5.503
C(PDBName=C12,ResName=UNK,ResNum=1) 1.01133 3.33304 -2.95326
H(PDBName=H12A,ResName=UNK,ResNum=1) 1.03452 3.17711 -2.00584
H(PDBName=H12B,ResName=UNK,ResNum=1) 0.62748 4.19482 -3.12687
H(PDBName=H12C,ResName=UNK,ResNum=1) 1.90718 3.30608 -3.30307
C(PDBName=C13,ResName=UNK,ResNum=1) -4.39706 -1.03942 -1.80102
C(PDBName=C14,ResName=UNK,ResNum=1) -5.87023 -1.23739 -1.78056
H(PDBName=H14A,ResName=UNK,ResNum=1) -6.09179 -1.92487 -1.14872
H(PDBName=H14B,ResName=UNK,ResNum=1) -6.17033 -1.49622 -2.65457
H(PDBName=H14C,ResName=UNK,ResNum=1) -6.29922 -0.41714 -1.52328
C(PDBName=C15,ResName=UNK,ResNum=1) -3.93053 -2.58047 -0.07494
C(PDBName=C16,ResName=UNK,ResNum=1) -3.53748 -3.9179 -0.18112
C(PDBName=C17,ResName=UNK,ResNum=1) -3.8687 -4.72256 0.91369
C(PDBName=C18,ResName=UNK,ResNum=1) -4.48677 -4.27322 2.0059
C(PDBName=C19,ResName=UNK,ResNum=1) -4.84453 -2.93896 2.1095
C(PDBName=C20,ResName=UNK,ResNum=1) -4.56116 -2.09601 1.05188
C(PDBName=C21,ResName=UNK,ResNum=1) -2.74341 -4.41709 -1.35104
C(PDBName=C22,ResName=UNK,ResNum=1) -3.2185 -5.7723 -1.87959
H(PDBName=H22A,ResName=UNK,ResNum=1) -3.23733 -6.40816 -1.16027
H(PDBName=H22B,ResName=UNK,ResNum=1) -2.61728 -6.0782 -2.56138
H(PDBName=H22C,ResName=UNK,ResNum=1) -4.10069 -5.67953 -2.24793
C(PDBName=C23,ResName=UNK,ResNum=1) -1.26525 -4.51311 -0.96548
H(PDBName=H23A,ResName=UNK,ResNum=1) -0.95162 -3.65163 -0.67897
H(PDBName=H23B,ResName=UNK,ResNum=1) -0.75404 -4.80119 -1.72705
H(PDBName=H23C,ResName=UNK,ResNum=1) -1.16076 -5.14668 -0.25256
C(PDBName=C24,ResName=UNK,ResNum=1) -3.94505 1.41021 -2.05461
C(PDBName=C25,ResName=UNK,ResNum=1) -4.20594 2.57565 -2.95337
H(PDBName=H25A,ResName=UNK,ResNum=1) -4.28081 3.37547 -2.42676
H(PDBName=H25B,ResName=UNK,ResNum=1) -5.02288 2.43207 -3.43593
H(PDBName=H25C,ResName=UNK,ResNum=1) -3.47999 2.66918 -3.57483
C(PDBName=C26,ResName=UNK,ResNum=1) -3.65267 2.67773 -0.07548
C(PDBName=C27,ResName=UNK,ResNum=1) -4.64116 2.96957 0.86836
C(PDBName=C28,ResName=UNK,ResNum=1) -4.44627 4.09908 1.65003
C(PDBName=C29,ResName=UNK,ResNum=1) -3.3294 4.89303 1.51657
C(PDBName=C30,ResName=UNK,ResNum=1) -2.38075 4.60023 0.57264
C(PDBName=C31,ResName=UNK,ResNum=1) -2.53584 3.48772 -0.22705
C(PDBName=C32,ResName=UNK,ResNum=1) -5.87096 2.09948 0.9688
C(PDBName=C33,ResName=UNK,ResNum=1) -6.90447 2.51962 -0.06675
H(PDBName=H33A,ResName=UNK,ResNum=1) -7.20256 3.4118 0.1237
H(PDBName=H33B,ResName=UNK,ResNum=1) -7.65283 1.91808 -0.03451
H(PDBName=H33C,ResName=UNK,ResNum=1) -6.51008 2.49367 -0.94099
C(PDBName=C34,ResName=UNK,ResNum=1) -6.50534 2.08402 2.36433
H(PDBName=H34A,ResName=UNK,ResNum=1) -5.82567 1.91157 3.0213
H(PDBName=H34B,ResName=UNK,ResNum=1) -7.17142 1.39279 2.40624
H(PDBName=H34C,ResName=UNK,ResNum=1) -6.91284 2.93323 2.53967
H(PDBName=H6,ResName=UNK,ResNum=1) 2.65523 1.19992 -3.84539
H(PDBName=H7,ResName=UNK,ResNum=1) 3.40432 -0.8729 -3.51517
H(PDBName=H8,ResName=UNK,ResNum=1) 1.83432 -2.47498 -2.84854
H(PDBName=H9,ResName=UNK,ResNum=1) -0.28755 -2.06844 -2.39748

H(PDBName=H10,ResName=UNK,ResNum=1) -0.62366 2.40685 -3.21666
H(PDBName=H17,ResName=UNK,ResNum=1) -3.52705 -5.49686 0.78099
H(PDBName=H18,ResName=UNK,ResNum=1) -4.7063 -4.73006 2.80339
H(PDBName=H19,ResName=UNK,ResNum=1) -5.2273 -2.59646 2.78491
H(PDBName=H20,ResName=UNK,ResNum=1) -4.79531 -1.21432 1.08126
H(PDBName=H21,ResName=UNK,ResNum=1) -2.82683 -3.81171 -2.10023
H(PDBName=H28,ResName=UNK,ResNum=1) -5.04175 4.34478 2.34344
H(PDBName=H29,ResName=UNK,ResNum=1) -3.3227 5.56188 2.12168
H(PDBName=H30,ResName=UNK,ResNum=1) -1.64143 5.18372 0.4565
H(PDBName=H31,ResName=UNK,ResNum=1) -1.89342 3.33643 -0.86695
H(PDBName=H32,ResName=UNK,ResNum=1) -5.61291 1.17463 0.71738
N(PDBName=N1,ResName=UNK,ResNum=1) -1.51924 0.15405 -2.58171
N(PDBName=N2,ResName=UNK,ResNum=1) -3.53596 -1.65812 -1.096
N(PDBName=N3,ResName=UNK,ResNum=1) -3.73643 1.45227 -0.81051
Tl(PDBName=Tl1,ResName=UNK,ResNum=1) -1.81636 -0.09599 0.13569
Tl(PDBName=Tl1,ResName=UNK,ResNum=1) 1.81632 0.09545 -0.13607
C(PDBName=C4,ResName=UNK,ResNum=1) 0.17068 0.15103 2.95819
C(PDBName=C5,ResName=UNK,ResNum=1) -0.68394 -0.87212 3.36055
C(PDBName=C6,ResName=UNK,ResNum=1) -2.01917 -0.53297 3.58233
C(PDBName=C7,ResName=UNK,ResNum=1) -2.48487 0.76464 3.38549
C(PDBName=C8,ResName=UNK,ResNum=1) -1.62662 1.74722 2.978
C(PDBName=C9,ResName=UNK,ResNum=1) -0.29297 1.44028 2.76521
C(PDBName=C1,ResName=UNK,ResNum=1) 3.90298 -0.05184 2.7376
H(PDBName=H1,ResName=UNK,ResNum=1) 4.51477 -0.08534 3.50355
C(PDBName=C2,ResName=UNK,ResNum=1) 2.50321 0.22689 3.27583
C(PDBName=C3,ResName=UNK,ResNum=1) 2.46013 0.97239 4.56911
H(PDBName=H3A,ResName=UNK,ResNum=1) 1.54585 1.12967 4.81767
H(PDBName=H3B,ResName=UNK,ResNum=1) 2.89254 0.45297 5.2526
H(PDBName=H3C,ResName=UNK,ResNum=1) 2.91438 1.81296 4.47093
C(PDBName=C10,ResName=UNK,ResNum=1) -0.184 -2.27066 3.6162
C(PDBName=C11,ResName=UNK,ResNum=1) -0.07506 -2.53782 5.09617
H(PDBName=H11A,ResName=UNK,ResNum=1) -0.95011 -2.51333 5.49081
H(PDBName=H11B,ResName=UNK,ResNum=1) 0.31559 -3.40222 5.23846
H(PDBName=H11C,ResName=UNK,ResNum=1) 0.47711 -1.86561 5.50262
C(PDBName=C12,ResName=UNK,ResNum=1) -1.01233 -3.33337 2.95307
H(PDBName=H12A,ResName=UNK,ResNum=1) -1.03428 -3.17685 2.006
H(PDBName=H12B,ResName=UNK,ResNum=1) -0.62721 -4.19514 3.12785
H(PDBName=H12C,ResName=UNK,ResNum=1) -1.90694 -3.30583 3.30323
C(PDBName=C13,ResName=UNK,ResNum=1) 4.3973 1.03967 1.80117
C(PDBName=C14,ResName=UNK,ResNum=1) 5.86951 1.23785 1.78091
H(PDBName=H14A,ResName=UNK,ResNum=1) 6.09203 1.92512 1.14888
H(PDBName=H14B,ResName=UNK,ResNum=1) 6.16961 1.49668 2.65492
H(PDBName=H14C,ResName=UNK,ResNum=1) 6.29918 0.4166 1.5229
C(PDBName=C15,ResName=UNK,ResNum=1) 3.92981 2.58093 0.07529
C(PDBName=C16,ResName=UNK,ResNum=1) 3.53744 3.91736 0.18074
C(PDBName=C17,ResName=UNK,ResNum=1) 3.86894 4.72281 -0.91353
C(PDBName=C18,ResName=UNK,ResNum=1) 4.48701 4.27347 -2.00574
C(PDBName=C19,ResName=UNK,ResNum=1) 4.84381 2.93943 -2.10916
C(PDBName=C20,ResName=UNK,ResNum=1) 4.56141 2.09626 -1.05172
C(PDBName=C21,ResName=UNK,ResNum=1) 2.74365 4.41734 1.35119
C(PDBName=C22,ResName=UNK,ResNum=1) 3.21874 5.77256 1.87975
H(PDBName=H22A,ResName=UNK,ResNum=1) 3.2373 6.40761 1.15989
H(PDBName=H22B,ResName=UNK,ResNum=1) 2.61752 6.07845 2.56154
H(PDBName=H22C,ResName=UNK,ResNum=1) 4.10065 5.67899 2.24755
C(PDBName=C23,ResName=UNK,ResNum=1) 1.26549 4.51336 0.96564
H(PDBName=H23A,ResName=UNK,ResNum=1) 0.95186 3.65188 0.67912
H(PDBName=H23B,ResName=UNK,ResNum=1) 0.75428 4.80144 1.7272
H(PDBName=H23C,ResName=UNK,ResNum=1) 1.161 5.14693 0.25272
C(PDBName=C24,ResName=UNK,ResNum=1) 3.94529 -1.40996 2.05477
C(PDBName=C25,ResName=UNK,ResNum=1) 4.20618 -2.5754 2.95353
H(PDBName=H25A,ResName=UNK,ResNum=1) 4.28106 -3.37521 2.42691
H(PDBName=H25B,ResName=UNK,ResNum=1) 5.02312 -2.43182 3.43609

H(PDBName=H25C,ResName=UNK,ResNum=1) 3.48027 -2.66949 3.5758
C(PDBName=C26,ResName=UNK,ResNum=1) 3.65291 -2.67748 0.07563
C(PDBName=C27,ResName=UNK,ResNum=1) 4.64044 -2.96911 -0.86802
C(PDBName=C28,ResName=UNK,ResNum=1) 4.44527 -4.09941 -1.65022
C(PDBName=C29,ResName=UNK,ResNum=1) 3.32964 -4.89278 -1.51641
C(PDBName=C30,ResName=UNK,ResNum=1) 2.38099 -4.59998 -0.57248
C(PDBName=C31,ResName=UNK,ResNum=1) 2.53608 -3.48747 0.2272
C(PDBName=C32,ResName=UNK,ResNum=1) 5.87024 -2.09902 -0.96845
C(PDBName=C33,ResName=UNK,ResNum=1) 6.90375 -2.51915 0.06709
H(PDBName=H33A,ResName=UNK,ResNum=1) 7.2028 -3.41155 -0.12354
H(PDBName=H33B,ResName=UNK,ResNum=1) 7.65307 -1.91783 0.03466
H(PDBName=H33C,ResName=UNK,ResNum=1) 6.50908 -2.494 0.9408
C(PDBName=C34,ResName=UNK,ResNum=1) 6.50559 -2.08377 -2.36417
H(PDBName=H34A,ResName=UNK,ResNum=1) 5.82591 -1.91132 -3.02115
H(PDBName=H34B,ResName=UNK,ResNum=1) 7.1707 -1.39233 -2.40589
H(PDBName=H34C,ResName=UNK,ResNum=1) 6.91308 -2.93298 -2.53952
H(PDBName=H6,ResName=UNK,ResNum=1) -2.65499 -1.19966 3.84555
H(PDBName=H7,ResName=UNK,ResNum=1) -3.40407 0.87315 3.51532
H(PDBName=H8,ResName=UNK,ResNum=1) -1.83407 2.47523 2.8487
H(PDBName=H9,ResName=UNK,ResNum=1) 0.2878 2.06869 2.39764
H(PDBName=H10,ResName=UNK,ResNum=1) 0.62391 -2.4066 3.21681
H(PDBName=H17,ResName=UNK,ResNum=1) 3.52701 5.49632 -0.78137
H(PDBName=H18,ResName=UNK,ResNum=1) 4.70654 4.73031 -2.80323
H(PDBName=H19,ResName=UNK,ResNum=1) 5.22754 2.59672 -2.78475
H(PDBName=H20,ResName=UNK,ResNum=1) 4.79555 1.21458 -1.0811
H(PDBName=H21,ResName=UNK,ResNum=1) 2.82707 3.81196 2.10039
H(PDBName=H28,ResName=UNK,ResNum=1) 5.04199 -4.34452 -2.34329
H(PDBName=H29,ResName=UNK,ResNum=1) 3.32199 -5.56142 -2.12133
H(PDBName=H30,ResName=UNK,ResNum=1) 1.64167 -5.18347 -0.45634
H(PDBName=H31,ResName=UNK,ResNum=1) 1.89366 -3.33618 0.86711
H(PDBName=H32,ResName=UNK,ResNum=1) 5.61315 -1.17438 -0.71722
N(PDBName=N1,ResName=UNK,ResNum=1) 1.51948 -0.1538 2.58187
N(PDBName=N2,ResName=UNK,ResNum=1) 3.5362 1.65838 1.09615
N(PDBName=N3,ResName=UNK,ResNum=1) 3.73667 -1.45202 0.81066

Residue 1 PDB Number 1_0 UNK charge 0.00000000 ave dist 0.000
Stoichiometry C68H86N6Tl2(2+)
Framework group C1[X(C68H86N6Tl2)]
Deg. of freedom 480
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.903023	0.051295	-2.737981
2	1	0	-4.514533	0.085596	-3.503394
3	6	0	-2.503247	-0.227432	-3.276213
4	6	0	-2.460164	-0.972930	-4.569492
5	1	0	-1.545611	-1.129417	-4.817515
6	1	0	-2.892297	-0.452722	-5.252444
7	1	0	-2.914133	-1.812707	-4.470777
8	6	0	-0.170439	-0.150782	-2.958032
9	6	0	0.684185	0.872376	-3.360395
10	6	0	2.019408	0.533222	-3.582174
11	6	0	2.485112	-0.764383	-3.385337
12	6	0	1.626865	-1.746963	-2.977845
13	6	0	0.293215	-1.440024	-2.765050
14	6	0	0.184239	2.270912	-3.616048
15	6	0	0.075302	2.538076	-5.096013

