

Supporting Information for:

**Carbon-Oxygen Bond Forming Mechanisms in Rhenium Oxo-Alkyl Complexes**

Mu-Jeng Cheng, Robert J. Nielsen\*, Marten Ahlquist, and William A Goddard III

***Computational methods***

The geometry optimizations and zero-point vibrational energy (ZPVE) were carried out with the B3LYP functional with the 6-31G\*\* basis set for all atoms except Re. For Re the first four shells of core electrons were described by the Los Alamos angular momentum projected effective core potential (ECP) using the double- $\zeta$  contraction of valence functions.

Solvation energies were calculated using the Poisson-Boltzmann self-consistent polarizable continuum method implemented in Jaguar to represent dichloromethane (dielectric constant = 8.93 and effective radius = 2.33 Å). The solvation calculations used the B3LYP/LACVP\*\* level of theory and the gas-phase optimized structures. For the most accurate energetics, singlet-point energy calculations were performed using the M06 functional with a larger basis set: Re was described with the triple- $\zeta$  contraction of valence functions augmented with two f-functions (exponents of 0.327 and 0.955, from Martin, J. M. L.; Sundermann, A. *J. Chem. Phys.* **2001**, 114, 3408) and the core electrons were described by the same ECP; S was described using the 6-311+G(3df) basis; the other atoms were described with the 6-311++G\*\* basis set.

Unless otherwise noted, all energies discussed are free energies, calculated as

$$G_{298K} = E_{\text{elec}} + G_{\text{solv}} + \text{ZPVE} + \sum_v \frac{h\nu}{e^{h\nu/kT} - 1} + \frac{n}{2}kT - T(S_{\text{vib}} + S_{\text{rot}} + S_{\text{trans}}) \text{ (equation (1))},$$

where  $n = 12$  accounts for the potential and kinetic energies of the translational and rotational modes.

The value of  $(S_{\text{rot}} + S_{\text{trans}}) = 47.4$  e.u. for DMSO was chosen by fitting our calculated  $\Delta S$  for the reaction  $(\text{HBpz}_3)\text{ReO}(\text{Ph})(\text{OTf}) + \text{DMSO} \rightarrow [(\text{HBpz}_3)\text{ReO}(\text{Ph})(\text{DMSO})]\text{OTf}$  to the value measured by Mayer *et al.* ( $\Delta S = -24.8$  e.u.). The values of  $(S_{\text{rot}} + S_{\text{trans}})$  for each Re intermediate were assumed to cancel.

The free energies of aqueous water and ammonia (1M) are the sum of the calculated free energy of the species in the gas phase at 1 atm (calculated with standard statistical mechanical formulae) and the appropriate experimental free energy of hydration ( $\Delta G_{\text{H}_2\text{O}}(1 \text{ atm} \rightarrow \text{liq}) = -2.05$  kcal/mol and  $\Delta G_{\text{NH}_3}(1 \text{ atm} \rightarrow 1\text{M}) = -2.4$  kcal/mol, from *J. Phys. Chem. Ref. Data*, Vol. 11, Suppl.2, 1982.).

We compared the performance of this M06(electronic energy)//B3LYP(geometry optimization) approach with that of M06//M06, and found both levels of theory gave similar results (with less computational cost using M06//B3LYP). Two reactions were used for this comparison: (1) 1,2-phenyl migration of  $[(\text{HBpz}_3)\text{ReO}_2(\text{Ph})]\text{OTf}$ ,  $\Delta G^\ddagger(\text{M06//M06}) = 20.2$  kcal/mol,  $\Delta G^\ddagger(\text{M06//B3LYP}) = 17.9$  kcal/mol,  $\Delta G^\ddagger(\text{exp}) = 20.9$  kcal/mol; (2)  $\text{DMS}_{(\text{g})}(1 \text{ atm}) + 0.5 \text{ O}_{2(\text{g})}(1 \text{ atm}) \rightarrow \text{DMSO}_{(\text{g})}(1 \text{ atm})$ ,

$\Delta H(\text{M06//M06}) = -28.3 \text{ kcal/mol}$ ,  $\Delta H(\text{M06//B3LYP}) = -27.8 \text{ kcal/mol}$ ,  $\Delta H(\text{exp}) = -27.0 \text{ kcal/mol}$ .

We also compared the Gibbs free energy profiles from this M06//B3LYP with those from B3LYP//B3LYP. We found both levels of theory give similar results in the unimolecular reactions with 1.9 kcal/mol discrepancy in barriers and 2.0 kcal/mol in reaction energies (Table 1S), but show significant difference after DMSO participated the reaction (Figure 1S). We believe that M06 gives more accurate results for such cases because of its improvements in treating van der Waals interactions and redox thermochemistry of main group elements and metals (Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, 41, 157).

At the request of a reviewer, free energy surfaces derived from both Eq (1) and again assuming ideal gas statistical mechanics for all species are presented in Figure 2S and Table 2S.