16	1	0	0.950346	2.513578	-5.490651
17	1	0	-0.315350	3.402468	-5.238301
18	1	0	-0.477148	1.865062	-5.502998
19	6	0	1.011329	3.333035	-2.953263
20	1	0	1.034524	3.177106	-2.005839
21	1	0	0.627484	4.194823	-3.126870
22	1	0	1.907183	3.306084	-3.303069
23	6	0	-4.397058	-1.039420	-1.801017
24	6	0	-5.870231	-1.237389	-1.780559
25	1	0	-6.091786	-1.924870	-1.148722
26	1	0	-6.170325	-1.496216	-2.654573
27	1	0	-6.299217	-0.417141	-1.523277
28	6	0	-3.930526	-2.580467	-0.074942
29	6	0	-3.537481	-3.917900	-0.181117
30	6	0	-3.868700	-4.722562	0.913689
31	6	0	-4.486773	-4.273217	2.005895
32	6	0	-4.844529	-2.938962	2.109501
33	6	0	-4.561165	-2.096006	1.051875
34	6	0	-2.743405	-4.417091	-1.351036
35	6	0	-3.218501	-5.772304	-1.879589
36	1	0	-3.237334	-6.408158	-1.160273
37	1	0	-2.617282	-6.078198	-2.561382
38	1	0	-4.100692	-5.679533	-2.247930
39	6	0	-1.265249	-4.513108	-0.965484
40	1	0	-0.951616	-3.651630	-0.678966
41	1	0	-0.754039	-4.801185	-1.727045
42	1	0	-1.160762	-5.146678	-0.252564
43	6	0	-3.945046	1.410207	-2.054612
44	6	0	-4.205935	2.575653	-2.953371
45	1	0	-4.280814	3.375466	-2.426758
46	1	0	-5.022881	2.432070	-3.435929
47	1	0	-3.479994	2.669176	-3.574825
48	6	0	-3.652669	2.677734	-0.075475
49	6	0	-4.641162	2.969572	0.868363
50	6	0	-4.446268	4.099082	1.650030
51	6	0	-3.329395	4.893029	1.516565
52	6	0	-2.380753	4.600231	0.572637
53	6	0	-2.535840	3.487717	-0.227047
54	6	0	-5.870955	2.099481	0.968797
55	6	0	-6.904465	2.519616	-0.066748
56	1	0	-7.202563	3.411803	0.123697
57	1	0	-7.652825	1.918078	-0.034507
58	1	0	-6.510077	2.493668	-0.940994
59	6	0	-6.505344	2.084019	2.364325
60	1	0	-5.825671	1.911567	3.021302
61	1	0	-7.171417	1.392791	2.406236
62	1	0	-6.912835	2.933227	2.539671
63	1	0	2.655230	1.199916	-3.845393
64	1	0	3.404316	-0.872897	-3.515165
65	1	0	1.834315	-2.474982	-2.848538
66	1	0	-0.287553	-2.068439	-2.397481
67	1	0	-0.623664	2.406848	-3.216657
68	1	0	-3.527049	-5.496860	0.780988
69	1	0	-4.706301	-4.730062	2.803385
70	1	0	-5.227296	-2.596463	2.784907
71	1	0	-4.795310	-1.214323	1.081259
72	1	0	-2.826831	-3.811705	-2.100233
73	1	0	-5.041747	4.344775	2.343442
74	1	0	-3.322704	5.561882	2.121677
75	1	0	-1.641429	5.183719	0.456500
76	1	0	-1.893421	3.336427	-0.866954
77	1	0	-5.612911	1.174631	0.717379

78	7	0	-1.519237	0.154047	-2.581712
79	7	0	-3.535959	-1.658124	-1.095997
80	7	0	-3.736426	1.452274	-0.810506
81	81	0	-1.816362	-0.095993	0.135685
82	81	0	1.816323	0.095450	-0.136066
83	6	0	0.170681	0.151034	2.958188
84	6	0	-0.683944	-0.872124	3.360551
85	6	0	-2.019167	-0.532970	3.582331
86	6	0	-2.484871	0.764635	3.385494
87	6	0	-1.626623	1.747215	2.978002
88	6	0	-0.292974	1.440276	2.765207
89	6	0	3.902984	-0.051837	2.737600
90	1	0	4.514774	-0.085344	3.503551
91	6	0	2.503207	0.226889	3.275832
92	6	0	2.460125	0.972387	4.569111
93	1	0	1.545852	1.129669	4.817671
94	1	0	2.892539	0.452974	5.252601
95	1	0	2.914375	1.812959	4.470934
96	6	0	-0.183997	-2.270660	3.616204
97	6	0	-0.075061	-2.537824	5.096170
98	1	0	-0.950105	-2.513326	5.490807
99	1	0	0.315592	-3.402216	5.238458
100	1	0	0.477109	-1.865605	5.502617
101	6	0	-1.012327	-3.333367	2.953071
102	1	0	-1.034283	-3.176854	2.005995
103	1	0	-0.627206	-4.195139	3.127848
104	1	0	-1.906942	-3.305832	3.303225
105	6	0	4.397299	1.039672	1.801173
106	6	0	5.869514	1.237852	1.780905
107	1	0	6.092028	1.925122	1.148879
108	1	0	6.169608	1.496679	2.654918
109	1	0	6.299178	0.416598	1.522896
110	6	0	3.929808	2.580930	0.075287
111	6	0	3.537442	3.917358	0.180736
112	6	0	3.868942	4.722814	-0.913532
113	6	0	4.487014	4.273469	-2.005739
114	6	0	4.843811	2.939425	-2.109156
115	6	0	4.561407	2.096258	-1.051719
116	6	0	2.743647	4.417343	1.351192
117	6	0	3.218742	5.772556	1.879746
118	1	0	3.237295	6.407615	1.159892
119	1	0	2.617523	6.078450	2.561539
120	1	0	4.100653	5.678990	2.247549
121	6	0	1.265490	4.513361	0.965640
122	1	0	0.951858	3.651882	0.679122
123	1	0	0.754281	4.801437	1.727201
124	1	0	1.161003	5.146930	0.252721
125	6	0	3.945288	-1.409955	2.054769
126	6	0	4.206177	-2.575401	2.953528
127	1	0	4.281056	-3.375214	2.426914
128	1	0	5.023122	-2.431818	3.436086
129	1	0	3.480273	-2.669493	3.575803
130	6	0	3.652911	-2.677482	0.075632
131	6	0	4.640444	-2.969109	-0.868017
132	6	0	4.445269	-4.099414	-1.650222
133	6	0	3.329636	-4.892777	-1.516408
134	6	0	2.380994	-4.599979	-0.572480
135	6	0	2.536082	-3.487465	0.227203
136	6	0	5.870238	-2.099018	-0.968451
137	6	0	6.903748	-2.519153	0.067093
138	1	0	7.202804	-3.411550	-0.123541
139	1	0	7.653067	-1.917826	0.034663

140	1	0	6.509079	-2.494000	0.940802
141	6	0	6.505586	-2.083767	-2.364168
142	1	0	5.825913	-1.911315	-3.021146
143	1	0	7.170699	-1.392328	-2.405890
144	1	0	6.913077	-2.932975	-2.539515
145	1	0	-2.654988	-1.199664	3.845550
146	1	0	-3.404074	0.873149	3.515322
147	1	0	-1.834074	2.475234	2.848695
148	1	0	0.287795	2.068691	2.397638
149	1	0	0.623905	-2.406596	3.216814
150	1	0	3.527009	5.496317	-0.781369
151	1	0	4.706543	4.730314	-2.803228
152	1	0	5.227537	2.596715	-2.784751
153	1	0	4.795551	1.214575	-1.081102
154	1	0	2.827073	3.811957	2.100390
155	1	0	5.041988	-4.344523	-2.343285
156	1	0	3.321986	-5.561420	-2.121332
157	1	0	1.641671	-5.183467	-0.456343
158	1	0	1.893663	-3.336175	0.867111
159	1	0	5.613153	-1.174379	-0.717222
160	7	0	1.519479	-0.153795	2.581869
161	7	0	3.536200	1.658376	1.096154
162	7	0	3.736668	-1.452022	0.810662

Rotational constants (GHZ): 0.0363398 0.0248776 0.0221224
Standard basis: LANL2DZ (5D, 7F)
There are 874 symmetry adapted basis functions of A symmetry.
Integral buffers will be 262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
874 basis functions, 2254 primitive gaussians, 878 cartesian basis functions
280 alpha electrons 280 beta electrons
nuclear repulsion energy 14838.1291604468 Hartrees.
NAtoms= 162 NActive= 162 NUniq= 162 SFac= 1.00D+00 NAtFMM= 50 NAOKFM=T Big=T
One-electron integrals computed using PRISM.
1 Symmetry operations used in ECPInt.
ECPInt: NShTT= 153735 NPrTT= 1086464 LenC2= 123334 LenP2D= 411860.
LDataN: DoStor=T MaxTD1= 6 Len= 172
NBasis= 874 RedAO= T NBF= 874
NBsUse= 874 1.00D-06 NBFU= 874
Defaulting to unpruned grid for atomic number 81.
Initial guess orbitals will be localized using method 0.
Harris functional with IExCor= 402 diagonalized for initial guess.
ExpMin= 4.44D-02 ExpMax= 5.91D+03 ExpMxC= 2.05D+02 IAcc=2 IRadAn= 0 AccDes= 0.00D+00
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 0 IDoV= 1
ScaDFX= 1.000000 1.000000 1.000000 1.000000
Defaulting to unpruned grid for atomic number 81.
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
Omega= 0.000000 0.000000 1.000000 0.000000 0.000000 ICntrl= 500 IOpCl= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
I1Cent= 4 NGrid= 0.
Petite list used in FoFCou.
LocMO: Using Boys method
Initial Trace= 0.32522505D-01 Initial TraceA= 0.27077929D+04
RMSG= 0.21473963D-06
LocMO: Using Boys method
Initial Trace= 0.61330906D-01 Initial TraceA= 0.72931985D+02
Initial Trace= 0.61330906D-01 Initial TraceA= 0.72931985D+02
Initial Trace= 0.61330906D-01 Initial TraceA= 0.72931985D+02
Localization failed after 3 tries of 1000 iterations each. Last change= 0.10625022D-05
RMSG= 0.12549320D-03

Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state of the initial guess is 1-A.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Defaulting to unpruned grid for atomic number 81.
SCF Done: E(RB3LYP) = -3072.05797944 A.U. after 14 cycles
Convg = 0.5507D-08 -V/T = 2.0090

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Population analysis using the SCF density.

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Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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The electronic state is 1-A.
Alpha occ. eigenvalues -- -14.51809 -14.51802 -14.51734 -14.51730 -14.51294
Alpha occ. eigenvalues -- -14.51287 -10.43823 -10.43815 -10.43781 -10.43774
Alpha occ. eigenvalues -- -10.43537 -10.43533 -10.39489 -10.39488 -10.38660
Alpha occ. eigenvalues -- -10.38651 -10.37996 -10.37992 -10.37832 -10.37828
Alpha occ. eigenvalues -- -10.36166 -10.36164 -10.34992 -10.34991 -10.34664
Alpha occ. eigenvalues -- -10.34655 -10.34594 -10.34591 -10.34257 -10.34254
Alpha occ. eigenvalues -- -10.34158 -10.34155 -10.33689 -10.33687 -10.33461
Alpha occ. eigenvalues -- -10.33457 -10.33256 -10.33256 -10.33056 -10.33055
Alpha occ. eigenvalues -- -10.32482 -10.32481 -10.32466 -10.32461 -10.32447
Alpha occ. eigenvalues -- -10.32444 -10.32440 -10.32435 -10.32318 -10.32317
Alpha occ. eigenvalues -- -10.32264 -10.32262 -10.32147 -10.32147 -10.32144
Alpha occ. eigenvalues -- -10.32144 -10.32117 -10.32107 -10.31906 -10.31897
Alpha occ. eigenvalues -- -10.31643 -10.31640 -10.28620 -10.28615 -10.27884
Alpha occ. eigenvalues -- -10.27883 -10.27838 -10.27829 -10.27518 -10.27513
Alpha occ. eigenvalues -- -10.27245 -10.27243 -10.27001 -10.26994 -1.15726
Alpha occ. eigenvalues --   -1.15716 -1.13751 -1.13739 -1.13278 -1.13276
Alpha occ. eigenvalues --   -1.04561 -1.04488 -1.03414 -1.03321 -1.02859
Alpha occ. eigenvalues --   -1.02847 -0.99370 -0.99337 -0.99029 -0.99018
Alpha occ. eigenvalues --   -0.97657 -0.97651 -0.97223 -0.97218 -0.95595
Alpha occ. eigenvalues --   -0.95576 -0.95367 -0.95366 -0.93149 -0.93135

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Alpha  occ. eigenvalues --   -0.92744  -0.92732  -0.92341  -0.92331  -0.92287
Alpha  occ. eigenvalues --   -0.92278  -0.91463  -0.91429  -0.90795  -0.90737
Alpha  occ. eigenvalues --   -0.90155  -0.90144  -0.89108  -0.89064  -0.88944
Alpha  occ. eigenvalues --   -0.88941  -0.88807  -0.88704  -0.88696  -0.88663
Alpha  occ. eigenvalues --   -0.88573  -0.88567  -0.87391  -0.87387  -0.86948
Alpha  occ. eigenvalues --   -0.86944  -0.86602  -0.86598  -0.82440  -0.82439
Alpha  occ. eigenvalues --   -0.81670  -0.81648  -0.81542  -0.81505  -0.81034
Alpha  occ. eigenvalues --   -0.81008  -0.80503  -0.80492  -0.80079  -0.80072
Alpha  occ. eigenvalues --   -0.76676  -0.76646  -0.76070  -0.76066  -0.75826
Alpha  occ. eigenvalues --   -0.75769  -0.75303  -0.75299  -0.74504  -0.74485
Alpha  occ. eigenvalues --   -0.73110  -0.73092  -0.70433  -0.70399  -0.69621
Alpha  occ. eigenvalues --   -0.69591  -0.68097  -0.67977  -0.67712  -0.67651
Alpha  occ. eigenvalues --   -0.67024  -0.67012  -0.66699  -0.66682  -0.65952
Alpha  occ. eigenvalues --   -0.65932  -0.65657  -0.65625  -0.64790  -0.64746
Alpha  occ. eigenvalues --   -0.64563  -0.64550  -0.64247  -0.64206  -0.63954
Alpha  occ. eigenvalues --   -0.63944  -0.63257  -0.63231  -0.63120  -0.63101
Alpha  occ. eigenvalues --   -0.62743  -0.62721  -0.62596  -0.62548  -0.62076
Alpha  occ. eigenvalues --   -0.62068  -0.61856  -0.61824  -0.61299  -0.61248
Alpha  occ. eigenvalues --   -0.61145  -0.61113  -0.61051  -0.60979  -0.60731
Alpha  occ. eigenvalues --   -0.60706  -0.60400  -0.60375  -0.59966  -0.59962
Alpha  occ. eigenvalues --   -0.59702  -0.59467  -0.58807  -0.58760  -0.58115
Alpha  occ. eigenvalues --   -0.58090  -0.57680  -0.57659  -0.57377  -0.57317
Alpha  occ. eigenvalues --   -0.57173  -0.57146  -0.57060  -0.57031  -0.56826
Alpha  occ. eigenvalues --   -0.56744  -0.56563  -0.56356  -0.56249  -0.56103
Alpha  occ. eigenvalues --   -0.56025  -0.55793  -0.55783  -0.55584  -0.55142
Alpha  occ. eigenvalues --   -0.54786  -0.54428  -0.54408  -0.54184  -0.54056
Alpha  occ. eigenvalues --   -0.53784  -0.53727  -0.53079  -0.52880  -0.52169
Alpha  occ. eigenvalues --   -0.51965  -0.51805  -0.51765  -0.51116  -0.51022
Alpha  occ. eigenvalues --   -0.50606  -0.50554  -0.50412  -0.50373  -0.50224
Alpha  occ. eigenvalues --   -0.50065  -0.49592  -0.49523  -0.49371  -0.49171
Alpha  occ. eigenvalues --   -0.49045  -0.48975  -0.48783  -0.48771  -0.48640
Alpha  occ. eigenvalues --   -0.48514  -0.48139  -0.48105  -0.47900  -0.47821
Alpha  occ. eigenvalues --   -0.46926  -0.46858  -0.46439  -0.46081  -0.45857
Alpha  occ. eigenvalues --   -0.45814  -0.43850  -0.42198  -0.42106  -0.41993
Alpha  occ. eigenvalues --   -0.40857  -0.40854  -0.40701  -0.40633  -0.40384
Alpha  occ. eigenvalues --   -0.39574  -0.39191  -0.38793  -0.38724  -0.38377
Alpha virt. eigenvalues --  -0.20936  -0.20915  -0.20462  -0.20342  -0.19216
Alpha virt. eigenvalues --  -0.18772  -0.18666  -0.18090  -0.17601  -0.17303
Alpha virt. eigenvalues --  -0.16757  -0.16469  -0.16102  -0.15861  -0.15490
Alpha virt. eigenvalues --  -0.15467  -0.15111  -0.14917  -0.14525  -0.14234
Alpha virt. eigenvalues --  -0.12717  -0.12068  -0.09146  -0.07700  -0.07589
Alpha virt. eigenvalues --  -0.06694  -0.06619  -0.05934  -0.05891  -0.05587
Alpha virt. eigenvalues --  -0.05233  -0.04810  -0.04676  -0.04147  -0.03717
Alpha virt. eigenvalues --  -0.03411  -0.02844  -0.02623  -0.02181  -0.02158
Alpha virt. eigenvalues --  -0.01873  -0.01836  -0.01791  -0.01698  -0.01402
Alpha virt. eigenvalues --  -0.01319  -0.00945  -0.00712  -0.00681  -0.00536
Alpha virt. eigenvalues --  -0.00287  -0.00256  -0.00078   0.00141   0.00144
Alpha virt. eigenvalues --   0.00457   0.00538   0.00647   0.00649   0.00675
Alpha virt. eigenvalues --   0.00847   0.01025   0.01224   0.01399   0.01890
Alpha virt. eigenvalues --   0.01902   0.01967   0.02221   0.02299   0.02507
Alpha virt. eigenvalues --   0.02648   0.02690   0.02772   0.03045   0.03148
Alpha virt. eigenvalues --   0.03302   0.03446   0.03523   0.03823   0.04042
Alpha virt. eigenvalues --   0.04317   0.04563   0.04716   0.04735   0.04788
Alpha virt. eigenvalues --   0.04861   0.05207   0.05296   0.05417   0.05529
Alpha virt. eigenvalues --   0.05818   0.05949   0.06271   0.06278   0.06623
Alpha virt. eigenvalues --   0.06676   0.06699   0.06906   0.07007   0.07036
Alpha virt. eigenvalues --   0.07111   0.07449   0.07541   0.07751   0.07933
Alpha virt. eigenvalues --   0.08001   0.08128   0.08450   0.08517   0.08790
Alpha virt. eigenvalues --   0.08861   0.08987   0.09112   0.09218   0.09460
Alpha virt. eigenvalues --   0.09595   0.09943   0.09952   0.10013   0.10085
Alpha virt. eigenvalues --   0.10650   0.10699   0.10740   0.10869   0.10930
Alpha virt. eigenvalues --   0.11034   0.11147   0.11279   0.11529   0.11649
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Alpha virt. eigenvalues -- 0.11659 0.11794 0.11855 0.12050 0.12117
Alpha virt. eigenvalues -- 0.12528 0.12656 0.12760 0.12922 0.12989
Alpha virt. eigenvalues -- 0.13170 0.13338 0.13517 0.13722 0.13802
Alpha virt. eigenvalues -- 0.13996 0.14226 0.14404 0.14470 0.14645
Alpha virt. eigenvalues -- 0.14916 0.15166 0.15267 0.15705 0.15770
Alpha virt. eigenvalues -- 0.16001 0.16081 0.16271 0.16387 0.16554
Alpha virt. eigenvalues -- 0.16602 0.16656 0.16860 0.16865 0.17101
Alpha virt. eigenvalues -- 0.17198 0.17475 0.17555 0.17750 0.17926
Alpha virt. eigenvalues -- 0.17993 0.18029 0.18324 0.18489 0.18682
Alpha virt. eigenvalues -- 0.18741 0.18857 0.18954 0.19036 0.19171
Alpha virt. eigenvalues -- 0.19327 0.19355 0.19726 0.19798 0.20036
Alpha virt. eigenvalues -- 0.20193 0.20204 0.20396 0.20408 0.20448
Alpha virt. eigenvalues -- 0.20756 0.20852 0.20978 0.21185 0.21321
Alpha virt. eigenvalues -- 0.21587 0.21592 0.21878 0.21904 0.22069
Alpha virt. eigenvalues -- 0.22449 0.22641 0.22990 0.23143 0.23240
Alpha virt. eigenvalues -- 0.23426 0.23614 0.23811 0.23904 0.23950
Alpha virt. eigenvalues -- 0.24115 0.24139 0.24388 0.24640 0.24709
Alpha virt. eigenvalues -- 0.24724 0.24803 0.24903 0.24991 0.25595
Alpha virt. eigenvalues -- 0.25618 0.25632 0.26003 0.26227 0.26277
Alpha virt. eigenvalues -- 0.26465 0.26508 0.26657 0.27045 0.27129
Alpha virt. eigenvalues -- 0.27165 0.27212 0.27253 0.27538 0.27952
Alpha virt. eigenvalues -- 0.28037 0.28045 0.28068 0.28190 0.28387
Alpha virt. eigenvalues -- 0.28411 0.28797 0.29082 0.29139 0.29555
Alpha virt. eigenvalues -- 0.29624 0.29750 0.29919 0.30079 0.30367
Alpha virt. eigenvalues -- 0.30593 0.30800 0.31071 0.31322 0.31479
Alpha virt. eigenvalues -- 0.31520 0.31565 0.31889 0.31973 0.32145
Alpha virt. eigenvalues -- 0.32149 0.32419 0.32490 0.32904 0.32919
Alpha virt. eigenvalues -- 0.32993 0.33473 0.33479 0.33548 0.34151
Alpha virt. eigenvalues -- 0.34259 0.34384 0.34483 0.34503 0.35066
Alpha virt. eigenvalues -- 0.35464 0.35693 0.36086 0.36304 0.36464
Alpha virt. eigenvalues -- 0.36664 0.36765 0.37043 0.37093 0.37152
Alpha virt. eigenvalues -- 0.37577 0.37621 0.37827 0.37989 0.38010
Alpha virt. eigenvalues -- 0.38406 0.38592 0.38643 0.38646 0.39189
Alpha virt. eigenvalues -- 0.39458 0.39670 0.39714 0.40141 0.40157
Alpha virt. eigenvalues -- 0.40491 0.40572 0.40729 0.40938 0.41347
Alpha virt. eigenvalues -- 0.41451 0.41579 0.41936 0.42097 0.42319
Alpha virt. eigenvalues -- 0.42386 0.42631 0.42669 0.42705 0.43325
Alpha virt. eigenvalues -- 0.43504 0.43640 0.43706 0.43969 0.44251
Alpha virt. eigenvalues -- 0.44324 0.44363 0.44771 0.44942 0.45069
Alpha virt. eigenvalues -- 0.45140 0.45205 0.45450 0.46186 0.46344
Alpha virt. eigenvalues -- 0.46457 0.46586 0.46972 0.47018 0.47321
Alpha virt. eigenvalues -- 0.47444 0.47574 0.48378 0.48413 0.48727
Alpha virt. eigenvalues -- 0.48773 0.49098 0.49244 0.49497 0.49730
Alpha virt. eigenvalues -- 0.50093 0.50183 0.50547 0.50611 0.51143
Alpha virt. eigenvalues -- 0.51391 0.51529 0.52429 0.52443 0.52776
Alpha virt. eigenvalues -- 0.52860 0.53273 0.53709 0.53782 0.54759
Alpha virt. eigenvalues -- 0.54847 0.55289 0.55437 0.56202 0.56414
Alpha virt. eigenvalues -- 0.56499 0.57230 0.57494 0.57754 0.57956
Alpha virt. eigenvalues -- 0.58280 0.58375 0.58821 0.58982 0.59249
Alpha virt. eigenvalues -- 0.59573 0.60239 0.60709 0.61146 0.61455
Alpha virt. eigenvalues -- 0.61651 0.61703 0.62241 0.62248 0.62440
Alpha virt. eigenvalues -- 0.62525 0.63265 0.63647 0.64072 0.64798
Alpha virt. eigenvalues -- 0.64942 0.65473 0.65767 0.65774 0.66250
Alpha virt. eigenvalues -- 0.67347 0.68057 0.68132 0.69071 0.69207
Alpha virt. eigenvalues -- 0.69672 0.69919 0.70735 0.71015 0.71201
Alpha virt. eigenvalues -- 0.71629 0.73334 0.73783 0.74693 0.74802
Alpha virt. eigenvalues -- 0.74974 0.75405 0.75878 0.77910 0.78093
Alpha virt. eigenvalues -- 0.80237 0.81578 0.83458 0.84315 0.84347
Alpha virt. eigenvalues -- 0.85357 0.87869 0.88538 0.88692 0.89460
Alpha virt. eigenvalues -- 0.92657 0.92863 0.93627 0.96740 0.98649
Alpha virt. eigenvalues -- 0.99402 0.99562 0.99970 1.00054 1.00220
Alpha virt. eigenvalues -- 1.00289 1.00975 1.01602 1.01908 1.02421

Alpha virt. eigenvalues -- 1.03000 1.03997 1.04210 1.04702 1.04962
Alpha virt. eigenvalues -- 1.05979 1.06223 1.06444 1.07249 1.07619
Alpha virt. eigenvalues -- 1.08465 1.08532 1.09459 1.09835 1.10183
Alpha virt. eigenvalues -- 1.10224 1.10941 1.11052 1.11325 1.11663
Alpha virt. eigenvalues -- 1.12082 1.12220 1.12378 1.12698 1.12905
Alpha virt. eigenvalues -- 1.12969 1.13949 1.14295 1.14324 1.14534
Alpha virt. eigenvalues -- 1.14569 1.14855 1.15212 1.15701 1.15770
Alpha virt. eigenvalues -- 1.15794 1.15901 1.16169 1.16759 1.16949
Alpha virt. eigenvalues -- 1.17017 1.17477 1.17611 1.17887 1.18307
Alpha virt. eigenvalues -- 1.18500 1.18508 1.19049 1.19188 1.19602
Alpha virt. eigenvalues -- 1.19770 1.20334 1.20553 1.20900 1.21069
Alpha virt. eigenvalues -- 1.21338 1.21478 1.21932 1.22192 1.22540
Alpha virt. eigenvalues -- 1.22852 1.22899 1.23497 1.23543 1.23921
Alpha virt. eigenvalues -- 1.24108 1.24345 1.24632 1.25332 1.25403
Alpha virt. eigenvalues -- 1.26279 1.26343 1.27136 1.27180 1.27341
Alpha virt. eigenvalues -- 1.27478 1.27666 1.28232 1.28434 1.28971
Alpha virt. eigenvalues -- 1.29354 1.29858 1.29920 1.30307 1.31105
Alpha virt. eigenvalues -- 1.31111 1.31501 1.31613 1.32025 1.32178
Alpha virt. eigenvalues -- 1.32844 1.33352 1.33383 1.33787 1.33984
Alpha virt. eigenvalues -- 1.35529 1.35534 1.35773 1.36179 1.36824
Alpha virt. eigenvalues -- 1.36889 1.37857 1.38193 1.38705 1.39545
Alpha virt. eigenvalues -- 1.39570 1.40821 1.41402 1.41666 1.41730
Alpha virt. eigenvalues -- 1.42215 1.42756 1.43488 1.44205 1.45233
Alpha virt. eigenvalues -- 1.45987 1.46965 1.47466 1.48410 1.48962
Alpha virt. eigenvalues -- 1.50054 1.50500 1.51207 1.51560 1.52074
Alpha virt. eigenvalues -- 1.53354 1.55025 1.55077 1.56166 1.56530
Alpha virt. eigenvalues -- 1.56925 1.57306 1.58205 1.58694 1.59198
Alpha virt. eigenvalues -- 1.59278 1.60676 1.61880 1.62417 1.64141
Alpha virt. eigenvalues -- 1.64840 1.65555 1.66559 1.69267 1.74599
Alpha virt. eigenvalues -- 1.75002 1.78851 1.78966 1.79909 1.81076
Alpha virt. eigenvalues -- 1.87930 1.89120 11.12065 11.15176
Condensed to atoms (all electrons):
Mulliken atomic charges:

		1
1	C	-0.333911
2	H	0.265782
3	C	0.127837
4	C	-0.780046
5	H	0.297158
6	H	0.284250
7	H	0.281275
8	C	0.011102
9	C	0.327394
10	C	-0.467888
11	C	-0.339764
12	C	-0.536073
13	C	-0.452126
14	C	-0.288567
15	C	-0.731062
16	H	0.250191
17	H	0.249865
18	H	0.239525
19	C	-0.745451
20	H	0.244420
21	H	0.256114
22	H	0.249806
23	C	0.135312
24	C	-0.787881
25	H	0.301723
26	H	0.286571
27	H	0.285099
28	C	0.034581

29	C	0.306330
30	C	-0.467734
31	C	-0.308329
32	C	-0.414991
33	C	-0.460677
34	C	-0.272945
35	C	-0.740638
36	H	0.241202
37	H	0.248146
38	H	0.254732
39	C	-0.758627
40	H	0.236766
41	H	0.251303
42	H	0.255408
43	C	0.125836
44	C	-0.782316
45	H	0.299187
46	H	0.284487
47	H	0.277726
48	C	0.086060
49	C	0.311069
50	C	-0.448951
51	C	-0.377576
52	C	-0.261371
53	C	-0.483340
54	C	-0.234559
55	C	-0.742056
56	H	0.262206
57	H	0.252734
58	H	0.238845
59	C	-0.752076
60	H	0.233642
61	H	0.255805
62	H	0.247188
63	H	0.330560
64	H	0.322589
65	H	0.591807
66	H	0.355698
67	H	0.273663
68	H	0.384422
69	H	0.312428
70	H	0.420651
71	H	0.372535
72	H	0.243027
73	H	0.327664
74	H	0.358452
75	H	0.307297
76	H	0.369920
77	H	0.215491
78	N	-0.197911
79	N	-0.232535
80	N	-0.233998
81	Tl	0.650540
82	Tl	0.650548
83	C	0.011362
84	C	0.327311
85	C	-0.467876
86	C	-0.339763
87	C	-0.536052
88	C	-0.452201
89	C	-0.333158
90	H	0.265199

91	C	0.127634
92	C	-0.780647
93	H	0.297313
94	H	0.284381
95	H	0.281053
96	C	-0.289442
97	C	-0.731310
98	H	0.250160
99	H	0.249821
100	H	0.239983
101	C	-0.744731
102	H	0.244392
103	H	0.255544
104	H	0.250238
105	C	0.135290
106	C	-0.787938
107	H	0.301810
108	H	0.286681
109	H	0.284569
110	C	0.034285
111	C	0.306052
112	C	-0.468198
113	C	-0.308613
114	C	-0.413913
115	C	-0.460742
116	C	-0.273140
117	C	-0.740243
118	H	0.241122
119	H	0.248072
120	H	0.254763
121	C	-0.758739
122	H	0.236770
123	H	0.251335
124	H	0.255370
125	C	0.126099
126	C	-0.782435
127	H	0.299201
128	H	0.284571
129	H	0.277579
130	C	0.086418
131	C	0.310248
132	C	-0.448260
133	C	-0.377588
134	C	-0.261409
135	C	-0.483449
136	C	-0.235026
137	C	-0.742096
138	H	0.262066
139	H	0.252513
140	H	0.239148
141	C	-0.752139
142	H	0.233609
143	H	0.255983
144	H	0.247189
145	H	0.330513
146	H	0.322563
147	H	0.591797
148	H	0.355719
149	H	0.273802
150	H	0.385192
151	H	0.312463
152	H	0.419807

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 153  H    0.372590
 154  H    0.242978
 155  H    0.327373
 156  H    0.358736
 157  H    0.307282
 158  H    0.369913
 159  H    0.215813
 160  N   -0.197158
 161  N   -0.231984
 162  N   -0.233992
Sum of Mulliken atomic charges =   2.00000
Mulliken charges with hydrogens summed into heavy atoms:
              1
     1  C   -0.068129
     3  C    0.127837
     4  C    0.082638
     8  C    0.011102
     9  C    0.327394
    10  C   -0.137327
    11  C   -0.017175
    12  C    0.055734
    13  C   -0.096427
    14  C   -0.014904
    15  C    0.008519
    19  C    0.004888
    23  C    0.135312
    24  C    0.085512
    28  C    0.034581
    29  C    0.306330
    30  C   -0.083312
    31  C    0.004099
    32  C    0.005660
    33  C   -0.088141
    34  C   -0.029919
    35  C    0.003442
    39  C   -0.015150
    43  C    0.125836
    44  C    0.079084
    48  C    0.086060
    49  C    0.311069
    50  C   -0.121287
    51  C   -0.019123
    52  C    0.045926
    53  C   -0.113420
    54  C   -0.019068
    55  C    0.011729
    59  C   -0.015441
    78  N   -0.197911
    79  N   -0.232535
    80  N   -0.233998
    81  Tl   0.650540
    82  Tl   0.650548
    83  C    0.011362
    84  C    0.327311
    85  C   -0.137363
    86  C   -0.017201
    87  C    0.055745
    88  C   -0.096481
    89  C   -0.067958
    91  C    0.127634
    92  C    0.082099
    96  C   -0.015640
```

```
   97  C    0.008654
  101  C    0.005442
  105  C    0.135290
  106  C    0.085122
  110  C    0.034285
  111  C    0.306052
  112  C   -0.083006
  113  C    0.003850
  114  C    0.005895
  115  C   -0.088153
  116  C   -0.030162
  117  C    0.003713
  121  C   -0.015265
  125  C    0.126099
  126  C    0.078916
  130  C    0.086418
  131  C    0.310248
  132  C   -0.120887
  133  C   -0.018852
  134  C    0.045873
  135  C   -0.113536
  136  C   -0.019213
  137  C    0.011631
  141  C   -0.015358
  160  N   -0.197158
  161  N   -0.231984
  162  N   -0.233992
Sum of Mulliken charges with hydrogens summed into heavy atoms =   2.00000
Electronic spatial extent (au):  <R**2>=          55179.7615
Charge=              2.0000 electrons
Dipole moment (field-independent basis, Debye):
   X=             -0.0008    Y=             -0.0012    Z=             -0.0030  Tot=              0.0033
Quadrupole moment (field-independent basis, Debye-Ang):
  XX=           -290.4308   YY=           -377.6805   ZZ=           -373.5408
  XY=             -5.3358   XZ=             27.7707   YZ=             -0.3635
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
  XX=             56.7866   YY=            -30.4631   ZZ=            -26.3234
  XY=             -5.3358   XZ=             27.7707   YZ=             -0.3635
Octapole moment (field-independent basis, Debye-Ang**2):
 XXX=              0.0082  YYY=             -0.1873  ZZZ=              0.0124  XYY=             -0.0458
 XXY=              0.0306  XXZ=             -0.0442  XZZ=             -0.0317  YZZ=             -0.0179
 YYZ=             -0.0730  XYZ=             -0.0507
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=        -30982.2777 YYYY=        -20106.9176 ZZZZ=        -14318.3487 XXXY=           -630.0522
XXXZ=           287.9859 YYYX=           164.9672 YYYZ=           260.4428 ZZZX=           536.5887
ZZZY=          -241.5723 XXYY=         -8751.7082 XXZZ=         -7092.4410 YYZZ=         -5618.2510
XXYZ=           141.7306 YYXZ=          -307.9519 ZZXY=            80.4701
N-N= 1.483812916045D+04 E-N=-3.673304832783D+04  KE= 3.044672329488D+03
******************************Gaussian NBO Version 3.1******************************
         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
******************************Gaussian NBO Version 3.1******************************
 /RESON  / : Allow strongly delocalized NBO set

Analyzing the SCF density

Job title: CSD ENTRY ofm27p-1

Storage needed:   2371396 in NPA (  33481086 available)