Figure 1S. M06//B3LYP (blue line) and B3LYP//B3LYP (red line) free energy

surfaces (including solvation by dichloromethane) of the oxidation of

(HBpz<sub>3</sub>)ReO(Et)(OTf) by DMSO (kcal/mol) at 298K

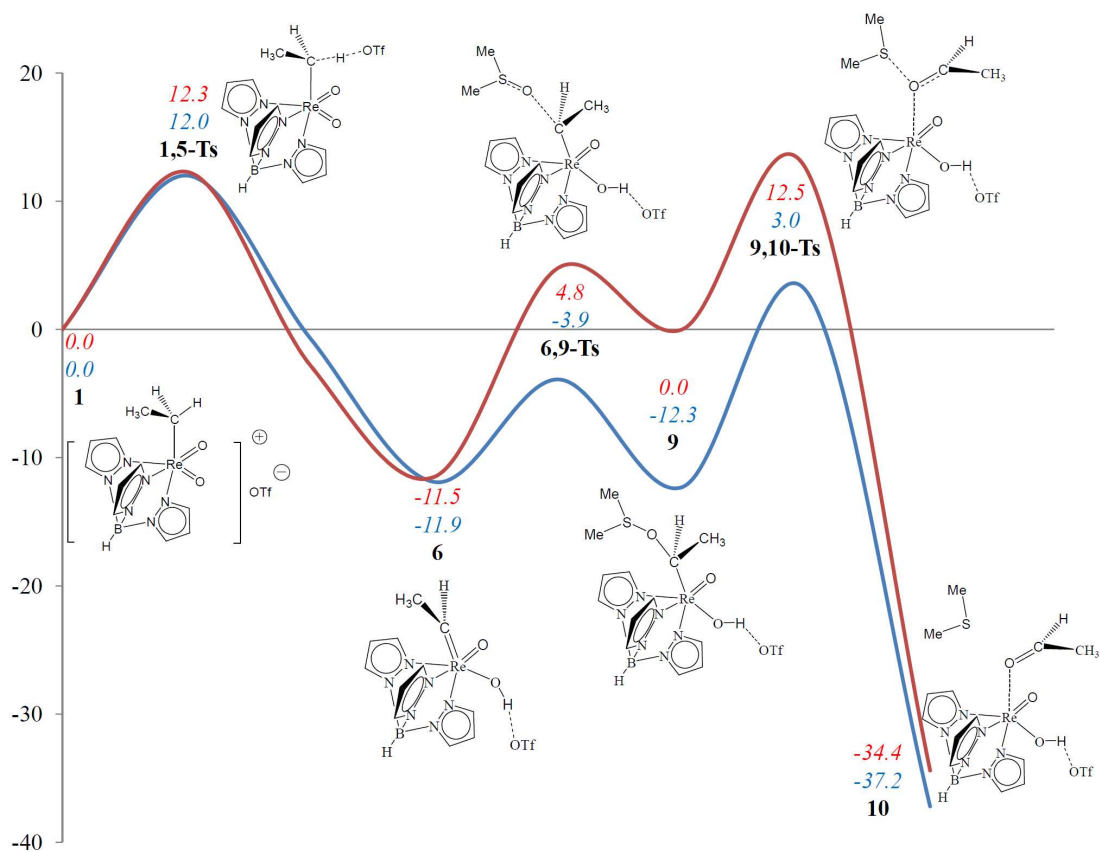


Figure 2S. Overall free energy surfaces of the oxidation of (HBpZ<sub>3</sub>)ReO(Et)(OTf) by DMSO (kcal/mol) at 298K (including solvation by dichloromethane). The green line is based on thermal corrections from the ideal gas model, while the blue line is based on equation (1).

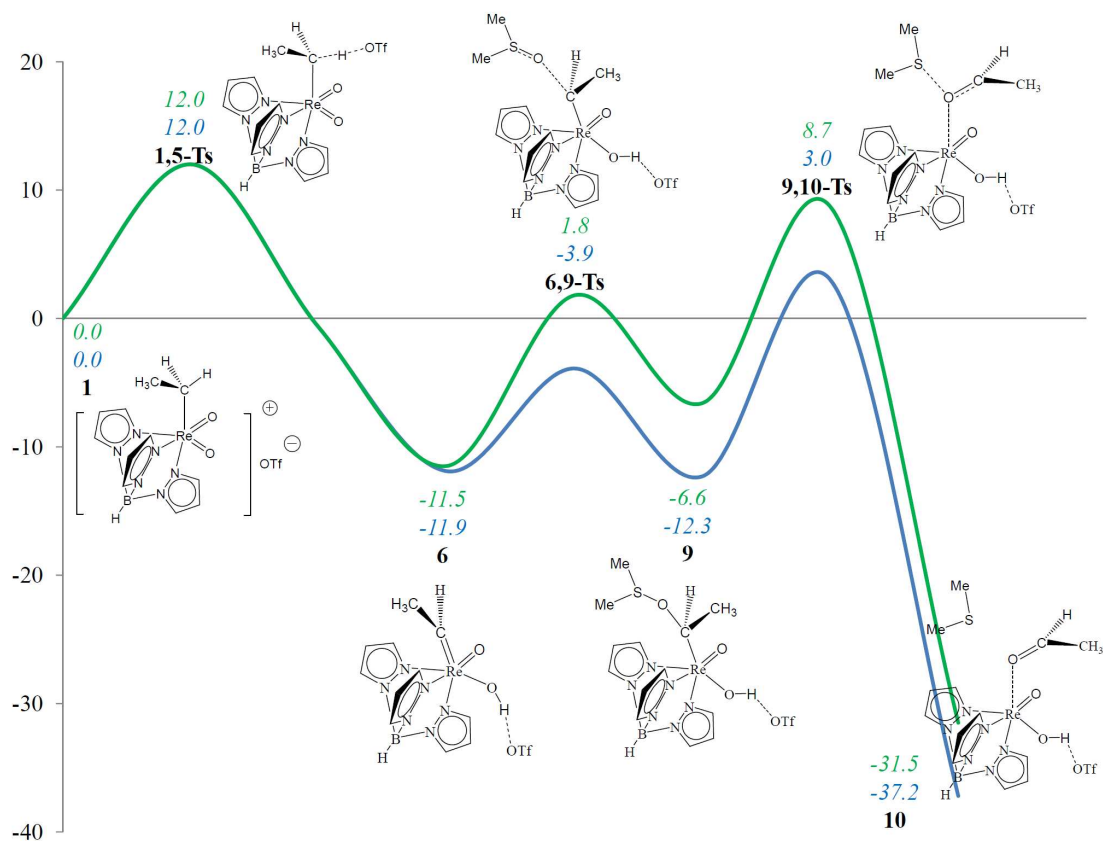
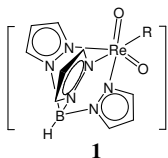
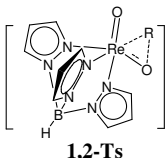
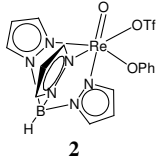


Table S1. The reaction barrier and free energy (including solvation by dichloromethane) for alkyl 1,2-migration at 298K (unit: kcal/mol) by B3LYP//B3LYP and M06//B3LYP (in parentheses)

Alkyl			
	<b>1</b>	<b>1,2-Ts</b>	<b>2</b>
Me	0.0 (0.0)	26.3 (29.1)	-23.3 (-26.1)
Et	0.0 (0.0)	18.6 (22.1)	-24.5 (-25.0)
<i>i</i> Pr	0.0 (0.0)	8.9 (11.8)	-29.7 (-28.4)