NATURAL POPULATIONS:  Natural atomic orbital occupancies
```

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	S	Cor(1S)	1.99882	-10.23427
2	C	1	S	Val(2S)	0.96075	-0.35897
3	C	1	S	Ryd(3S)	0.00111	1.35451
4	C	1	px	Val(2p)	1.12008	-0.26082
5	C	1	px	Ryd(3p)	0.01055	0.39243
6	C	1	py	Val(2p)	1.07297	-0.28135
7	C	1	py	Ryd(3p)	0.00594	0.34299
8	C	1	pz	Val(2p)	1.15114	-0.24983
9	C	1	pz	Ryd(3p)	0.01367	0.41365
10	H	2	S	Val(1S)	0.77092	0.01379
11	H	2	S	Ryd(2S)	0.00188	0.89805
12	C	3	S	Cor(1S)	1.99900	-10.30754
13	C	3	S	Val(2S)	0.85587	-0.32376
14	C	3	S	Ryd(3S)	0.00474	0.94734
15	C	3	px	Val(2p)	0.91499	-0.20614
16	C	3	px	Ryd(3p)	0.00700	0.45204
17	C	3	py	Val(2p)	0.84205	-0.27685
18	C	3	py	Ryd(3p)	0.00798	0.35828
19	C	3	pz	Val(2p)	0.92087	-0.23319
20	C	3	pz	Ryd(3p)	0.00677	0.41287
21	C	4	S	Cor(1S)	1.99907	-10.16140
22	C	4	S	Val(2S)	1.02345	-0.29132
23	C	4	S	Ryd(3S)	0.00053	1.05488
24	C	4	px	Val(2p)	1.26715	-0.20659
25	C	4	px	Ryd(3p)	0.00260	0.15957
26	C	4	py	Val(2p)	1.20848	-0.21458
27	C	4	py	Ryd(3p)	0.00201	0.18319
28	C	4	pz	Val(2p)	1.13477	-0.23240
29	C	4	pz	Ryd(3p)	0.00351	0.16823
30	H	5	S	Val(1S)	0.77349	0.03085
31	H	5	S	Ryd(2S)	0.00144	0.81496
32	H	6	S	Val(1S)	0.76876	0.02294
33	H	6	S	Ryd(2S)	0.00102	0.74571
34	H	7	S	Val(1S)	0.77062	0.02020
35	H	7	S	Ryd(2S)	0.00101	0.75225
36	C	8	S	Cor(1S)	1.99873	-10.25755
37	C	8	S	Val(2S)	0.84207	-0.27531
38	C	8	S	Ryd(3S)	0.00198	1.07008
39	C	8	px	Val(2p)	0.89434	-0.20233
40	C	8	px	Ryd(3p)	0.01412	0.57295
41	C	8	py	Val(2p)	1.07307	-0.21663
42	C	8	py	Ryd(3p)	0.00510	0.43334
43	C	8	pz	Val(2p)	1.03116	-0.27444
44	C	8	pz	Ryd(3p)	0.00801	0.35060
45	C	9	S	Cor(1S)	1.99891	-10.22240
46	C	9	S	Val(2S)	0.89121	-0.28186
47	C	9	S	Ryd(3S)	0.00175	1.12664
48	C	9	px	Val(2p)	1.06187	-0.20170
49	C	9	px	Ryd(3p)	0.00744	0.48019
50	C	9	py	Val(2p)	1.06118	-0.21040
51	C	9	py	Ryd(3p)	0.00959	0.58686

52	C	9	pz	Val(2p)	0.98440	-0.25346
53	C	9	pz	Ryd(3p)	0.00685	0.39912
54	C	10	S	Cor(1S)	1.99906	-10.19632
55	C	10	S	Val(2S)	0.93745	-0.27267
56	C	10	S	Ryd(3S)	0.00130	1.02671
57	C	10	px	Val(2p)	1.10929	-0.16743
58	C	10	px	Ryd(3p)	0.00641	0.38470
59	C	10	py	Val(2p)	1.11083	-0.16791
60	C	10	py	Ryd(3p)	0.00448	0.46244
61	C	10	pz	Val(2p)	1.00019	-0.25693
62	C	10	pz	Ryd(3p)	0.00351	0.27207
63	C	11	S	Cor(1S)	1.99917	-10.19601
64	C	11	S	Val(2S)	0.93831	-0.25988
65	C	11	S	Ryd(3S)	0.00150	0.95053
66	C	11	px	Val(2p)	1.15915	-0.10801
67	C	11	px	Ryd(3p)	0.00685	0.43549
68	C	11	py	Val(2p)	1.04953	-0.18528
69	C	11	py	Ryd(3p)	0.00382	0.34433
70	C	11	pz	Val(2p)	1.00319	-0.25676
71	C	11	pz	Ryd(3p)	0.00372	0.28236
72	C	12	S	Cor(1S)	1.99858	-10.15233
73	C	12	S	Val(2S)	0.87393	-0.11866
74	C	12	S	Ryd(3S)	0.00108	0.96431
75	C	12	px	Val(2p)	1.06280	-0.17858
76	C	12	px	Ryd(3p)	0.00404	0.42785
77	C	12	py	Val(2p)	1.12700	-0.01159
78	C	12	py	Ryd(3p)	0.00713	0.33730
79	C	12	pz	Val(2p)	0.99869	-0.25361
80	C	12	pz	Ryd(3p)	0.00405	0.33470
81	C	13	S	Cor(1S)	1.99904	-10.19692
82	C	13	S	Val(2S)	0.92823	-0.26055
83	C	13	S	Ryd(3S)	0.00138	1.08466
84	C	13	px	Val(2p)	1.10023	-0.17272
85	C	13	px	Ryd(3p)	0.00520	0.48594
86	C	13	py	Val(2p)	1.10399	-0.17481
87	C	13	py	Ryd(3p)	0.00724	0.37207
88	C	13	pz	Val(2p)	1.04828	-0.25589
89	C	13	pz	Ryd(3p)	0.00395	0.36796
90	C	14	S	Cor(1S)	1.99896	-10.17752
91	C	14	S	Val(2S)	0.91775	-0.24279
92	C	14	S	Ryd(3S)	0.00053	1.36681
93	C	14	px	Val(2p)	1.14115	-0.13973
94	C	14	px	Ryd(3p)	0.00867	0.33968
95	C	14	py	Val(2p)	1.01731	-0.19789
96	C	14	py	Ryd(3p)	0.00434	0.33814
97	C	14	pz	Val(2p)	1.04581	-0.18590
98	C	14	pz	Ryd(3p)	0.00315	0.39390
99	C	15	S	Cor(1S)	1.99918	-10.11990
100	C	15	S	Val(2S)	1.01165	-0.23312
101	C	15	S	Ryd(3S)	0.00051	1.02956
102	C	15	px	Val(2p)	1.24284	-0.15573
103	C	15	px	Ryd(3p)	0.00248	0.16004
104	C	15	py	Val(2p)	1.23533	-0.15386
105	C	15	py	Ryd(3p)	0.00279	0.20106
106	C	15	pz	Val(2p)	1.07768	-0.18481
107	C	15	pz	Ryd(3p)	0.00290	0.18908

108	H	16	S	Val(1S)	0.79821	0.05817
109	H	16	S	Ryd(2S)	0.00152	0.75032
110	H	17	S	Val(1S)	0.79391	0.06437
111	H	17	S	Ryd(2S)	0.00122	0.74153
112	H	18	S	Val(1S)	0.80358	0.05321
113	H	18	S	Ryd(2S)	0.00128	0.78190
114	C	19	S	Cor(1S)	1.99921	-10.11942
115	C	19	S	Val(2S)	1.00349	-0.22629
116	C	19	S	Ryd(3S)	0.00045	1.06664
117	C	19	px	Val(2p)	1.19655	-0.16870
118	C	19	px	Ryd(3p)	0.00229	0.29795
119	C	19	py	Val(2p)	1.16494	-0.17342
120	C	19	py	Ryd(3p)	0.00317	0.29118
121	C	19	pz	Val(2p)	1.19914	-0.16208
122	C	19	pz	Ryd(3p)	0.00324	0.26417
123	H	20	S	Val(1S)	0.81143	0.04469
124	H	20	S	Ryd(2S)	0.00145	0.91511
125	H	21	S	Val(1S)	0.79308	0.06497
126	H	21	S	Ryd(2S)	0.00128	0.79256
127	H	22	S	Val(1S)	0.80320	0.04837
128	H	22	S	Ryd(2S)	0.00180	0.86595
129	C	23	S	Cor(1S)	1.99899	-10.30473
130	C	23	S	Val(2S)	0.85654	-0.32328
131	C	23	S	Ryd(3S)	0.00496	0.98224
132	C	23	px	Val(2p)	0.94981	-0.20699
133	C	23	px	Ryd(3p)	0.00706	0.44214
134	C	23	py	Val(2p)	0.86994	-0.25263
135	C	23	py	Ryd(3p)	0.00899	0.38652
136	C	23	pz	Val(2p)	0.85920	-0.25120
137	C	23	pz	Ryd(3p)	0.00640	0.38854
138	C	24	S	Cor(1S)	1.99907	-10.15620
139	C	24	S	Val(2S)	1.02082	-0.28520
140	C	24	S	Ryd(3S)	0.00055	1.08178
141	C	24	px	Val(2p)	1.10118	-0.23787
142	C	24	px	Ryd(3p)	0.00413	0.15620
143	C	24	py	Val(2p)	1.25338	-0.20370
144	C	24	py	Ryd(3p)	0.00213	0.16080
145	C	24	pz	Val(2p)	1.25978	-0.20331
146	C	24	pz	Ryd(3p)	0.00217	0.20372
147	H	25	S	Val(1S)	0.76956	0.03800
148	H	25	S	Ryd(2S)	0.00130	0.82303
149	H	26	S	Val(1S)	0.76802	0.02947
150	H	26	S	Ryd(2S)	0.00108	0.75421
151	H	27	S	Val(1S)	0.77263	0.01826
152	H	27	S	Ryd(2S)	0.00117	0.81650
153	C	28	S	Cor(1S)	1.99877	-10.24349
154	C	28	S	Val(2S)	0.84459	-0.26332
155	C	28	S	Ryd(3S)	0.00207	1.04583
156	C	28	px	Val(2p)	1.04372	-0.25197

157	C	28	px	Ryd(3p)	0.00666	0.40465
158	C	28	py	Val(2p)	1.00567	-0.19710
159	C	28	py	Ryd(3p)	0.00718	0.51745
160	C	28	pz	Val(2p)	0.95595	-0.20324
161	C	28	pz	Ryd(3p)	0.01041	0.52898
162	C	29	S	Cor(1S)	1.99899	-10.21076
163	C	29	S	Val(2S)	0.89205	-0.26761
164	C	29	S	Ryd(3S)	0.00139	1.11335
165	C	29	px	Val(2p)	0.99405	-0.22967
166	C	29	px	Ryd(3p)	0.00762	0.42570
167	C	29	py	Val(2p)	1.04364	-0.18445
168	C	29	py	Ryd(3p)	0.00654	0.48167
169	C	29	pz	Val(2p)	1.03886	-0.19866
170	C	29	pz	Ryd(3p)	0.00843	0.52924
171	C	30	S	Cor(1S)	1.99889	-10.15233
172	C	30	S	Val(2S)	0.89472	-0.16917
173	C	30	S	Ryd(3S)	0.00093	0.97774
174	C	30	px	Val(2p)	1.02190	-0.20503
175	C	30	px	Ryd(3p)	0.00252	0.32440
176	C	30	py	Val(2p)	1.14851	-0.08294
177	C	30	py	Ryd(3p)	0.00768	0.26759
178	C	30	pz	Val(2p)	1.06639	-0.18198
179	C	30	pz	Ryd(3p)	0.00297	0.45086
180	C	31	S	Cor(1S)	1.99921	-10.17727
181	C	31	S	Val(2S)	0.93342	-0.23034
182	C	31	S	Ryd(3S)	0.00089	0.89781
183	C	31	px	Val(2p)	1.00626	-0.21900
184	C	31	px	Ryd(3p)	0.00298	0.27519
185	C	31	py	Val(2p)	1.08341	-0.15648
186	C	31	py	Ryd(3p)	0.00455	0.30994
187	C	31	pz	Val(2p)	1.12364	-0.11033
188	C	31	pz	Ryd(3p)	0.00541	0.34449
189	C	32	S	Cor(1S)	1.99904	-10.16401
190	C	32	S	Val(2S)	0.91220	-0.18502
191	C	32	S	Ryd(3S)	0.00075	0.89437
192	C	32	px	Val(2p)	1.02124	-0.20666
193	C	32	px	Ryd(3p)	0.00402	0.26067
194	C	32	py	Val(2p)	1.06117	-0.15001
195	C	32	py	Ryd(3p)	0.00343	0.35270
196	C	32	pz	Val(2p)	1.09786	-0.10058
197	C	32	pz	Ryd(3p)	0.00569	0.29191
198	C	33	S	Cor(1S)	1.99907	-10.17873
199	C	33	S	Val(2S)	0.92137	-0.23660
200	C	33	S	Ryd(3S)	0.00121	1.01641
201	C	33	px	Val(2p)	1.04295	-0.24337
202	C	33	px	Ryd(3p)	0.00442	0.31812
203	C	33	py	Val(2p)	1.15849	-0.11235
204	C	33	py	Ryd(3p)	0.00683	0.51603
205	C	33	pz	Val(2p)	1.07167	-0.20609
206	C	33	pz	Ryd(3p)	0.00466	0.44128
207	C	34	S	Cor(1S)	1.99911	-10.18966
208	C	34	S	Val(2S)	0.94564	-0.28345
209	C	34	S	Ryd(3S)	0.00052	1.35521
210	C	34	px	Val(2p)	1.00836	-0.19886
211	C	34	px	Ryd(3p)	0.00272	0.31802
212	C	34	py	Val(2p)	1.08863	-0.18196

213	C	34	py	Ryd(3p)	0.00735	0.45107
214	C	34	pz	Val(2p)	1.10051	-0.16176
215	C	34	pz	Ryd(3p)	0.00587	0.27539
216	C	35	S	Cor(1S)	1.99917	-10.11250
217	C	35	S	Val(2S)	1.01313	-0.22724
218	C	35	S	Ryd(3S)	0.00041	1.02022
219	C	35	px	Val(2p)	1.22944	-0.14792
220	C	35	px	Ryd(3p)	0.00294	0.20060
221	C	35	py	Val(2p)	1.10372	-0.17052
222	C	35	py	Ryd(3p)	0.00269	0.18602
223	C	35	pz	Val(2p)	1.22101	-0.15129
224	C	35	pz	Ryd(3p)	0.00249	0.18062
225	H	36	S	Val(1S)	0.80572	0.05818
226	H	36	S	Ryd(2S)	0.00141	0.77765
227	H	37	S	Val(1S)	0.79524	0.07114
228	H	37	S	Ryd(2S)	0.00125	0.75152
229	H	38	S	Val(1S)	0.79419	0.07425
230	H	38	S	Ryd(2S)	0.00118	0.74307
231	C	39	S	Cor(1S)	1.99918	-10.12829
232	C	39	S	Val(2S)	1.01080	-0.23849
233	C	39	S	Ryd(3S)	0.00051	1.02927
234	C	39	px	Val(2p)	1.09587	-0.19700
235	C	39	px	Ryd(3p)	0.00379	0.37972
236	C	39	py	Val(2p)	1.22861	-0.15981
237	C	39	py	Ryd(3p)	0.00292	0.22824
238	C	39	pz	Val(2p)	1.23561	-0.16171
239	C	39	pz	Ryd(3p)	0.00227	0.32099
240	H	40	S	Val(1S)	0.81581	0.03854
241	H	40	S	Ryd(2S)	0.00150	0.89133
242	H	41	S	Val(1S)	0.79483	0.05659
243	H	41	S	Ryd(2S)	0.00138	0.77936
244	H	42	S	Val(1S)	0.79958	0.05439
245	H	42	S	Ryd(2S)	0.00150	0.79942
246	C	43	S	Cor(1S)	1.99898	-10.30614
247	C	43	S	Val(2S)	0.85448	-0.32225
248	C	43	S	Ryd(3S)	0.00488	0.95167
249	C	43	px	Val(2p)	0.80819	-0.29302
250	C	43	px	Ryd(3p)	0.00761	0.34571
251	C	43	py	Val(2p)	0.98559	-0.24260
252	C	43	py	Ryd(3p)	0.00632	0.49835
253	C	43	pz	Val(2p)	0.88388	-0.18050
254	C	43	pz	Ryd(3p)	0.00802	0.42276
255	C	44	S	Cor(1S)	1.99907	-10.16054
256	C	44	S	Val(2S)	1.02262	-0.29020
257	C	44	S	Ryd(3S)	0.00054	1.06163
258	C	44	px	Val(2p)	1.24258	-0.20525
259	C	44	px	Ryd(3p)	0.00149	0.21599
260	C	44	py	Val(2p)	1.16523	-0.22726
261	C	44	py	Ryd(3p)	0.00379	0.18126
262	C	44	pz	Val(2p)	1.20513	-0.21972
263	C	44	pz	Ryd(3p)	0.00276	0.13999

264	H	45	S	Val(1S)	0.77005	0.03427
265	H	45	S	Ryd(2S)	0.00126	0.80851
266	H	46	S	Val(1S)	0.77014	0.02659
267	H	46	S	Ryd(2S)	0.00100	0.75232
268	H	47	S	Val(1S)	0.77147	0.01884
269	H	47	S	Ryd(2S)	0.00104	0.78255
270	C	48	S	Cor(1S)	1.99878	-10.25139
271	C	48	S	Val(2S)	0.84199	-0.26805
272	C	48	S	Ryd(3S)	0.00210	1.06407
273	C	48	px	Val(2p)	1.07871	-0.22305
274	C	48	px	Ryd(3p)	0.00511	0.43222
275	C	48	py	Val(2p)	0.90470	-0.20131
276	C	48	py	Ryd(3p)	0.00771	0.48783
277	C	48	pz	Val(2p)	1.01707	-0.23851
278	C	48	pz	Ryd(3p)	0.01077	0.55558
279	C	49	S	Cor(1S)	1.99897	-10.21149
280	C	49	S	Val(2S)	0.89039	-0.26733
281	C	49	S	Ryd(3S)	0.00140	1.11279
282	C	49	px	Val(2p)	1.04112	-0.20769
283	C	49	px	Ryd(3p)	0.00824	0.57463
284	C	49	py	Val(2p)	1.04258	-0.20741
285	C	49	py	Ryd(3p)	0.00685	0.44991
286	C	49	pz	Val(2p)	1.02408	-0.21424
287	C	49	pz	Ryd(3p)	0.00695	0.42913
288	C	50	S	Cor(1S)	1.99907	-10.17686
289	C	50	S	Val(2S)	0.93223	-0.24308
290	C	50	S	Ryd(3S)	0.00099	0.97926
291	C	50	px	Val(2p)	1.08847	-0.17199
292	C	50	px	Ryd(3p)	0.00423	0.36828
293	C	50	py	Val(2p)	1.04257	-0.19125
294	C	50	py	Ryd(3p)	0.00362	0.34058
295	C	50	pz	Val(2p)	1.08605	-0.17157
296	C	50	pz	Ryd(3p)	0.00545	0.28876
297	C	51	S	Cor(1S)	1.99914	-10.17026
298	C	51	S	Val(2S)	0.92654	-0.21781
299	C	51	S	Ryd(3S)	0.00073	0.88052
300	C	51	px	Val(2p)	1.03637	-0.18468
301	C	51	px	Ryd(3p)	0.00293	0.31452
302	C	51	py	Val(2p)	1.09676	-0.14756
303	C	51	py	Ryd(3p)	0.00566	0.26692
304	C	51	pz	Val(2p)	1.07130	-0.15510
305	C	51	pz	Ryd(3p)	0.00413	0.28887
306	C	52	S	Cor(1S)	1.99921	-10.18795
307	C	52	S	Val(2S)	0.93838	-0.24833
308	C	52	S	Ryd(3S)	0.00084	0.89380
309	C	52	px	Val(2p)	1.11394	-0.15476
310	C	52	px	Ryd(3p)	0.00645	0.41687
311	C	52	py	Val(2p)	1.06987	-0.16746
312	C	52	py	Ryd(3p)	0.00438	0.29831
313	C	52	pz	Val(2p)	1.02873	-0.20630
314	C	52	pz	Ryd(3p)	0.00327	0.29916
315	C	53	S	Cor(1S)	1.99906	-10.18583
316	C	53	S	Val(2S)	0.92120	-0.24351
317	C	53	S	Ryd(3S)	0.00128	1.02224

318	C	53	px	Val(2p)	1.11282	-0.17221
319	C	53	px	Ryd(3p)	0.00641	0.40996
320	C	53	py	Val(2p)	1.06101	-0.21870
321	C	53	py	Ryd(3p)	0.00416	0.40047
322	C	53	pz	Val(2p)	1.10248	-0.18765
323	C	53	pz	Ryd(3p)	0.00492	0.39497
324	C	54	S	Cor(1S)	1.99916	-10.19254
325	C	54	S	Val(2S)	0.95064	-0.29306
326	C	54	S	Ryd(3S)	0.00052	1.37887
327	C	54	px	Val(2p)	1.02515	-0.19674
328	C	54	px	Ryd(3p)	0.00392	0.36320
329	C	54	py	Val(2p)	1.13815	-0.15971
330	C	54	py	Ryd(3p)	0.00680	0.30045
331	C	54	pz	Val(2p)	1.02763	-0.19656
332	C	54	pz	Ryd(3p)	0.00445	0.43287
333	C	55	S	Cor(1S)	1.99916	-10.11642
334	C	55	S	Val(2S)	1.01167	-0.23017
335	C	55	S	Ryd(3S)	0.00050	1.04528
336	C	55	px	Val(2p)	1.16131	-0.16752
337	C	55	px	Ryd(3p)	0.00285	0.19637
338	C	55	py	Val(2p)	1.23887	-0.15362
339	C	55	py	Ryd(3p)	0.00209	0.21422
340	C	55	pz	Val(2p)	1.15310	-0.16396
341	C	55	pz	Ryd(3p)	0.00324	0.21214
342	H	56	S	Val(1S)	0.79315	0.07319
343	H	56	S	Ryd(2S)	0.00160	0.76206
344	H	57	S	Val(1S)	0.79381	0.06715
345	H	57	S	Ryd(2S)	0.00128	0.74376
346	H	58	S	Val(1S)	0.81631	0.04570
347	H	58	S	Ryd(2S)	0.00155	0.88304
348	C	59	S	Cor(1S)	1.99918	-10.11448
349	C	59	S	Val(2S)	1.01244	-0.22964
350	C	59	S	Ryd(3S)	0.00045	1.03862
351	C	59	px	Val(2p)	1.21585	-0.15189
352	C	59	px	Ryd(3p)	0.00292	0.21337
353	C	59	py	Val(2p)	1.24878	-0.14784
354	C	59	py	Ryd(3p)	0.00212	0.19897
355	C	59	pz	Val(2p)	1.10229	-0.17624
356	C	59	pz	Ryd(3p)	0.00313	0.19331
357	H	60	S	Val(1S)	0.80430	0.05717
358	H	60	S	Ryd(2S)	0.00122	0.79814
359	H	61	S	Val(1S)	0.79019	0.07466
360	H	61	S	Ryd(2S)	0.00115	0.77483
361	H	62	S	Val(1S)	0.79736	0.06731
362	H	62	S	Ryd(2S)	0.00162	0.74359
363	H	63	S	Val(1S)	0.80495	0.07443
364	H	63	S	Ryd(2S)	0.00166	0.90368
365	H	64	S	Val(1S)	0.81429	0.09900
366	H	64	S	Ryd(2S)	0.00185	0.85226
367	H	65	S	Val(1S)	0.89645	0.25763

368	H	65	S	Ryd(2S)	0.00241	0.76964
369	H	66	S	Val(1S)	0.81647	0.08335
370	H	66	S	Ryd(2S)	0.00212	0.94052
371	H	67	S	Val(1S)	0.83099	0.12041
372	H	67	S	Ryd(2S)	0.00311	0.84525
373	H	68	S	Val(1S)	0.84688	0.18262
374	H	68	S	Ryd(2S)	0.00229	0.84793
375	H	69	S	Val(1S)	0.80599	0.10969
376	H	69	S	Ryd(2S)	0.00185	0.82832
377	H	70	S	Val(1S)	0.85944	0.19019
378	H	70	S	Ryd(2S)	0.00164	0.78101
379	H	71	S	Val(1S)	0.83028	0.10282
380	H	71	S	Ryd(2S)	0.00200	0.97501
381	H	72	S	Val(1S)	0.81233	0.07566
382	H	72	S	Ryd(2S)	0.00270	0.84079
383	H	73	S	Val(1S)	0.81006	0.09647
384	H	73	S	Ryd(2S)	0.00168	0.85884
385	H	74	S	Val(1S)	0.82548	0.14707
386	H	74	S	Ryd(2S)	0.00186	0.80068
387	H	75	S	Val(1S)	0.81182	0.08994
388	H	75	S	Ryd(2S)	0.00156	0.85032
389	H	76	S	Val(1S)	0.82243	0.09643
390	H	76	S	Ryd(2S)	0.00180	0.91401
391	H	77	S	Val(1S)	0.81487	0.04036
392	H	77	S	Ryd(2S)	0.00262	0.92009
393	N	78	S	Cor(1S)	1.99934	-14.33068
394	N	78	S	Val(2S)	1.35143	-0.70496
395	N	78	S	Ryd(3S)	0.00213	1.60489
396	N	78	px	Val(2p)	1.27342	-0.38750
397	N	78	px	Ryd(3p)	0.00533	0.81598
398	N	78	py	Val(2p)	1.36611	-0.39498
399	N	78	py	Ryd(3p)	0.00586	0.62585
400	N	78	pz	Val(2p)	1.57635	-0.42712
401	N	78	pz	Ryd(3p)	0.01112	0.58931
402	N	79	S	Cor(1S)	1.99936	-14.32591
403	N	79	S	Val(2S)	1.36040	-0.70670
404	N	79	S	Ryd(3S)	0.00225	1.61380
405	N	79	px	Val(2p)	1.67828	-0.43229
406	N	79	px	Ryd(3p)	0.01074	0.58684
407	N	79	py	Val(2p)	1.28212	-0.38468
408	N	79	py	Ryd(3p)	0.00716	0.76562
409	N	79	pz	Val(2p)	1.27148	-0.38490
410	N	79	pz	Ryd(3p)	0.00403	0.70625
411	N	80	S	Cor(1S)	1.99932	-14.32952
412	N	80	S	Val(2S)	1.34865	-0.70525
413	N	80	S	Ryd(3S)	0.00234	1.60373
414	N	80	px	Val(2p)	1.28046	-0.39229

415	N	80	px	Ryd(3p)	0.00570	0.65387
416	N	80	py	Val(2p)	1.55221	-0.40797
417	N	80	py	Ryd(3p)	0.01127	0.78230
418	N	80	pz	Val(2p)	1.40781	-0.41882
419	N	80	pz	Ryd(3p)	0.00628	0.64215
420	Tl	81	S	Val(6S)	1.85744	-0.44078
421	Tl	81	S	Ryd(7S)	0.00024	10.05804
422	Tl	81	px	Val(6p)	0.16466	0.18917
423	Tl	81	px	Ryd(7p)	0.00725	0.55856
424	Tl	81	py	Val(6p)	0.06333	-0.04354
425	Tl	81	py	Ryd(7p)	0.00370	0.26373
426	Tl	81	pz	Val(6p)	0.08944	0.01155
427	Tl	81	pz	Ryd(7p)	0.00549	0.39030
428	Tl	81	dxy	Cor(5d)	1.99618	-0.88539
429	Tl	81	dxy	Ryd(6d)	0.00014	1.46576
430	Tl	81	dxz	Cor(5d)	1.99654	-0.88393
431	Tl	81	dxz	Ryd(6d)	0.00012	1.45910
432	Tl	81	dyz	Cor(5d)	1.99787	-0.88448
433	Tl	81	dyz	Ryd(6d)	0.00013	1.40965
434	Tl	81	dx2y2	Cor(5d)	1.99769	-0.88718
435	Tl	81	dx2y2	Ryd(6d)	0.00008	1.35619
436	Tl	81	dz2	Cor(5d)	1.99698	-0.88292
437	Tl	81	dz2	Ryd(6d)	0.00018	1.47586
438	Tl	82	S	Val(6S)	1.85753	-0.44080
439	Tl	82	S	Ryd(7S)	0.00024	10.05808
440	Tl	82	px	Val(6p)	0.16467	0.18921
441	Tl	82	px	Ryd(7p)	0.00725	0.55867
442	Tl	82	py	Val(6p)	0.06334	-0.04355
443	Tl	82	py	Ryd(7p)	0.00370	0.26373
444	Tl	82	pz	Val(6p)	0.08945	0.01158
445	Tl	82	pz	Ryd(7p)	0.00549	0.39023
446	Tl	82	dxy	Cor(5d)	1.99618	-0.88540
447	Tl	82	dxy	Ryd(6d)	0.00014	1.46578
448	Tl	82	dxz	Cor(5d)	1.99655	-0.88394
449	Tl	82	dxz	Ryd(6d)	0.00012	1.45904
450	Tl	82	dyz	Cor(5d)	1.99787	-0.88449
451	Tl	82	dyz	Ryd(6d)	0.00013	1.40962
452	Tl	82	dx2y2	Cor(5d)	1.99769	-0.88719
453	Tl	82	dx2y2	Ryd(6d)	0.00008	1.35624
454	Tl	82	dz2	Cor(5d)	1.99698	-0.88293
455	Tl	82	dz2	Ryd(6d)	0.00018	1.47588
456	C	83	S	Cor(1S)	1.99873	-10.25755
457	C	83	S	Val(2S)	0.84209	-0.27528
458	C	83	S	Ryd(3S)	0.00198	1.07011
459	C	83	px	Val(2p)	0.89430	-0.20227
460	C	83	px	Ryd(3p)	0.01412	0.57306
461	C	83	py	Val(2p)	1.07306	-0.21661
462	C	83	py	Ryd(3p)	0.00510	0.43338
463	C	83	pz	Val(2p)	1.03118	-0.27441
464	C	83	pz	Ryd(3p)	0.00801	0.35060
465	C	84	S	Cor(1S)	1.99891	-10.22236
466	C	84	S	Val(2S)	0.89121	-0.28185
467	C	84	S	Ryd(3S)	0.00175	1.12663
468	C	84	px	Val(2p)	1.06189	-0.20169
469	C	84	px	Ryd(3p)	0.00743	0.48020
470	C	84	py	Val(2p)	1.06123	-0.21041
471	C	84	py	Ryd(3p)	0.00958	0.58681
472	C	84	pz	Val(2p)	0.98444	-0.25343

473	C	84	pz	Ryd(3p)	0.00685	0.39913
474	C	85	S	Cor(1S)	1.99906	-10.19629
475	C	85	S	Val(2S)	0.93745	-0.27265
476	C	85	S	Ryd(3S)	0.00130	1.02666
477	C	85	px	Val(2p)	1.10928	-0.16740
478	C	85	px	Ryd(3p)	0.00641	0.38469
479	C	85	py	Val(2p)	1.11083	-0.16788
480	C	85	py	Ryd(3p)	0.00448	0.46245
481	C	85	pz	Val(2p)	1.00023	-0.25691
482	C	85	pz	Ryd(3p)	0.00351	0.27209
483	C	86	S	Cor(1S)	1.99917	-10.19598
484	C	86	S	Val(2S)	0.93831	-0.25985
485	C	86	S	Ryd(3S)	0.00150	0.95057
486	C	86	px	Val(2p)	1.15915	-0.10798
487	C	86	px	Ryd(3p)	0.00685	0.43546
488	C	86	py	Val(2p)	1.04953	-0.18525
489	C	86	py	Ryd(3p)	0.00382	0.34432
490	C	86	pz	Val(2p)	1.00320	-0.25673
491	C	86	pz	Ryd(3p)	0.00372	0.28239
492	C	87	S	Cor(1S)	1.99858	-10.15230
493	C	87	S	Val(2S)	0.87394	-0.11863
494	C	87	S	Ryd(3S)	0.00108	0.96434
495	C	87	px	Val(2p)	1.06279	-0.17854
496	C	87	px	Ryd(3p)	0.00403	0.42785
497	C	87	py	Val(2p)	1.12700	-0.01156
498	C	87	py	Ryd(3p)	0.00713	0.33730
499	C	87	pz	Val(2p)	0.99868	-0.25357
500	C	87	pz	Ryd(3p)	0.00405	0.33473
501	C	88	S	Cor(1S)	1.99904	-10.19689
502	C	88	S	Val(2S)	0.92823	-0.26051
503	C	88	S	Ryd(3S)	0.00138	1.08470
504	C	88	px	Val(2p)	1.10023	-0.17269
505	C	88	px	Ryd(3p)	0.00520	0.48597
506	C	88	py	Val(2p)	1.10399	-0.17477
507	C	88	py	Ryd(3p)	0.00724	0.37208
508	C	88	pz	Val(2p)	1.04827	-0.25585
509	C	88	pz	Ryd(3p)	0.00395	0.36803
510	C	89	S	Cor(1S)	1.99882	-10.23425
511	C	89	S	Val(2S)	0.96073	-0.35906
512	C	89	S	Ryd(3S)	0.00112	1.35468
513	C	89	px	Val(2p)	1.12006	-0.26089
514	C	89	px	Ryd(3p)	0.01055	0.39269
515	C	89	py	Val(2p)	1.07303	-0.28127
516	C	89	py	Ryd(3p)	0.00594	0.34303
517	C	89	pz	Val(2p)	1.15122	-0.24995
518	C	89	pz	Ryd(3p)	0.01368	0.41420
519	H	90	S	Val(1S)	0.77074	0.01322
520	H	90	S	Ryd(2S)	0.00188	0.89791
521	C	91	S	Cor(1S)	1.99900	-10.30734
522	C	91	S	Val(2S)	0.85553	-0.32327
523	C	91	S	Ryd(3S)	0.00475	0.94721
524	C	91	px	Val(2p)	0.91513	-0.20595
525	C	91	px	Ryd(3p)	0.00700	0.45230
526	C	91	py	Val(2p)	0.84216	-0.27678
527	C	91	py	Ryd(3p)	0.00799	0.35842

528	C	91	pz	Val(2p)	0.92107	-0.23311
529	C	91	pz	Ryd(3p)	0.00677	0.41277
530	C	92	S	Cor(1S)	1.99907	-10.16149
531	C	92	S	Val(2S)	1.02359	-0.29153
532	C	92	S	Ryd(3S)	0.00053	1.05528
533	C	92	px	Val(2p)	1.26716	-0.20660
534	C	92	px	Ryd(3p)	0.00260	0.15974
535	C	92	py	Val(2p)	1.20851	-0.21477
536	C	92	py	Ryd(3p)	0.00201	0.18325
537	C	92	pz	Val(2p)	1.13485	-0.23226
538	C	92	pz	Ryd(3p)	0.00351	0.16820
539	H	93	S	Val(1S)	0.77348	0.03100
540	H	93	S	Ryd(2S)	0.00144	0.81483
541	H	94	S	Val(1S)	0.76875	0.02302
542	H	94	S	Ryd(2S)	0.00102	0.74572
543	H	95	S	Val(1S)	0.77045	0.01954
544	H	95	S	Ryd(2S)	0.00101	0.75255
545	C	96	S	Cor(1S)	1.99896	-10.17764
546	C	96	S	Val(2S)	0.91799	-0.24298
547	C	96	S	Ryd(3S)	0.00053	1.36676
548	C	96	px	Val(2p)	1.14093	-0.13967
549	C	96	px	Ryd(3p)	0.00867	0.33981
550	C	96	py	Val(2p)	1.01715	-0.19792
551	C	96	py	Ryd(3p)	0.00434	0.33816
552	C	96	pz	Val(2p)	1.04571	-0.18587
553	C	96	pz	Ryd(3p)	0.00315	0.39386
554	C	97	S	Cor(1S)	1.99918	-10.11970
555	C	97	S	Val(2S)	1.01145	-0.23272
556	C	97	S	Ryd(3S)	0.00051	1.02951
557	C	97	px	Val(2p)	1.24287	-0.15560
558	C	97	px	Ryd(3p)	0.00248	0.16005
559	C	97	py	Val(2p)	1.23538	-0.15373
560	C	97	py	Ryd(3p)	0.00279	0.20108
561	C	97	pz	Val(2p)	1.07776	-0.18477
562	C	97	pz	Ryd(3p)	0.00290	0.18913