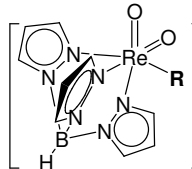
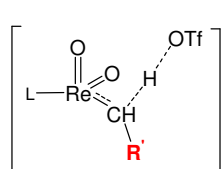
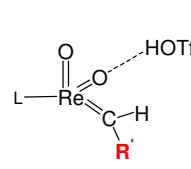
			
	<b>1</b>	<b>1,2-Ts</b>	<b>2</b>
Me	0.0 (0.0)	11.1 (12.0)	3.5 (4.6)
Et	0.0 (0.0)	12.3 (12.0)	-2.8 (-0.7)
<i>i</i> Pr	0.0 (0.0)	12.4 (13.5)	-7.8 (-4.2)

Table S2. The reaction barrier and energy (including solvation by dichloromethane) for alkyl 1,2-migration at 298K based on the ideal gas model. For comparison, we also showed the numbers based on equation (1) in parentheses (unit: kcal/mol).

Alkyl			
Me	0.0 (0.0)	29.1 (29.1)	-26.0 (-26.1)
Et	0.0 (0.0)	22.1 (22.1)	-24.9 (-25.0)
<i>i</i> Pr	0.0 (0.0)	11.6 (11.8)	-28.4 (-28.4)
Alkyl			
Me	0.0 (0.0)	12.0 (12.0)	4.5 (4.6)
Et	0.0 (0.0)	12.0 (12.0)	-0.7 (-0.7)
<i>i</i> Pr	0.0 (0.0)	13.5 (13.5)	-4.3 (-4.2)

*Cartesian coordinates of optimized geometries and corresponding electronic energy ( $E_{elec}$ ) from M06 level of theory (the unit is hartree for  $E_{elec}$  and Å for Cartesian coordinates)*

<b><i>I-Ph</i></b>	<b><math>E_{elec} = -2124.59182551877</math></b>		
Re	0.136863704	0.2586078990	0.2691612982
N	-0.294342430	-0.2594426939	2.3329166990
N	2.177715548	-0.1713647406	1.1195347226
N	0.171149473	-2.0209547770	0.1769855827
N	0.229224287	-1.3066756555	3.0189038679
N	2.460354992	-1.2163010763	1.9517412594
N	0.734665974	-2.8240849903	1.1164472989
B	1.348362827	-2.1790591718	2.3757374847
H	1.735670994	-3.0063674444	3.1473115692
C	-1.1672767592	0.3772870127	3.1367307114
C	3.2858233396	0.5823922103	1.0094007860
C	-0.4126482537	-2.8161359726	-0.7341930303
C	-0.3149876994	-1.3311971164	4.2474903571
C	3.7423136553	-1.1151715451	2.3595864064
C	0.5119316863	-4.1128761921	0.7953787089
C	-1.2172787090	-0.2772212732	4.3657776880
C	4.3047572035	0.0134689124	1.7815305148
C	-0.2137339081	-4.1552262935	-0.3903181250
H	-1.8163054370	-0.0162781907	5.2242909859
H	5.3114853854	0.3824120218	1.9021278644
H	-0.5519225230	-5.0302140187	-0.9234683041
O	-1.4304119495	0.0561197189	-0.3801993889
O	0.2302426980	1.8969783697	0.7068807168
H	-0.9317895873	-2.3829141376	-1.5763941124
H	0.8791886794	-4.9060249370	1.4301488882
H	-1.6886677522	1.2573977168	2.7897239728
H	-0.0197954245	-2.0909675444	4.9561842004
H	3.2892740673	1.4836977117	0.3992608076
H	4.1575389431	-1.8521873280	3.0317119614
O	0.7967000266	3.9473398105	-0.5850538513
S	2.2388032961	4.3285322422	-0.4397295166
O	3.1775708352	3.1945396702	-0.6318021828
O	2.6011316554	5.5906057831	-1.0988968870



C	2.3934687399	4.6795648064	1.3815806999
F	2.1899009987	3.5537842001	2.1019231676
F	1.5000073585	5.5930388927	1.7836950455
F	3.6229590739	5.1314280593	1.6731639884
C	1.2453249489	0.2764230632	-1.4972421021
C	2.0550127283	-0.7801980434	-1.9513788950
C	1.0790452363	1.4256386510	-2.2934349685
C	2.6447882486	-0.7107207564	-3.2088379672
H	2.2278896540	-1.6485227268	-1.3267270989
C	1.6696901200	1.4761643759	-3.5577821874
H	0.5449809210	2.2938135333	-1.9214756657
C	2.4468031360	0.4150397405	-4.0177474228
H	3.2688301762	-1.5290812519	-3.5567604907
H	1.5446416267	2.3706302565	-4.1604985885
H	2.9195964479	0.4709793013	-4.9942277607

***1,2-Ts-Ph***  $E_{elec} = -2124.56079570858$

C	-0.040245975	0.0056465001	-0.0436601625
O	0.017236522	-0.0039238270	1.9794150066
Re	1.693338868	-0.0002060752	1.4720343667
N	3.540757068	-0.2961084628	2.5788189070
N	2.818197976	-0.9762707224	-0.0137833466
N	1.486622081	-2.1423476166	2.2157499164
N	4.304615975	-1.4179269862	2.5391082949
N	3.669400458	-2.0273385007	0.2207677790
N	2.489817420	-3.0563034446	2.1645552492
B	3.8642763198	-2.5958389176	1.6392208514
H	4.6658947151	-3.4824874299	1.6519516521
C	4.1346901824	0.5770282089	3.4117877629
C	2.9022462720	-0.6505738528	-1.3240359696
C	0.4263582378	-2.7435927176	2.7856336118
C	5.3658518082	-1.2560233810	3.3505984354
C	4.2693134312	-2.3520106154	-0.9367909082
C	2.0664644030	-4.2204306670	2.6896900918
C	5.2964337990	0.0056071322	3.9314952819
C	3.8153694501	-1.5031438911	-1.9404636820
C	0.7447924552	-4.0667010034	3.0973318132
H	5.9949466791	0.4511703081	4.6225125059