563	H	98	S	Val(1S)	0.79820	0.05812
564	H	98	S	Ryd(2S)	0.00151	0.75051
565	H	99	S	Val(1S)	0.79391	0.06430
566	H	99	S	Ryd(2S)	0.00122	0.74169
567	H	100	S	Val(1S)	0.80368	0.05417
568	H	100	S	Ryd(2S)	0.00128	0.78147
569	C	101	S	Cor(1S)	1.99921	-10.11945
570	C	101	S	Val(2S)	1.00366	-0.22634
571	C	101	S	Ryd(3S)	0.00045	1.06644
572	C	101	px	Val(2p)	1.19644	-0.16836
573	C	101	px	Ryd(3p)	0.00229	0.29822
574	C	101	py	Val(2p)	1.16473	-0.17379
575	C	101	py	Ryd(3p)	0.00317	0.29128
576	C	101	pz	Val(2p)	1.19905	-0.16187
577	C	101	pz	Ryd(3p)	0.00324	0.26425
578	H	102	S	Val(1S)	0.81153	0.04487

579	H	102	S	Ryd(2S)	0.00145	0.91487
580	H	103	S	Val(1S)	0.79304	0.06411
581	H	103	S	Ryd(2S)	0.00128	0.79275
582	H	104	S	Val(1S)	0.80335	0.04938
583	H	104	S	Ryd(2S)	0.00180	0.86514
584	C	105	S	Cor(1S)	1.99899	-10.30463
585	C	105	S	Val(2S)	0.85632	-0.32304
586	C	105	S	Ryd(3S)	0.00495	0.98205
587	C	105	px	Val(2p)	0.94982	-0.20687
588	C	105	px	Ryd(3p)	0.00705	0.44203
589	C	105	py	Val(2p)	0.87013	-0.25259
590	C	105	py	Ryd(3p)	0.00899	0.38653
591	C	105	pz	Val(2p)	0.85917	-0.25120
592	C	105	pz	Ryd(3p)	0.00640	0.38851
593	C	106	S	Cor(1S)	1.99907	-10.15638
594	C	106	S	Val(2S)	1.02100	-0.28574
595	C	106	S	Ryd(3S)	0.00055	1.08197
596	C	106	px	Val(2p)	1.10160	-0.23796
597	C	106	px	Ryd(3p)	0.00412	0.15602
598	C	106	py	Val(2p)	1.25336	-0.20419
599	C	106	py	Ryd(3p)	0.00213	0.16076
600	C	106	pz	Val(2p)	1.25978	-0.20334
601	C	106	pz	Ryd(3p)	0.00218	0.20360
602	H	107	S	Val(1S)	0.76945	0.03791
603	H	107	S	Ryd(2S)	0.00130	0.82303
604	H	108	S	Val(1S)	0.76795	0.02955
605	H	108	S	Ryd(2S)	0.00108	0.75417
606	H	109	S	Val(1S)	0.77231	0.01690
607	H	109	S	Ryd(2S)	0.00117	0.81740
608	C	110	S	Cor(1S)	1.99877	-10.24339
609	C	110	S	Val(2S)	0.84438	-0.26301
610	C	110	S	Ryd(3S)	0.00207	1.04583
611	C	110	px	Val(2p)	1.04373	-0.25195
612	C	110	px	Ryd(3p)	0.00667	0.40467
613	C	110	py	Val(2p)	1.00600	-0.19703
614	C	110	py	Ryd(3p)	0.00718	0.51731
615	C	110	pz	Val(2p)	0.95597	-0.20327
616	C	110	pz	Ryd(3p)	0.01041	0.52894
617	C	111	S	Cor(1S)	1.99899	-10.21059
618	C	111	S	Val(2S)	0.89193	-0.26732
619	C	111	S	Ryd(3S)	0.00140	1.11363
620	C	111	px	Val(2p)	0.99416	-0.22964
621	C	111	px	Ryd(3p)	0.00763	0.42590
622	C	111	py	Val(2p)	1.04396	-0.18434
623	C	111	py	Ryd(3p)	0.00654	0.48151
624	C	111	pz	Val(2p)	1.03891	-0.19867
625	C	111	pz	Ryd(3p)	0.00844	0.52943
626	C	112	S	Cor(1S)	1.99889	-10.15219
627	C	112	S	Val(2S)	0.89454	-0.16865
628	C	112	S	Ryd(3S)	0.00093	0.97792
629	C	112	px	Val(2p)	1.02185	-0.20484
630	C	112	px	Ryd(3p)	0.00252	0.32441

631	C	112	py	Val(2p)	1.14828	-0.08255
632	C	112	py	Ryd(3p)	0.00768	0.26735
633	C	112	pz	Val(2p)	1.06626	-0.18197
634	C	112	pz	Ryd(3p)	0.00297	0.45096
635	C	113	S	Cor(1S)	1.99921	-10.17717
636	C	113	S	Val(2S)	0.93334	-0.23020
637	C	113	S	Ryd(3S)	0.00089	0.89777
638	C	113	px	Val(2p)	1.00629	-0.21900
639	C	113	px	Ryd(3p)	0.00298	0.27508
640	C	113	py	Val(2p)	1.08351	-0.15642
641	C	113	py	Ryd(3p)	0.00455	0.30984
642	C	113	pz	Val(2p)	1.12364	-0.11033
643	C	113	pz	Ryd(3p)	0.00541	0.34437
644	C	114	S	Cor(1S)	1.99905	-10.16404
645	C	114	S	Val(2S)	0.91232	-0.18538
646	C	114	S	Ryd(3S)	0.00075	0.89412
647	C	114	px	Val(2p)	1.02131	-0.20661
648	C	114	px	Ryd(3p)	0.00402	0.26096
649	C	114	py	Val(2p)	1.06133	-0.15004
650	C	114	py	Ryd(3p)	0.00343	0.35297
651	C	114	pz	Val(2p)	1.09808	-0.10102
652	C	114	pz	Ryd(3p)	0.00569	0.29200
653	C	115	S	Cor(1S)	1.99907	-10.17879
654	C	115	S	Val(2S)	0.92144	-0.23670
655	C	115	S	Ryd(3S)	0.00121	1.01643
656	C	115	px	Val(2p)	1.04288	-0.24337
657	C	115	px	Ryd(3p)	0.00442	0.31804
658	C	115	py	Val(2p)	1.15839	-0.11229
659	C	115	py	Ryd(3p)	0.00683	0.51600
660	C	115	pz	Val(2p)	1.07145	-0.20603
661	C	115	pz	Ryd(3p)	0.00466	0.44134
662	C	116	S	Cor(1S)	1.99912	-10.18966
663	C	116	S	Val(2S)	0.94573	-0.28347
664	C	116	S	Ryd(3S)	0.00052	1.35511
665	C	116	px	Val(2p)	1.00824	-0.19880
666	C	116	px	Ryd(3p)	0.00272	0.31799
667	C	116	py	Val(2p)	1.08852	-0.18187
668	C	116	py	Ryd(3p)	0.00735	0.45113
669	C	116	pz	Val(2p)	1.10033	-0.16167
670	C	116	pz	Ryd(3p)	0.00586	0.27538
671	C	117	S	Cor(1S)	1.99917	-10.11236
672	C	117	S	Val(2S)	1.01304	-0.22704
673	C	117	S	Ryd(3S)	0.00041	1.02006
674	C	117	px	Val(2p)	1.22940	-0.14776
675	C	117	px	Ryd(3p)	0.00294	0.20060
676	C	117	py	Val(2p)	1.10376	-0.17056
677	C	117	py	Ryd(3p)	0.00269	0.18615
678	C	117	pz	Val(2p)	1.22100	-0.15117
679	C	117	pz	Ryd(3p)	0.00248	0.18057
680	H	118	S	Val(1S)	0.80577	0.05823
681	H	118	S	Ryd(2S)	0.00141	0.77774
682	H	119	S	Val(1S)	0.79525	0.07111
683	H	119	S	Ryd(2S)	0.00125	0.75162
684	H	120	S	Val(1S)	0.79428	0.07460

685	H	120	S	Ryd(2S)	0.00119	0.74297
686	C	121	S	Cor(1S)	1.99918	-10.12824
687	C	121	S	Val(2S)	1.01080	-0.23846
688	C	121	S	Ryd(3S)	0.00051	1.02935
689	C	121	px	Val(2p)	1.09598	-0.19697
690	C	121	px	Ryd(3p)	0.00379	0.37977
691	C	121	py	Val(2p)	1.22860	-0.15976
692	C	121	py	Ryd(3p)	0.00292	0.22826
693	C	121	pz	Val(2p)	1.23559	-0.16167
694	C	121	pz	Ryd(3p)	0.00227	0.32096
695	H	122	S	Val(1S)	0.81582	0.03857
696	H	122	S	Ryd(2S)	0.00150	0.89134
697	H	123	S	Val(1S)	0.79484	0.05664
698	H	123	S	Ryd(2S)	0.00138	0.77940
699	H	124	S	Val(1S)	0.79961	0.05439
700	H	124	S	Ryd(2S)	0.00150	0.79944
701	C	125	S	Cor(1S)	1.99898	-10.30600
702	C	125	S	Val(2S)	0.85423	-0.32197
703	C	125	S	Ryd(3S)	0.00487	0.95177
704	C	125	px	Val(2p)	0.80822	-0.29298
705	C	125	px	Ryd(3p)	0.00761	0.34579
706	C	125	py	Val(2p)	0.98589	-0.24258
707	C	125	py	Ryd(3p)	0.00631	0.49833
708	C	125	pz	Val(2p)	0.88403	-0.18051
709	C	125	pz	Ryd(3p)	0.00801	0.42286
710	C	126	S	Cor(1S)	1.99907	-10.16063
711	C	126	S	Val(2S)	1.02271	-0.29038
712	C	126	S	Ryd(3S)	0.00054	1.06181
713	C	126	px	Val(2p)	1.24258	-0.20539
714	C	126	px	Ryd(3p)	0.00149	0.21609
715	C	126	py	Val(2p)	1.16521	-0.22721
716	C	126	py	Ryd(3p)	0.00379	0.18121
717	C	126	pz	Val(2p)	1.20513	-0.21973
718	C	126	pz	Ryd(3p)	0.00276	0.13996
719	H	127	S	Val(1S)	0.77008	0.03430
720	H	127	S	Ryd(2S)	0.00126	0.80846
721	H	128	S	Val(1S)	0.77013	0.02665
722	H	128	S	Ryd(2S)	0.00100	0.75225
723	H	129	S	Val(1S)	0.77136	0.01835
724	H	129	S	Ryd(2S)	0.00103	0.78278
725	C	130	S	Cor(1S)	1.99878	-10.25121
726	C	130	S	Val(2S)	0.84180	-0.26772
727	C	130	S	Ryd(3S)	0.00210	1.06407
728	C	130	px	Val(2p)	1.07886	-0.22307
729	C	130	px	Ryd(3p)	0.00510	0.43223
730	C	130	py	Val(2p)	0.90484	-0.20131
731	C	130	py	Ryd(3p)	0.00771	0.48787
732	C	130	pz	Val(2p)	1.01728	-0.23848
733	C	130	pz	Ryd(3p)	0.01076	0.55566
734	C	131	S	Cor(1S)	1.99897	-10.21150
735	C	131	S	Val(2S)	0.89044	-0.26738

736	C	131	S	Ryd(3S)	0.00140	1.11321
737	C	131	px	Val(2p)	1.04110	-0.20766
738	C	131	px	Ryd(3p)	0.00825	0.57457
739	C	131	py	Val(2p)	1.04246	-0.20746
740	C	131	py	Ryd(3p)	0.00685	0.45028
741	C	131	pz	Val(2p)	1.02408	-0.21422
742	C	131	pz	Ryd(3p)	0.00695	0.42913
743	C	132	S	Cor(1S)	1.99907	-10.17691
744	C	132	S	Val(2S)	0.93223	-0.24315
745	C	132	S	Ryd(3S)	0.00099	0.97913
746	C	132	px	Val(2p)	1.08867	-0.17186
747	C	132	px	Ryd(3p)	0.00422	0.36838
748	C	132	py	Val(2p)	1.04237	-0.19122
749	C	132	py	Ryd(3p)	0.00362	0.34063
750	C	132	pz	Val(2p)	1.08590	-0.17181
751	C	132	pz	Ryd(3p)	0.00545	0.28863
752	C	133	S	Cor(1S)	1.99914	-10.16997
753	C	133	S	Val(2S)	0.92620	-0.21725
754	C	133	S	Ryd(3S)	0.00073	0.88050
755	C	133	px	Val(2p)	1.03671	-0.18468
756	C	133	px	Ryd(3p)	0.00293	0.31453
757	C	133	py	Val(2p)	1.09696	-0.14749
758	C	133	py	Ryd(3p)	0.00566	0.26665
759	C	133	pz	Val(2p)	1.07136	-0.15504
760	C	133	pz	Ryd(3p)	0.00413	0.28889
761	C	134	S	Cor(1S)	1.99921	-10.18795
762	C	134	S	Val(2S)	0.93838	-0.24833
763	C	134	S	Ryd(3S)	0.00084	0.89387
764	C	134	px	Val(2p)	1.11384	-0.15473
765	C	134	px	Ryd(3p)	0.00645	0.41692
766	C	134	py	Val(2p)	1.06983	-0.16746
767	C	134	py	Ryd(3p)	0.00438	0.29833
768	C	134	pz	Val(2p)	1.02864	-0.20626
769	C	134	pz	Ryd(3p)	0.00327	0.29920
770	C	135	S	Cor(1S)	1.99906	-10.18581
771	C	135	S	Val(2S)	0.92119	-0.24349
772	C	135	S	Ryd(3S)	0.00128	1.02238
773	C	135	px	Val(2p)	1.11277	-0.17217
774	C	135	px	Ryd(3p)	0.00641	0.40997
775	C	135	py	Val(2p)	1.06102	-0.21869
776	C	135	py	Ryd(3p)	0.00416	0.40046
777	C	135	pz	Val(2p)	1.10248	-0.18765
778	C	135	pz	Ryd(3p)	0.00492	0.39500
779	C	136	S	Cor(1S)	1.99916	-10.19251
780	C	136	S	Val(2S)	0.95064	-0.29294
781	C	136	S	Ryd(3S)	0.00052	1.37896
782	C	136	px	Val(2p)	1.02514	-0.19677
783	C	136	px	Ryd(3p)	0.00392	0.36319
784	C	136	py	Val(2p)	1.13817	-0.15946
785	C	136	py	Ryd(3p)	0.00680	0.30047
786	C	136	pz	Val(2p)	1.02760	-0.19661
787	C	136	pz	Ryd(3p)	0.00446	0.43314
788	C	137	S	Cor(1S)	1.99916	-10.11655
789	C	137	S	Val(2S)	1.01182	-0.23047
790	C	137	S	Ryd(3S)	0.00050	1.04542
791	C	137	px	Val(2p)	1.16129	-0.16750

792	C	137	px	Ryd(3p)	0.00285	0.19627
793	C	137	py	Val(2p)	1.23890	-0.15400
794	C	137	py	Ryd(3p)	0.00209	0.21438
795	C	137	pz	Val(2p)	1.15308	-0.16382
796	C	137	pz	Ryd(3p)	0.00324	0.21231
797	H	138	S	Val(1S)	0.79305	0.07274
798	H	138	S	Ryd(2S)	0.00159	0.76222
799	H	139	S	Val(1S)	0.79371	0.06656
800	H	139	S	Ryd(2S)	0.00128	0.74396
801	H	140	S	Val(1S)	0.81638	0.04616
802	H	140	S	Ryd(2S)	0.00156	0.88288
803	C	141	S	Cor(1S)	1.99917	-10.11444
804	C	141	S	Val(2S)	1.01243	-0.22948
805	C	141	S	Ryd(3S)	0.00045	1.03849
806	C	141	px	Val(2p)	1.21578	-0.15184
807	C	141	px	Ryd(3p)	0.00291	0.21338
808	C	141	py	Val(2p)	1.24877	-0.14763
809	C	141	py	Ryd(3p)	0.00211	0.19902
810	C	141	pz	Val(2p)	1.10220	-0.17625
811	C	141	pz	Ryd(3p)	0.00313	0.19339
812	H	142	S	Val(1S)	0.80432	0.05714
813	H	142	S	Ryd(2S)	0.00122	0.79815
814	H	143	S	Val(1S)	0.79032	0.07518
815	H	143	S	Ryd(2S)	0.00115	0.77455
816	H	144	S	Val(1S)	0.79739	0.06731
817	H	144	S	Ryd(2S)	0.00161	0.74356
818	H	145	S	Val(1S)	0.80497	0.07443
819	H	145	S	Ryd(2S)	0.00166	0.90367
820	H	146	S	Val(1S)	0.81431	0.09901
821	H	146	S	Ryd(2S)	0.00185	0.85229
822	H	147	S	Val(1S)	0.89645	0.25767
823	H	147	S	Ryd(2S)	0.00241	0.76967
824	H	148	S	Val(1S)	0.81647	0.08338
825	H	148	S	Ryd(2S)	0.00212	0.94056
826	H	149	S	Val(1S)	0.83113	0.12044
827	H	149	S	Ryd(2S)	0.00310	0.84512
828	H	150	S	Val(1S)	0.84726	0.18329
829	H	150	S	Ryd(2S)	0.00229	0.84735
830	H	151	S	Val(1S)	0.80598	0.10966
831	H	151	S	Ryd(2S)	0.00185	0.82840
832	H	152	S	Val(1S)	0.85901	0.18964
833	H	152	S	Ryd(2S)	0.00165	0.78182
834	H	153	S	Val(1S)	0.83035	0.10282
835	H	153	S	Ryd(2S)	0.00200	0.97489
836	H	154	S	Val(1S)	0.81242	0.07570

837	H	154	S	Ryd(2S)	0.00270	0.84073
838	H	155	S	Val(1S)	0.80994	0.09609
839	H	155	S	Ryd(2S)	0.00167	0.85914
840	H	156	S	Val(1S)	0.82547	0.14733
841	H	156	S	Ryd(2S)	0.00187	0.80094
842	H	157	S	Val(1S)	0.81185	0.08992
843	H	157	S	Ryd(2S)	0.00156	0.85030
844	H	158	S	Val(1S)	0.82244	0.09645
845	H	158	S	Ryd(2S)	0.00180	0.91401
846	H	159	S	Val(1S)	0.81495	0.04083
847	H	159	S	Ryd(2S)	0.00262	0.91973
848	N	160	S	Cor(1S)	1.99934	-14.33049
849	N	160	S	Val(2S)	1.35098	-0.70465
850	N	160	S	Ryd(3S)	0.00213	1.60481
851	N	160	px	Val(2p)	1.27354	-0.38753
852	N	160	px	Ryd(3p)	0.00533	0.81598
853	N	160	py	Val(2p)	1.36594	-0.39494
854	N	160	py	Ryd(3p)	0.00587	0.62589
855	N	160	pz	Val(2p)	1.57653	-0.42713
856	N	160	pz	Ryd(3p)	0.01114	0.58926
857	N	161	S	Cor(1S)	1.99936	-14.32586
858	N	161	S	Val(2S)	1.36013	-0.70648
859	N	161	S	Ryd(3S)	0.00225	1.61381
860	N	161	px	Val(2p)	1.67830	-0.43219
861	N	161	px	Ryd(3p)	0.01074	0.58690
862	N	161	py	Val(2p)	1.28220	-0.38461
863	N	161	py	Ryd(3p)	0.00716	0.76581
864	N	161	pz	Val(2p)	1.27139	-0.38481
865	N	161	pz	Ryd(3p)	0.00403	0.70645
866	N	162	S	Cor(1S)	1.99932	-14.32949
867	N	162	S	Val(2S)	1.34866	-0.70518
868	N	162	S	Ryd(3S)	0.00234	1.60391
869	N	162	px	Val(2p)	1.28046	-0.39227
870	N	162	px	Ryd(3p)	0.00570	0.65396
871	N	162	py	Val(2p)	1.55219	-0.40791
872	N	162	py	Ryd(3p)	0.01127	0.78240
873	N	162	pz	Val(2p)	1.40773	-0.41874
874	N	162	pz	Ryd(3p)	0.00628	0.64220

[136 electrons found in the effective core potential]

WARNING: 1 low occupancy (<1.9990e) core orbital found on C 1
1 low occupancy (<1.9990e) core orbital found on C 3
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 12
1 low occupancy (<1.9990e) core orbital found on C 14
1 low occupancy (<1.9990e) core orbital found on C 23
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 43
1 low occupancy (<1.9990e) core orbital found on C 48
1 low occupancy (<1.9990e) core orbital found on C 49

5 low occupancy (<1.9990e) core orbitals found on Tl 81
5 low occupancy (<1.9990e) core orbitals found on Tl 82
1 low occupancy (<1.9990e) core orbital found on C 83
1 low occupancy (<1.9990e) core orbital found on C 84
1 low occupancy (<1.9990e) core orbital found on C 87
1 low occupancy (<1.9990e) core orbital found on C 89
1 low occupancy (<1.9990e) core orbital found on C 91
1 low occupancy (<1.9990e) core orbital found on C 96
1 low occupancy (<1.9990e) core orbital found on C 105
1 low occupancy (<1.9990e) core orbital found on C 110
1 low occupancy (<1.9990e) core orbital found on C 111
1 low occupancy (<1.9990e) core orbital found on C 112
1 low occupancy (<1.9990e) core orbital found on C 125
1 low occupancy (<1.9990e) core orbital found on C 130
1 low occupancy (<1.9990e) core orbital found on C 131

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.33502	1.99882	4.30493	0.03127	6.33502
H	2	0.22720	0.00000	0.77092	0.00188	0.77280
C	3	0.44075	1.99900	3.53377	0.02648	5.55925
C	4	-0.64156	1.99907	4.63384	0.00864	6.64156
H	5	0.22507	0.00000	0.77349	0.00144	0.77493
H	6	0.23022	0.00000	0.76876	0.00102	0.76978
H	7	0.22837	0.00000	0.77062	0.00101	0.77163
C	8	0.13143	1.99873	3.84064	0.02921	5.86857
C	9	-0.02319	1.99891	3.99865	0.02563	6.02319
C	10	-0.17252	1.99906	4.15776	0.01570	6.17252
C	11	-0.16526	1.99917	4.15019	0.01589	6.16526
C	12	-0.07731	1.99858	4.06243	0.01630	6.07731
C	13	-0.19756	1.99904	4.18074	0.01777	6.19756
C	14	-0.13768	1.99896	4.12202	0.01670	6.13768
C	15	-0.57537	1.99918	4.56751	0.00869	6.57537
H	16	0.20028	0.00000	0.79821	0.00152	0.79972
H	17	0.20487	0.00000	0.79391	0.00122	0.79513
H	18	0.19515	0.00000	0.80358	0.00128	0.80485
C	19	-0.57249	1.99921	4.56412	0.00915	6.57249
H	20	0.18712	0.00000	0.81143	0.00145	0.81288
H	21	0.20564	0.00000	0.79308	0.00128	0.79436
H	22	0.19500	0.00000	0.80320	0.00180	0.80500
C	23	0.43811	1.99899	3.53549	0.02741	5.56189
C	24	-0.64322	1.99907	4.63517	0.00897	6.64322
H	25	0.22914	0.00000	0.76956	0.00130	0.77086
H	26	0.23090	0.00000	0.76802	0.00108	0.76910
H	27	0.22620	0.00000	0.77263	0.00117	0.77380
C	28	0.12497	1.99877	3.84993	0.02633	5.87503
C	29	0.00842	1.99899	3.96861	0.02398	5.99158
C	30	-0.14450	1.99889	4.13151	0.01410	6.14450
C	31	-0.15976	1.99921	4.14673	0.01382	6.15976
C	32	-0.10540	1.99904	4.09247	0.01388	6.10540
C	33	-0.21067	1.99907	4.19448	0.01712	6.21067
C	34	-0.15871	1.99911	4.14313	0.01646	6.15871
C	35	-0.57500	1.99917	4.56730	0.00853	6.57500
H	36	0.19287	0.00000	0.80572	0.00141	0.80713
H	37	0.20351	0.00000	0.79524	0.00125	0.79649
H	38	0.20463	0.00000	0.79419	0.00118	0.79537
C	39	-0.57955	1.99918	4.57088	0.00949	6.57955

H	40	0.18269	0.00000	0.81581	0.00150	0.81731
H	41	0.20379	0.00000	0.79483	0.00138	0.79621
H	42	0.19892	0.00000	0.79958	0.00150	0.80108
C	43	0.44205	1.99898	3.53214	0.02683	5.55795
C	44	-0.64322	1.99907	4.63557	0.00858	6.64322
H	45	0.22869	0.00000	0.77005	0.00126	0.77131
H	46	0.22885	0.00000	0.77014	0.00100	0.77115
H	47	0.22750	0.00000	0.77147	0.00104	0.77250
C	48	0.13306	1.99878	3.84247	0.02569	5.86694
C	49	-0.02058	1.99897	3.99817	0.02344	6.02058
C	50	-0.16267	1.99907	4.14932	0.01428	6.16267
C	51	-0.14355	1.99914	4.13096	0.01345	6.14355
C	52	-0.16506	1.99921	4.15091	0.01494	6.16506
C	53	-0.21333	1.99906	4.19751	0.01676	6.21333
C	54	-0.15643	1.99916	4.14157	0.01570	6.15643
C	55	-0.57278	1.99916	4.56494	0.00867	6.57278
H	56	0.20525	0.00000	0.79315	0.00160	0.79475
H	57	0.20491	0.00000	0.79381	0.00128	0.79509
H	58	0.18214	0.00000	0.81631	0.00155	0.81786
C	59	-0.58716	1.99918	4.57937	0.00861	6.58716
H	60	0.19449	0.00000	0.80430	0.00122	0.80551
H	61	0.20866	0.00000	0.79019	0.00115	0.79134
H	62	0.20102	0.00000	0.79736	0.00162	0.79898
H	63	0.19340	0.00000	0.80495	0.00166	0.80660
H	64	0.18385	0.00000	0.81429	0.00185	0.81615
H	65	0.10115	0.00000	0.89645	0.00241	0.89885
H	66	0.18141	0.00000	0.81647	0.00212	0.81859
H	67	0.16590	0.00000	0.83099	0.00311	0.83410
H	68	0.15083	0.00000	0.84688	0.00229	0.84917
H	69	0.19216	0.00000	0.80599	0.00185	0.80784
H	70	0.13892	0.00000	0.85944	0.00164	0.86108
H	71	0.16772	0.00000	0.83028	0.00200	0.83228
H	72	0.18498	0.00000	0.81233	0.00270	0.81502
H	73	0.18826	0.00000	0.81006	0.00168	0.81174
H	74	0.17266	0.00000	0.82548	0.00186	0.82734
H	75	0.18662	0.00000	0.81182	0.00156	0.81338
H	76	0.17577	0.00000	0.82243	0.00180	0.82423
H	77	0.18251	0.00000	0.81487	0.00262	0.81749
N	78	-0.59109	1.99934	5.56731	0.02444	7.59109
N	79	-0.61582	1.99936	5.59228	0.02418	7.61582
N	80	-0.61403	1.99932	5.58912	0.02559	7.61403
Tl	81	0.82255	77.98527	2.17486	0.01732	80.17745
Tl	82	0.82242	77.98527	2.17498	0.01733	80.17758
C	83	0.13144	1.99873	3.84063	0.02920	5.86856
C	84	-0.02330	1.99891	3.99878	0.02562	6.02330
C	85	-0.17253	1.99906	4.15778	0.01570	6.17253
C	86	-0.16527	1.99917	4.15020	0.01589	6.16527
C	87	-0.07728	1.99858	4.06241	0.01630	6.07728
C	88	-0.19753	1.99904	4.18072	0.01777	6.19753
C	89	-0.33515	1.99882	4.30504	0.03129	6.33515
H	90	0.22738	0.00000	0.77074	0.00188	0.77262
C	91	0.44060	1.99900	3.53389	0.02651	5.55940
C	92	-0.64183	1.99907	4.63411	0.00865	6.64183
H	93	0.22509	0.00000	0.77348	0.00144	0.77491
H	94	0.23023	0.00000	0.76875	0.00102	0.76977
H	95	0.22854	0.00000	0.77045	0.00101	0.77146
C	96	-0.13743	1.99896	4.12178	0.01669	6.13743
C	97	-0.57533	1.99918	4.56747	0.00869	6.57533
H	98	0.20028	0.00000	0.79820	0.00151	0.79972
H	99	0.20487	0.00000	0.79391	0.00122	0.79513
H	100	0.19504	0.00000	0.80368	0.00128	0.80496
C	101	-0.57224	1.99921	4.56388	0.00915	6.57224

H	102	0.18701	0.00000	0.81153	0.00145	0.81299
H	103	0.20569	0.00000	0.79304	0.00128	0.79431
H	104	0.19484	0.00000	0.80335	0.00180	0.80516
C	105	0.43817	1.99899	3.53544	0.02740	5.56183
C	106	-0.64379	1.99907	4.63573	0.00898	6.64379
H	107	0.22924	0.00000	0.76945	0.00130	0.77076
H	108	0.23097	0.00000	0.76795	0.00108	0.76903
H	109	0.22653	0.00000	0.77231	0.00117	0.77347
C	110	0.12484	1.99877	3.85007	0.02632	5.87516
C	111	0.00806	1.99899	3.96895	0.02400	5.99194
C	112	-0.14391	1.99889	4.13093	0.01410	6.14391
C	113	-0.15981	1.99921	4.14678	0.01382	6.15981
C	114	-0.10597	1.99905	4.09304	0.01389	6.10597
C	115	-0.21035	1.99907	4.19416	0.01711	6.21035
C	116	-0.15838	1.99912	4.14281	0.01646	6.15838
C	117	-0.57490	1.99917	4.56721	0.00852	6.57490
H	118	0.19282	0.00000	0.80577	0.00141	0.80718
H	119	0.20350	0.00000	0.79525	0.00125	0.79650
H	120	0.20454	0.00000	0.79428	0.00119	0.79546
C	121	-0.57965	1.99918	4.57098	0.00949	6.57965
H	122	0.18269	0.00000	0.81582	0.00150	0.81731
H	123	0.20378	0.00000	0.79484	0.00138	0.79622
H	124	0.19888	0.00000	0.79961	0.00150	0.80112
C	125	0.44183	1.99898	3.53237	0.02681	5.55817
C	126	-0.64328	1.99907	4.63563	0.00858	6.64328
H	127	0.22866	0.00000	0.77008	0.00126	0.77134
H	128	0.22887	0.00000	0.77013	0.00100	0.77113
H	129	0.22761	0.00000	0.77136	0.00103	0.77239
C	130	0.13277	1.99878	3.84278	0.02567	5.86723
C	131	-0.02051	1.99897	3.99808	0.02345	6.02051
C	132	-0.16253	1.99907	4.14918	0.01428	6.16253
C	133	-0.14383	1.99914	4.13124	0.01345	6.14383
C	134	-0.16484	1.99921	4.15068	0.01494	6.16484
C	135	-0.21329	1.99906	4.19747	0.01677	6.21329
C	136	-0.15642	1.99916	4.14155	0.01571	6.15642
C	137	-0.57292	1.99916	4.56509	0.00867	6.57292
H	138	0.20536	0.00000	0.79305	0.00159	0.79464
H	139	0.20501	0.00000	0.79371	0.00128	0.79499
H	140	0.18206	0.00000	0.81638	0.00156	0.81794
C	141	-0.58697	1.99917	4.57918	0.00861	6.58697
H	142	0.19446	0.00000	0.80432	0.00122	0.80554
H	143	0.20854	0.00000	0.79032	0.00115	0.79146
H	144	0.20100	0.00000	0.79739	0.00161	0.79900
H	145	0.19338	0.00000	0.80497	0.00166	0.80662
H	146	0.18384	0.00000	0.81431	0.00185	0.81616
H	147	0.10115	0.00000	0.89645	0.00241	0.89885
H	148	0.18141	0.00000	0.81647	0.00212	0.81859
H	149	0.16577	0.00000	0.83113	0.00310	0.83423
H	150	0.15045	0.00000	0.84726	0.00229	0.84955
H	151	0.19217	0.00000	0.80598	0.00185	0.80783
H	152	0.13935	0.00000	0.85901	0.00165	0.86065
H	153	0.16766	0.00000	0.83035	0.00200	0.83234
H	154	0.18488	0.00000	0.81242	0.00270	0.81512
H	155	0.18839	0.00000	0.80994	0.00167	0.81161
H	156	0.17266	0.00000	0.82547	0.00187	0.82734
H	157	0.18659	0.00000	0.81185	0.00156	0.81341
H	158	0.17576	0.00000	0.82244	0.00180	0.82424
H	159	0.18244	0.00000	0.81495	0.00262	0.81756
N	160	-0.59080	1.99934	5.56699	0.02447	7.59080
N	161	-0.61556	1.99936	5.59202	0.02418	7.61556
N	162	-0.61396	1.99932	5.58905	0.02559	7.61396

===