H	4.1138433836	-1.4908884611	-2.9770059967
H	0.1071287792	-4.8085527729	3.5526796779
O	2.1790392701	1.6145693377	1.4140405710
H	-0.4910771675	-2.1913773444	2.9238876167
H	2.7277047013	-5.0736231995	2.7358997183
H	3.7066194238	1.5563469651	3.5671039462
H	6.0968913830	-2.0444564530	3.4545776019
H	2.3555517067	0.2008113254	-1.7300394875
H	4.9807736476	-3.1648274851	-0.9658433109
O	1.5115446750	3.5592435504	-0.5401696272
S	2.1422177156	3.3219810981	-1.8672673413
O	1.8892894457	1.9599916173	-2.4201967018
O	2.0328907351	4.4222897399	-2.8339856993
C	3.9553494464	3.2385458624	-1.4498020471
F	4.2154266130	2.1629355546	-0.6627116293
F	4.3644013239	4.3302234901	-0.7895876374
F	4.7030782582	3.1106696208	-2.5579368466
C	-0.5240855861	-1.2265893284	-0.4845408620
C	-0.4427868846	1.2322170731	-0.5543855849
C	-1.3772427062	-1.2202060705	-1.5865641646
H	-0.2302556639	-2.1564870875	-0.0126915805
C	-1.2987038738	1.2031794125	-1.6606240120
H	-0.0418917660	2.1745660509	-0.1914420973
C	-1.7642128627	-0.0078218233	-2.1706014192
H	-1.7438745312	-2.1627972306	-1.9827586442
H	-1.5826582367	2.1438400273	-2.1217191136
H	-2.4370232458	-0.0116000990	-3.0230541363

**2-Ph**  $E_{elec} = -2124.67504675881$

Re	-0.198330658	-0.0785173290	-0.0866228078
N	0.396962684	0.1086241468	1.9653605319
N	2.090922318	-0.2219645359	-0.1252110998
N	0.051727910	-2.1449734922	-0.0293808031
N	1.125383779	-0.8674176339	2.5742158392
N	2.728356457	-1.0954315033	0.6961492071
N	0.865975485	-2.7471482161	0.8846320633
B	1.880680919	-1.9030984226	1.7078532928
H	2.559128679	-2.6182723608	2.3866032526

C	0.0576105965	1.0084249739	2.8966723447
C	3.0247071891	0.4328849108	-0.8247828254
C	-0.5223613455	-3.1066261124	-0.7708976748
C	1.2491787155	-0.5692223453	3.8838872663
C	4.0612756582	-0.9917273264	0.5109598596
C	0.7983085717	-4.0785903028	0.7092397100
C	0.5702514646	0.6153083606	4.1380718103
C	4.2972473040	-0.0258832883	-0.4590578548
C	-0.0897942167	-4.3556803647	-0.3272666263
H	0.4656748280	1.1229793564	5.0844011607
H	5.2515081409	0.3017083627	-0.8420651037
H	-0.3745636360	-5.3246945288	-0.7066960467
O	-1.8051461695	-0.0904365528	0.4154401231
O	0.2804959584	1.9095361662	-0.2255132844
S	-0.3249419649	3.1381865511	-0.9906174993
O	-1.7711020151	3.0250849405	-1.1570423952
O	0.5330141053	3.5636985146	-2.0906812804
C	-0.0706894915	4.3823359557	0.3734264655
F	-0.7746077483	4.0298071031	1.4629710832
F	1.2194365537	4.4704607268	0.7038892871
F	-0.5000248500	5.5752127275	-0.0432362913
H	-1.1987584171	-2.8346659347	-1.5670461966
H	1.3936970911	-4.7391675453	1.3223049398
H	-0.5219190087	1.8769165160	2.6222554019
H	1.8190987993	-1.2125483800	4.5381835084
H	2.7325647794	1.1934720387	-1.5351901058
H	4.7437816417	-1.6062957430	1.0797320033
O	-0.1186099061	-0.4106905660	-2.0054150539
C	-0.2091138623	0.3722184123	-3.1216711123
C	-1.4153622229	0.9937103019	-3.4642246447
C	0.8943061117	0.4513476714	-3.9823977512
C	-1.5033847304	1.7123370288	-4.6555825052
H	-2.2607762695	0.9251917918	-2.7887100650
C	0.7945211535	1.1804300055	-5.1651452078
H	1.8119729097	-0.0615904194	-3.7110813052
C	-0.4025795572	1.8141698175	-5.5067275050
H	-2.4378454198	2.2039580061	-4.9115497593
H	1.6555600406	1.2527525580	-5.8244027584

H	-0.4751869082	2.3850805076	-6.4279127759
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***I***     ***E<sub>elec</sub>*** = **-1972.25945257161**

Re	0.057989341	0.3630935969	0.5835865032
N	-0.316305275	-0.4548484866	2.5057745486
N	2.131486870	-0.1955333223	1.2868044048
N	0.076596197	-1.9004844694	0.1437805244
N	0.227124480	-1.5792473286	3.0393305147
N	2.430468123	-1.3547929704	1.9438634830
N	0.672127151	-2.8257939323	0.9388705397
B	1.325518969	-2.3653846385	2.2527861572
H	1.722603511	-3.2887039427	2.8998293624
C	-1.1942750623	0.0550929325	3.3978134229
C	3.2479210768	0.5544192890	1.2488448485
C	-0.4807431602	-2.5571135439	-0.8844220338
C	-0.3043291743	-1.7759852284	4.2544968111
C	3.7274800679	-1.3269874389	2.3151638316
C	0.4943884058	-4.0540461610	0.4122328837
C	-1.2195493351	-0.7580972511	4.5249108098
C	4.2857655221	-0.1313669477	1.8891714903
C	-0.2365717757	-3.9284043371	-0.7624199221
H	-1.8125492189	-0.6260436141	5.4164569786
H	5.3021477078	0.2059129280	2.0204570495
H	-0.5515657540	-4.7161205198	-1.4290172040
O	-1.4867718613	0.2987172844	-0.1295987171
O	0.3394284831	1.9715808299	1.0278250116
H	-1.0238140292	-2.0147481502	-1.6443036539
H	0.8949236893	-4.9258655001	0.9084363637
H	-1.7380253312	0.9621156663	3.1766303309
H	0.0044674449	-2.6225692764	4.8502073522
H	3.2529793921	1.5227663256	0.7523824481
H	4.1552953598	-2.1591923581	2.8551681704
O	0.9227920151	3.5989688879	-1.0051160237
S	2.3619217592	3.9796011122	-0.9854236475
O	3.2732569470	2.8153088877	-0.7543790420
O	2.7928560866	4.9191944098	-2.0279149358
C	2.5262068391	4.9212267264	0.6111207178
F	2.2754821356	4.1111910944	1.6641127782

F	1.6630872264	5.9449888901	0.6650283061
F	3.7687387703	5.4066040716	0.7577876570
C	1.2084702447	0.4167342764	-1.2842404463
H	1.9748326882	1.1685186770	-1.0691321828
H	1.6467011552	-0.5724103988	-1.4006119756
C	0.3309233891	0.8650283902	-2.4457262233
H	0.9923834688	0.9589607953	-3.3188771459
H	-0.4635395868	0.1538100230	-2.6883983520
H	-0.0876171546	1.8553478634	-2.2607167504

***1,3-Ts*  $E_{elec} = -1972.18406835147$**

H	-0.050300049	0.0498669101	0.0498573712
O	0.050912610	0.0535793037	1.4759009045
C	0.986985112	0.0624413037	-1.1543292917
Re	1.352509173	0.9276307533	0.5535570930
N	2.201205239	1.7760822762	2.4491198683
N	3.395078881	1.4714415962	-0.1369777921
N	2.596921848	-0.8194124424	1.2399449347
N	3.467626241	1.5624761953	2.8850693284
N	4.511061641	1.3422955412	0.6291565395
N	3.8029143524	-0.6878547537	1.8572447915
B	4.4314604683	0.7027421072	2.0296066958
H	5.5109457633	0.6390357884	2.5404010829
C	1.5765251315	2.5337697494	3.3643700534
C	3.7721981406	1.9938808139	-1.3153071340
C	2.2844332209	-2.1262613587	1.2446800285
C	3.6395075011	2.1810866237	4.0675916311
C	5.5767496174	1.7782526110	-0.0675667614
C	4.2400488745	-1.9018294365	2.2397476086
C	2.4513250075	2.8165004347	4.4156255730
C	5.1497085104	2.2115939735	-1.3157706545
C	3.2993817225	-2.8528234166	1.8672239904
H	2.2525122615	3.4000651735	5.3011355854
H	5.7513590322	2.6097375586	-2.1176041773
H	3.3530393001	-3.9215894932	2.0017329009
O	0.8664972476	2.5006662742	0.0983556717
H	1.3773280842	-2.4808442057	0.7821937319
H	5.1898037256	-2.0036790803	2.7439893182

H	0.5469994861	2.8280123848	3.2187191602
H	4.5898475582	2.1284895497	4.5782980325
H	3.0496629330	2.1806655777	-2.0934629463
H	6.5628073551	1.7456563581	0.3717207920
O	3.1137193744	-0.9349335154	-3.2684744041
S	2.9909325713	-2.3530399311	-2.8469399327
O	1.9192063798	-2.5682778817	-1.8139375420
O	3.0347157082	-3.3673594337	-3.9037985528
C	4.5541723392	-2.6152683046	-1.8722848368
F	4.6652951002	-1.6877827836	-0.8930277634
F	5.6322810639	-2.5057499947	-2.6594163847
F	4.5723669393	-3.8248393529	-1.2923216547
H	1.1756054388	-1.0333110643	-1.2714015611
C	0.7012236579	0.7157974711	-2.4536413044
H	-0.1477216292	0.1943961881	-2.9213858744
H	0.4986084731	1.7867025406	-2.3776934867
H	1.5553183467	0.4936696639	-3.1128789922

**3  $E_{elec} = -1972.29437774804$**

H	0.362604622	0.0469029537	-0.0678409699
O	0.209156618	0.1253115292	0.8845832252
C	2.838999500	-0.4239812291	0.1882749539
Re	1.816658520	0.1143004743	1.9847540475
N	0.379239084	-0.1082400305	3.5501399081
N	3.375896906	-0.5210807242	3.3594989057
N	1.532344105	-2.2243009104	2.1609318486
N	0.589467842	-0.8703210553	4.6572416779
N	3.092676419	-1.2241682479	4.4909257045
N	1.5115040463	-2.7993889380	3.3936863422
B	1.7277601868	-1.9249316021	4.6477866139
H	1.6985134188	-2.5796283493	5.6506310906
C	-0.7786185995	0.5485094631	3.7161302576
C	4.6705366022	-0.1807973714	3.4145600309
C	1.2426129587	-3.1896356379	1.2791402609
C	-0.4332191502	-0.6891428105	5.5135111016
C	4.2095191281	-1.3328776852	5.2394506990
C	1.2143244040	-4.1106969153	3.2817864923
C	-1.3271560129	0.2222062573	4.9590979208

C	5.2429118390	-0.6671650581	4.5947463959
C	1.0338720868	-4.4071808254	1.9390683832
H	-2.2442849031	0.5892497640	5.3934160205
H	6.2636925907	-0.5566223093	4.9265199135
H	0.7945220779	-5.3633680390	1.4999526718
O	2.3459461857	1.7031575665	2.1458090396
H	1.2113734847	-2.9809546304	0.2202994570
H	1.1532507447	-4.7347542515	4.1614303493
H	-1.1373713571	1.2005486209	2.9337297204
H	-0.4614898019	-1.2252270741	6.4510533616
H	5.1134300762	0.3864065327	2.6105646266
H	4.1919409995	-1.8853690867	6.1673915942
O	4.1606715196	-1.0488394019	0.5078965804
S	4.8180663635	-2.0870388618	-0.5325731142
O	3.7866521726	-2.7284984136	-1.3453355496
O	6.0163599079	-1.5254974715	-1.1398610231
C	5.3936781359	-3.3305679999	0.7333413815
F	4.3494252866	-3.8669796571	1.3642641713
F	6.1967055795	-2.7419866704	1.6198688878
F	6.0649607483	-4.2913345617	0.0944676179
H	2.2676827843	-1.1920154720	-0.3393748317
C	3.0878289774	0.7523871764	-0.7563461005
H	2.1383231536	1.2450100778	-0.9938043022
H	3.7423805407	1.4952979724	-0.2950723896
H	3.5394956318	0.4205827826	-1.6992854831