```
 * Total *    2.00000    303.90060   390.62231    1.47709   696.00000

                              Natural Population
 --------------------------------------------------------
   Effective Core          136.00000
   Core                    167.90060 ( 99.9408% of 168)
   Valence                 390.62231 ( 99.6485% of 392)
   Natural Minimal Basis   694.52291 ( 99.7878% of 696)
   Natural Rydberg Basis     1.47709 (  0.2122% of 696)
 --------------------------------------------------------

    Atom  No          Natural Electron Configuration
 ----------------------------------------------------------------------------
      C    1      [core]2S( 0.96)2p( 3.34)3p( 0.03)
      H    2            1S( 0.77)
      C    3      [core]2S( 0.86)2p( 2.68)3p( 0.02)
      C    4      [core]2S( 1.02)2p( 3.61)3p( 0.01)
      H    5            1S( 0.77)
      H    6            1S( 0.77)
      H    7            1S( 0.77)
      C    8      [core]2S( 0.84)2p( 3.00)3p( 0.03)
      C    9      [core]2S( 0.89)2p( 3.11)3p( 0.02)
      C   10      [core]2S( 0.94)2p( 3.22)3p( 0.01)
      C   11      [core]2S( 0.94)2p( 3.21)3p( 0.01)
      C   12      [core]2S( 0.87)2p( 3.19)3p( 0.02)
      C   13      [core]2S( 0.93)2p( 3.25)3p( 0.02)
      C   14      [core]2S( 0.92)2p( 3.20)3p( 0.02)
      C   15      [core]2S( 1.01)2p( 3.56)3p( 0.01)
      H   16            1S( 0.80)
      H   17            1S( 0.79)
      H   18            1S( 0.80)
      C   19      [core]2S( 1.00)2p( 3.56)3p( 0.01)
      H   20            1S( 0.81)
      H   21            1S( 0.79)
      H   22            1S( 0.80)
      C   23      [core]2S( 0.86)2p( 2.68)3p( 0.02)
      C   24      [core]2S( 1.02)2p( 3.61)3p( 0.01)
      H   25            1S( 0.77)
      H   26            1S( 0.77)
      H   27            1S( 0.77)
      C   28      [core]2S( 0.84)2p( 3.01)3p( 0.02)
      C   29      [core]2S( 0.89)2p( 3.08)3p( 0.02)
      C   30      [core]2S( 0.89)2p( 3.24)3p( 0.01)
      C   31      [core]2S( 0.93)2p( 3.21)3p( 0.01)
      C   32      [core]2S( 0.91)2p( 3.18)3p( 0.01)
      C   33      [core]2S( 0.92)2p( 3.27)3p( 0.02)
      C   34      [core]2S( 0.95)2p( 3.20)3p( 0.02)
      C   35      [core]2S( 1.01)2p( 3.55)3p( 0.01)
      H   36            1S( 0.81)
      H   37            1S( 0.80)
      H   38            1S( 0.79)
      C   39      [core]2S( 1.01)2p( 3.56)3p( 0.01)
      H   40            1S( 0.82)
      H   41            1S( 0.79)
      H   42            1S( 0.80)
      C   43      [core]2S( 0.85)2p( 2.68)3p( 0.02)
      C   44      [core]2S( 1.02)2p( 3.61)3p( 0.01)
      H   45            1S( 0.77)
      H   46            1S( 0.77)
      H   47            1S( 0.77)
      C   48      [core]2S( 0.84)2p( 3.00)3p( 0.02)
      C   49      [core]2S( 0.89)2p( 3.11)3p( 0.02)
```

C	50	[core]2S(0.93)2p(3.22)3p(0.01)
C	51	[core]2S(0.93)2p(3.20)3p(0.01)
C	52	[core]2S(0.94)2p(3.21)3p(0.01)
C	53	[core]2S(0.92)2p(3.28)3p(0.02)
C	54	[core]2S(0.95)2p(3.19)3p(0.02)
C	55	[core]2S(1.01)2p(3.55)3p(0.01)
H	56	1S(0.79)
H	57	1S(0.79)
H	58	1S(0.82)
C	59	[core]2S(1.01)2p(3.57)3p(0.01)
H	60	1S(0.80)
H	61	1S(0.79)
H	62	1S(0.80)
H	63	1S(0.80)
H	64	1S(0.81)
H	65	1S(0.90)
H	66	1S(0.82)
H	67	1S(0.83)
H	68	1S(0.85)
H	69	1S(0.81)
H	70	1S(0.86)
H	71	1S(0.83)
H	72	1S(0.81)
H	73	1S(0.81)
H	74	1S(0.83)
H	75	1S(0.81)
H	76	1S(0.82)
H	77	1S(0.81)
N	78	[core]2S(1.35)2p(4.22)3p(0.02)
N	79	[core]2S(1.36)2p(4.23)3p(0.02)
N	80	[core]2S(1.35)2p(4.24)3p(0.02)
Tl	81	[core]6S(1.86)6p(0.32)7p(0.02)
Tl	82	[core]6S(1.86)6p(0.32)7p(0.02)
C	83	[core]2S(0.84)2p(3.00)3p(0.03)
C	84	[core]2S(0.89)2p(3.11)3p(0.02)
C	85	[core]2S(0.94)2p(3.22)3p(0.01)
C	86	[core]2S(0.94)2p(3.21)3p(0.01)
C	87	[core]2S(0.87)2p(3.19)3p(0.02)
C	88	[core]2S(0.93)2p(3.25)3p(0.02)
C	89	[core]2S(0.96)2p(3.34)3p(0.03)
H	90	1S(0.77)
C	91	[core]2S(0.86)2p(2.68)3p(0.02)
C	92	[core]2S(1.02)2p(3.61)3p(0.01)
H	93	1S(0.77)
H	94	1S(0.77)
H	95	1S(0.77)
C	96	[core]2S(0.92)2p(3.20)3p(0.02)
C	97	[core]2S(1.01)2p(3.56)3p(0.01)
H	98	1S(0.80)
H	99	1S(0.79)
H	100	1S(0.80)
C	101	[core]2S(1.00)2p(3.56)3p(0.01)
H	102	1S(0.81)
H	103	1S(0.79)
H	104	1S(0.80)
C	105	[core]2S(0.86)2p(2.68)3p(0.02)
C	106	[core]2S(1.02)2p(3.61)3p(0.01)
H	107	1S(0.77)
H	108	1S(0.77)
H	109	1S(0.77)
C	110	[core]2S(0.84)2p(3.01)3p(0.02)
C	111	[core]2S(0.89)2p(3.08)3p(0.02)

C 112 [core]2S(0.89)2p(3.24)3p(0.01)
C 113 [core]2S(0.93)2p(3.21)3p(0.01)
C 114 [core]2S(0.91)2p(3.18)3p(0.01)
C 115 [core]2S(0.92)2p(3.27)3p(0.02)
C 116 [core]2S(0.95)2p(3.20)3p(0.02)
C 117 [core]2S(1.01)2p(3.55)3p(0.01)
H 118 1S(0.81)
H 119 1S(0.80)
H 120 1S(0.79)
C 121 [core]2S(1.01)2p(3.56)3p(0.01)
H 122 1S(0.82)
H 123 1S(0.79)
H 124 1S(0.80)
C 125 [core]2S(0.85)2p(2.68)3p(0.02)
C 126 [core]2S(1.02)2p(3.61)3p(0.01)
H 127 1S(0.77)
H 128 1S(0.77)
H 129 1S(0.77)
C 130 [core]2S(0.84)2p(3.00)3p(0.02)
C 131 [core]2S(0.89)2p(3.11)3p(0.02)
C 132 [core]2S(0.93)2p(3.22)3p(0.01)
C 133 [core]2S(0.93)2p(3.21)3p(0.01)
C 134 [core]2S(0.94)2p(3.21)3p(0.01)
C 135 [core]2S(0.92)2p(3.28)3p(0.02)
C 136 [core]2S(0.95)2p(3.19)3p(0.02)
C 137 [core]2S(1.01)2p(3.55)3p(0.01)
H 138 1S(0.79)
H 139 1S(0.79)
H 140 1S(0.82)
C 141 [core]2S(1.01)2p(3.57)3p(0.01)
H 142 1S(0.80)
H 143 1S(0.79)
H 144 1S(0.80)
H 145 1S(0.80)
H 146 1S(0.81)
H 147 1S(0.90)
H 148 1S(0.82)
H 149 1S(0.83)
H 150 1S(0.85)
H 151 1S(0.81)
H 152 1S(0.86)
H 153 1S(0.83)
H 154 1S(0.81)
H 155 1S(0.81)
H 156 1S(0.83)
H 157 1S(0.81)
H 158 1S(0.82)
H 159 1S(0.81)
N 160 [core]2S(1.35)2p(4.22)3p(0.02)
N 161 [core]2S(1.36)2p(4.23)3p(0.02)
N 162 [core]2S(1.35)2p(4.24)3p(0.02)

NBO analysis skipped by request.

1|1|UNPC-E-C07CYG43054|SP|RB3LYP|LANL2DZ|C68H86N6Tl2(2+)|MCDSTFM|03-Ap
r-2013|0||# b3lyp/lanl2dz guess=local pop=npa geom=connectivity||CSD E
NTRY ofm27p-1||2,1|C,0,-3.903023,0.051295,-2.737981|H,0,-4.514533,0.08
5596,-3.503394|C,0,-2.503247,-0.227432,-3.276213|C,0,-2.460164,-0.9729
3,-4.569492|H,0,-1.545611,-1.129417,-4.817515|H,0,-2.892297,-0.452722,
-5.252444|H,0,-2.914133,-1.812707,-4.470777|C,0,-0.170439,-0.150782,-2
.958032|C,0,0.684185,0.872376,-3.360395|C,0,2.019408,0.533222,-3.58217
4|C,0,2.485112,-0.764383,-3.385337|C,0,1.626865,-1.746963,-2.977845|C,

Electronic Supplementary Material (ESI) for Dalton Transactions

0,0.293215,-1.440024,-2.76505|C,0,0.184239,2.270912,-3.616048|C,0,0.07
5302,2.538076,-5.096013|H,0,0.950346,2.513578,-5.490651|H,0,-0.31535,3
.402468,-5.238301|H,0,-0.477148,1.865062,-5.502998|C,0,1.011329,3.3330
35,-2.953263|H,0,1.034524,3.177106,-2.005839|H,0,0.627484,4.194823,-3.
12687|H,0,1.907183,3.306084,-3.303069|C,0,-4.397058,-1.03942,-1.801017
|C,0,-5.870231,-1.237389,-1.780559|H,0,-6.091786,-1.92487,-1.148722|H,
0,-6.170325,-1.496216,-2.654573|H,0,-6.299217,-0.417141,-1.523277|C,0,
-3.930526,-2.580467,-0.074942|C,0,-3.537481,-3.9179,-0.181117|C,0,-3.8
687,-4.722562,0.913689|C,0,-4.486773,-4.273217,2.005895|C,0,-4.844529,
-2.938962,2.109501|C,0,-4.561165,-2.096006,1.051875|C,0,-2.743405,-4.4
17091,-1.351036|C,0,-3.218501,-5.772304,-1.879589|H,0,-3.237334,-6.408
158,-1.160273|H,0,-2.617282,-6.078198,-2.561382|H,0,-4.100692,-5.67953
3,-2.24793|C,0,-1.265249,-4.513108,-0.965484|H,0,-0.951616,-3.65163,-0
.678966|H,0,-0.754039,-4.801185,-1.727045|H,0,-1.160762,-5.146678,-0.2
52564|C,0,-3.945046,1.410207,-2.054612|C,0,-4.205935,2.575653,-2.95337
1|H,0,-4.280814,3.375466,-2.426758|H,0,-5.022881,2.43207,-3.435929|H,0
,-3.479994,2.669176,-3.574825|C,0,-3.652669,2.677734,-0.075475|C,0,-4.
641162,2.969572,0.868363|C,0,-4.446268,4.099082,1.65003|C,0,-3.329395,
4.893029,1.516565|C,0,-2.380753,4.600231,0.572637|C,0,-2.53584,3.48771
7,-0.227047|C,0,-5.870955,2.099481,0.968797|C,0,-6.904465,2.519616,-0.
066748|H,0,-7.202563,3.411803,0.123697|H,0,-7.652825,1.918078,-0.03450
7|H,0,-6.510077,2.493668,-0.940994|C,0,-6.505344,2.084019,2.364325|H,0
,-5.825671,1.911567,3.021302|H,0,-7.171417,1.392791,2.406236|H,0,-6.91
2835,2.933227,2.539671|H,0,2.65523,1.199916,-3.845393|H,0,3.404316,-0.
872897,-3.515165|H,0,1.834315,-2.474982,-2.848538|H,0,-0.287553,-2.068
439,-2.397481|H,0,-0.623664,2.406848,-3.216657|H,0,-3.527049,-5.49686,
0.780988|H,0,-4.706301,-4.730062,2.803385|H,0,-5.227296,-2.596463,2.78
4907|H,0,-4.79531,-1.214323,1.081259|H,0,-2.826831,-3.811705,-2.100233
|H,0,-5.041747,4.344775,2.343442|H,0,-3.322704,5.561882,2.121677|H,0,-
1.641429,5.183719,0.4565|H,0,-1.893421,3.336427,-0.866954|H,0,-5.61291
1,1.174631,0.717379|N,0,-1.519237,0.154047,-2.581712|N,0,-3.535959,-1.
658124,-1.095997|N,0,-3.736426,1.452274,-0.810506|Tl,0,-1.816362,-0.09
5993,0.135685|Tl,0,1.816323,0.09545,-0.136066|C,0,0.170681,0.151034,2.
958188|C,0,-0.683944,-0.872124,3.360551|C,0,-2.019167,-0.53297,3.58233
1|C,0,-2.484871,0.764635,3.385494|C,0,-1.626623,1.747215,2.978002|C,0,
-0.292974,1.440276,2.765207|C,0,3.902984,-0.051837,2.7376|H,0,4.514774
,-0.085344,3.503551|C,0,2.503207,0.226889,3.275832|C,0,2.460125,0.9723
87,4.569111|H,0,1.545852,1.129669,4.817671|H,0,2.892539,0.452974,5.252
601|H,0,2.914375,1.812959,4.470934|C,0,-0.183997,-2.27066,3.616204|C,0
,-0.075061,-2.537824,5.09617|H,0,-0.950105,-2.513326,5.490807|H,0,0.31
5592,-3.402216,5.238458|H,0,0.477109,-1.865605,5.502617|C,0,-1.012327,
-3.333367,2.953071|H,0,-1.034283,-3.176854,2.005995|H,0,-0.627206,-4.1
95139,3.127848|H,0,-1.906942,-3.305832,3.303225|C,0,4.397299,1.039672,
1.801173|C,0,5.869514,1.237852,1.780905|H,0,6.092028,1.925122,1.148879
|H,0,6.169608,1.496679,2.654918|H,0,6.299178,0.416598,1.522896|C,0,3.9
29808,2.58093,0.075287|C,0,3.537442,3.917358,0.180736|C,0,3.868942,4.7
22814,-0.913532|C,0,4.487014,4.273469,-2.005739|C,0,4.843811,2.939425,
-2.109156|C,0,4.561407,2.096258,-1.051719|C,0,2.743647,4.417343,1.3511
92|C,0,3.218742,5.772556,1.879746|H,0,3.237295,6.407615,1.159892|H,0,2
.617523,6.07845,2.561539|H,0,4.100653,5.67899,2.247549|C,0,1.26549,4.5
13361,0.96564|H,0,0.951858,3.651882,0.679122|H,0,0.754281,4.801437,1.7
27201|H,0,1.161003,5.14693,0.252721|C,0,3.945288,-1.409955,2.054769|C,
0,4.206177,-2.575401,2.953528|H,0,4.281056,-3.375214,2.426914|H,0,5.02
3122,-2.431818,3.436086|H,0,3.480273,-2.669493,3.575803|C,0,3.652911,-
2.677482,0.075632|C,0,4.640444,-2.969109,-0.868017|C,0,4.445269,-4.099
414,-1.650222|C,0,3.329636,-4.892777,-1.516408|C,0,2.380994,-4.599979,
-0.57248|C,0,2.536082,-3.487465,0.227203|C,0,5.870238,-2.099018,-0.968
451|C,0,6.903748,-2.519153,0.067093|H,0,7.202804,-3.41155,-0.123541|H,
0,7.653067,-1.917826,0.034663|H,0,6.509079,-2.494,0.940802|C,0,6.50558
6,-2.083767,-2.364168|H,0,5.825913,-1.911315,-3.021146|H,0,7.170699,-1
.392328,-2.40589|H,0,6.913077,-2.932975,-2.539515|H,0,-2.654988,-1.199
664,3.84555|H,0,-3.404074,0.873149,3.515322|H,0,-1.834074,2.475234,2.8

48695|H,0,0.287795,2.068691,2.397638|H,0,0.623905,-2.406596,3.216814|H
,0,3.527009,5.496317,-0.781369|H,0,4.706543,4.730314,-2.803228|H,0,5.2
27537,2.596715,-2.784751|H,0,4.795551,1.214575,-1.081102|H,0,2.827073,
3.811957,2.10039|H,0,5.041988,-4.344523,-2.343285|H,0,3.321986,-5.5614
2,-2.121332|H,0,1.641671,-5.183467,-0.456343|H,0,1.893663,-3.336175,0.
867111|H,0,5.613153,-1.174379,-0.717222|N,0,1.519479,-0.153795,2.58186
9|N,0,3.5362,1.658376,1.096154|N,0,3.736668,-1.452022,0.810662||Versio
n=IA32W-G09RevB.01|State=1-A|HF=-3072.0579794|RMSD=5.507e-009|Dipole=-
0.0003059,-0.0004876,-0.0011615|Quadrupole=42.2194261,-22.6486038,-19.
5708223,-3.9670195,20.6468479,-0.2702449|PG=C01 [X(C68H86N6Tl2)]||@

A HARD FALL SHOULD MEAN A HIGH BOUNCE
IF ONE IS MADE OF THE RIGHT MATERIAL.

-- THE CHEMIST ANALYST, MARCH 1950

Job cpu time: 0 days 9 hours 36 minutes 6.0 seconds.
File lengths (MBytes): RWF=   403 Int=   0 D2E=   0 Chk=   28 Scr=   1
Normal termination of Gaussian 09 at Wed Apr 03 22:53:43 2013.