***1,4-Ts*      $E_{elec} = -1972.20164907805$**

H	0.082037562	0.0479697888	0.0929738321
C	0.031643994	0.0666779197	1.4209442000
O	0.973335415	0.0365332737	-0.8348268285
Re	2.552423698	0.4166504841	-0.0222553716
N	3.376548467	0.7754088813	-1.9939869795
N	4.393638400	1.2791284272	0.7598771558
N	2.273160683	2.7185299537	-0.4248394463
N	4.350236189	1.6882281118	-2.2524935469
N	5.171501771	2.1698009666	0.0825892337
N	3.2949132530	3.4756819383	-0.9073881309
B	4.6525270380	2.8078120313	-1.2165664450

H	5.4404817391	3.5905509549	-1.6605168772
C	3.1719084753	0.0581780829	-3.1113268996
C	5.0256215580	0.9697377392	1.9087577060
C	1.1925220202	3.5109949792	-0.3697811630
C	4.7525464434	1.5435886541	-3.5290938745
C	6.2807664740	2.4193986723	0.8045555391
C	2.8586690594	4.7292726107	-1.1450769591
C	4.0344052873	0.5058260616	-4.1138761876
C	6.2305086940	1.6718768251	1.9754068313
C	1.5130740535	4.7988978542	-0.8114675452
H	4.1211777170	0.1333177252	-5.1226958592
H	6.9598999168	1.6432945159	2.7697938720
H	0.8609172712	5.6559648694	-0.8763218203
O	3.0530316837	-1.1240709799	0.4460099669
H	0.2453120752	3.1228400785	-0.0255758028
H	3.5332524479	5.4793677409	-1.5312477782
H	2.4276783348	-0.7247927997	-3.1211873854
H	5.5133801605	2.1934436373	-3.9361702926
H	4.5658470931	0.2918564975	2.6177412566
H	7.0229215836	3.1142238111	0.4395005776
O	0.3579875115	-0.6427961072	4.2459800485
S	1.7629093989	-0.9630504192	4.5803294325
O	2.7450455404	-0.1696206369	3.7486694894
O	2.1218975631	-1.0596634282	5.9964487227
C	1.9862178754	-2.6798218148	3.9011812618
F	1.6776409332	-2.7026827641	2.5843147354
F	1.1833761810	-3.5467655380	4.5288065246
F	3.2528172159	-3.0931136716	4.0352527006
C	1.2733676936	0.8563507437	1.5534452573
H	1.9152284237	0.4461116391	2.4124666698
H	1.1061038154	1.9215951535	1.6977331485
H	-0.9028060202	0.4914965132	1.7888926131
H	0.1060261304	-1.0043351186	1.6110198240

**4**  $E_{elec} = -1972.28411642821$

H	0.693368963	-0.8152673111	0.2008119912
C	0.777757904	-0.4374868327	2.6002140024
O	1.371109950	-0.4962606045	-0.4066209015



Re	3.005078161	0.1745388588	0.4231618113
N	3.431420261	0.6939067832	-1.6009065871
N	4.562863136	1.5167197971	1.1008209493
N	2.087205857	2.3500892324	0.1432242573
N	4.117688766	1.8154913939	-1.9534076512
N	5.044122208	2.5141097879	0.3073208126
N	2.8206050547	3.3178455103	-0.4637324259
B	4.2516468014	2.9791609042	-0.9359677569
H	4.7842133171	3.9229012474	-1.4465477077
C	3.2314622339	-0.0324789542	-2.7096454095
C	5.3603121271	1.4432755336	2.1759109537
C	0.8859869161	2.8778354833	0.4035443919
C	4.3439947663	1.7889140400	-3.2811109202
C	6.1243095744	3.0683501848	0.8943690507
C	2.0866587790	4.4448409504	-0.5792912264
C	3.8077533063	0.6173986057	-3.8050929547
C	6.3717945361	2.4056929620	2.0886903544
C	0.8332335440	4.2087013869	-0.0328928768
H	3.8282010421	0.2882733874	-4.8325370506
H	7.1669203453	2.5930558476	2.7934706707
H	0.0051463906	4.8968211579	0.0396748941
O	4.0019692048	-1.1508955512	0.6997217270
H	0.1231852866	2.2864572559	0.8885899671
H	2.5062147140	5.3283515387	-1.0377828905
H	2.6844029322	-0.9609522944	-2.6438104318
H	4.8594100949	2.6068340815	-3.7631432536
H	5.1769659147	0.6993960824	2.9371193813
H	6.6320573513	3.8991712775	0.4269800537
O	0.1346296976	-0.1018753825	3.9062194025
S	0.6611265412	-0.8038387412	5.2530086673
O	1.9353444126	-1.4782872562	5.0388443763
O	0.4410121233	0.1263137478	6.3450557542
C	-0.6205157204	-2.1511631226	5.4108260657
F	-0.5995725978	-2.9125147177	4.3093564211
F	-1.8332391286	-1.6227690315	5.5582650491
F	-0.3267741513	-2.9018492006	6.4716196486
C	2.0344035813	0.3601008881	2.3595315316
H	2.8002940190	0.0246310379	3.0667871628

H	1.8517892772	1.4175132795	2.5678652777
H	-0.0358811312	-0.1865426655	1.9138411994
H	0.9526615139	-1.5156571815	2.5760671306

***1,5-Ts***     ***E<sub>elec</sub> = -1972.24994819374***

H	-0.017174315	0.0157100116	0.0226869668
C	-0.006107179	0.0216034656	1.3405006435
O	0.268535708	-0.0086913108	-1.2404538498
Re	-2.023058637	0.0347532910	1.4159189980
O	-2.227539928	1.7093745889	1.1460006090
N	-4.042393903	-0.1968905506	2.2416444290
N	-1.688175957	0.5985491483	3.6302554429
N	-1.923426294	-2.0145847297	2.3988199160
N	-4.344867597	-0.7219517387	3.4559539445
N	-2.2789940576	-0.0413846036	4.6700366842
N	-2.4392003195	-2.3096582894	3.6235717543
B	-3.2149587007	-1.2315573644	4.3975374048
H	-3.6783686408	-1.6638114159	5.4125389042
C	-5.1939478083	0.1056065793	1.6201464396
C	-1.0030718176	1.6336500958	4.1379129787
C	-1.5284505110	-3.1670991428	1.8342405403
C	-5.6828860087	-0.7464037009	3.5974495986
C	-1.9633189764	0.5819491909	5.8231349209
C	-2.3551888203	-3.6409696958	3.8298863238
C	-6.2678581295	-0.2245225357	2.4481375566
C	-1.1429373729	1.6628478309	5.5293389100
C	-1.7691879088	-4.2264466328	2.7165469783
H	-7.3197923998	-0.1052872109	2.2402199942
H	-0.7117951940	2.3700494912	6.2207833834
H	-1.5533422815	-5.2720219317	2.5595984166
O	-2.4343159258	-0.8537065143	0.0142306192
H	-1.1090717292	-3.1657106163	0.8358472537
H	-2.7239015076	-4.0738585172	4.7484594962
H	-5.1821818545	0.5310988189	0.6272251396
H	-6.1263452776	-1.1352431081	4.5022458813
H	-0.4606738350	2.3025018972	3.4861427482
H	-2.3431184025	0.2136732558	6.7647692926
H	0.3283784434	1.0113215617	1.6671072943

C	0.9866193127	-1.0422522664	1.7517181640
H	0.9611949459	-1.1874999201	2.8393080280
H	0.8101627654	-1.9952427715	1.2566069798
H	1.9970143256	-0.7105397777	1.4859489396
S	0.2291943021	-1.3843116485	-1.9388515194
C	2.0329970407	-1.6139028007	-2.3318424723
F	2.4716878295	-0.6484447592	-3.1436599353
F	2.2169499078	-2.7983989244	-2.9252663039
F	2.7558998059	-1.5853269922	-1.1992835510
O	-0.4620923944	-1.3377735924	-3.2226189254
O	-0.0738361037	-2.4761747856	-0.9982210676

**5**      $E_{elec} = -1972.2804827202$

C	-0.303999206	-0.4040519766	0.1667845720
O	0.519839629	1.4090287408	-1.7809667209
H	1.955090092	1.2382668514	-1.8743261028
O	2.979658854	1.0846817049	-1.9937127810
Re	-0.996887125	0.8235350393	-1.1112733471
N	-2.007009019	2.5874347457	-2.4096417569
N	-0.767336431	2.5858438502	0.3189053226
N	-3.025448895	1.0002315305	-0.0925400469
N	-2.765752521	3.5501066789	-1.8266806545
N	-1.6839193389	3.5791640984	0.4488785695
N	-3.6883367093	2.1731464439	0.0689148073
B	-3.0285673403	3.5201896260	-0.3090315692
H	-3.7330969014	4.4346871508	0.0134117025
C	-1.9179198276	2.8885558204	-3.7083079306
C	0.2941152598	2.9176340911	1.0693014301
C	-3.8572732332	0.0179705670	0.2821177354
C	-3.1531988484	4.4506156375	-2.7579870084
C	-1.2059073434	4.5222138693	1.2850951292
C	-4.9220316410	1.9282460691	0.5534229710
C	-2.6323422952	4.0645264639	-3.9838220437
C	0.0593443502	4.1394760256	1.7086101138
C	-5.0750594265	0.5571589188	0.7075684527
H	-2.7513939815	4.5606346106	-4.9348535189
H	0.7172726652	4.6681600654	2.3808711674
H	-5.9410642232	0.0267394536	1.0722011302

H	-3.5479979228	-1.0135448531	0.2151260486
H	-5.5997476038	2.7450010781	0.7530711542
H	-1.3490372485	2.2538269282	-4.3731577107
H	-3.7667805234	5.2958491717	-2.4822308651
H	1.1647225074	2.2782927366	1.1011439319
H	-1.7991092394	5.3944459945	1.5171392444
C	-0.7862674683	-1.7664144139	0.5380275019
H	-1.4587661643	-2.1833404418	-0.2171756825
H	0.0666079383	-2.4409849005	0.6844644517
H	-1.3201989747	-1.7302112000	1.4994471623
H	0.5795749540	-0.0740834405	0.7205695319
O	-1.8260472161	-0.3205067833	-2.0710607237
S	3.7209577665	0.8359730143	-0.6291938434
O	2.7625490670	0.5750748277	0.4511597095
O	4.8633907755	-0.0335143385	-0.8425573374
C	4.3918430890	2.5376193476	-0.2849562764
F	5.0497720347	2.5155361671	0.8764260022
F	5.2180444717	2.9192673770	-1.2559086871
F	3.3787065463	3.4090170393	-0.1962123105

***I,7-Ts*      $E_{elec} = -1972.2284735689$**

O	0.013812731	-0.0123087566	0.0986566853
H	0.073486634	0.0755308776	1.4242078665
C	0.563825136	0.0953282102	2.6590288226
Re	-1.751869785	1.1356271481	3.0275749783
N	-3.795956146	1.7310651167	3.1963444666
N	-1.499603748	3.3957706503	3.2281858457
N	-1.970689789	1.4775747840	5.3204391407
N	-4.271844788	2.7270601489	3.9880020609
N	-2.250110329	4.1818268071	4.0412118220
N	-2.6544436564	2.5155240386	5.8609020818
B	-3.3253620929	3.5359229506	4.9254692502
H	-3.9473429681	4.3539518577	5.5380819732
C	-4.8218699127	1.2309931150	2.4878051494
C	-0.7357639645	4.1990767490	2.4733278665
C	-1.6131273516	0.6694080155	6.3271339444
C	-5.5951300092	2.8462400844	3.7789901191
C	-1.9512462558	5.4777993823	3.8080488544

C	-2.7193852587	2.3669964655	7.2005308449
C	-5.9910649761	1.9096669309	2.8293966683
C	-0.9824897921	5.5346781654	2.8164550021
C	-2.0574007085	1.1969703359	7.5452480763
H	-6.9835236475	1.7460112502	2.4393949271
H	-0.5245547649	6.4159081172	2.3945715094
H	-1.9226494507	0.7822657934	8.5321349416
O	-2.1287634528	-0.4834832506	3.4666415729
O	-1.8258646126	1.4979175516	1.3596691007
H	-1.0777972202	-0.2471315579	6.1255750840
H	-3.2313176053	3.0989980392	7.8076693680
H	-4.6573393752	0.4311353692	1.7811900997
H	-6.1634047723	3.5890575148	4.3189837597
H	-0.0761670251	3.7785613134	1.7232070723
H	-2.4492494841	6.2606359769	4.3612646174
S	0.8598015498	1.0792480949	-0.5779459622
O	1.2447255544	2.1323205571	0.3863639703
O	1.8910418013	0.5274431892	-1.4542361417
C	-0.3536462831	1.8950883603	-1.7374651013
F	-1.2666519167	2.6140976769	-1.0746731454
F	-0.9800570861	0.9756801886	-2.4783124347
F	0.3207385709	2.7207912847	-2.5490522697
C	0.3406164057	1.2013530232	3.5918403852
H	0.7958597214	2.1458153490	3.3074419805
H	0.3864495063	1.0258861259	4.6621834582
H	1.4994332952	0.2692161515	2.1142392607
H	0.4598404395	-0.9051234933	3.0759533542

7  $E_{elec} = -1972.28979530882$

O	0.141265083	-0.0682281960	0.1015741486
H	0.037898227	-0.0691930124	1.1465426293
C	0.674371171	0.0438057306	5.2006258255
Re	-0.295866393	1.4424928038	3.6100827857
N	-1.627107725	2.1634253095	2.0686048341
N	1.302690173	2.3349041390	2.2160466310
N	-0.173968129	3.6334163893	4.1797035544
N	-1.436839298	3.3544724920	1.4329640325
N	1.070983556	3.4632137802	1.5004401425

N	-0.2514744632	4.6168067626	3.2487616899
B	-0.2215290956	4.2612543916	1.7469543444
H	-0.2584716627	5.2494027282	1.0716570275
C	-2.7511735123	1.6164353977	1.5848722303
C	2.4522566365	1.8127640618	1.7664705543
C	-0.2859117120	4.2159099691	5.3811197274
C	-2.4418223959	3.5438880235	0.5553820211
C	2.0720618875	3.6559937351	0.6179475123
C	-0.3933803244	5.8096870819	3.8609726654
C	-3.3065569791	2.4594479677	0.6194062263
C	2.9863982660	2.6215734221	0.7575451914
C	-0.4183151271	5.6009945673	5.2329563787
H	-4.1992257577	2.2923663977	0.0372922995
H	3.8963636181	2.4668308195	0.1989499603
H	-0.5234087805	6.3415848007	6.0105374496
O	-1.5904805964	1.4861726396	4.7416829663
O	0.0370097402	0.0316666926	2.5810169603
H	-0.2944911601	3.6170356470	6.2796918965
H	-0.4659345947	6.7161641432	3.2782528886
H	-3.0792027770	0.6477945780	1.9284355392
H	-2.4676964089	4.4331066603	-0.0569858952
H	2.8202466173	0.8787073278	2.1652822871
H	2.0590883289	4.5079370359	-0.0456372111
S	-1.0064887723	-0.8419817819	-0.6506460948
O	-2.1455388982	-1.0977680966	0.2279215847
O	-1.1853090402	-0.2614748047	-1.9721937201
C	-0.1831859600	-2.4917882521	-0.9012239577
F	0.1510217648	-3.0159468698	0.2829715076
F	0.9164251079	-2.3566420267	-1.6453276016
F	-1.0345912240	-3.3137224349	-1.5198309263
C	1.4313781934	1.2033920571	5.0903234206
H	2.3410857824	1.2247515120	4.4996182475
H	1.3506659412	2.0012115490	5.8204620187
H	0.9408625365	-0.8496835585	4.6483344804
H	-0.0632113920	-0.0630847922	5.9883782413
<b>6</b>	<b><math>E_{elec} = -1972.29157922291</math></b>		
C	-0.057848613	0.1953299942	0.0088809359

O	0.394674045	1.9338318456	-2.1524778401
H	1.294723140	1.5634443561	-1.8721574134
O	2.526734382	0.7177937707	-1.4347461175
Re	-1.082792113	1.1930617839	-1.2744188117
N	-2.108982357	2.8700159257	-2.3199508792
N	-1.007303950	2.9073635808	0.2492830383
N	-3.010249861	0.9805288758	-0.1711617402
N	-3.115229804	3.5967790089	-1.7681000567
N	-2.0853635310	3.7061555441	0.4919214838
N	-3.8542729273	2.0186043984	0.0556341620
B	-3.4106904644	3.4666214718	-0.2527219537
H	-4.2535805445	4.2473139250	0.0825968602
C	-1.9269840753	3.3040336721	-3.5760089290
C	0.0285972968	3.4074340200	0.9452868486
C	-3.6228062863	-0.1364153092	0.2480103923
C	-3.5685794154	4.4804301472	-2.6789013646
C	-1.7267174157	4.6939046038	1.3368129395
C	-4.9845882497	1.5570417899	0.6258799768
C	-2.8435693916	4.3220167093	-3.8550445948
C	-0.3856156513	4.5392790318	1.6560908907
C	-4.8822532545	0.1787371731	0.7649416399
H	-2.9599420427	4.8704391702	-4.7770574394
H	0.2130250206	5.1573179161	2.3072407557
H	-5.6124690414	-0.4978710916	1.1810432424
H	-3.1366088791	-1.0953210887	0.1461084834
H	-5.7761935970	2.2400158717	0.8966383702
H	-1.1498349843	2.8695807360	-4.1875161593
H	-4.3664296389	5.1636133985	-2.4263927616
H	1.0064041118	2.9403817775	0.9017846753
H	-2.4502308185	5.4341453835	1.6462208839
C	0.1067036564	-1.2757734151	0.1476536895
H	-0.4124562470	-1.8516988500	-0.6196257262
H	1.1881301105	-1.4835806743	0.1193293829
H	-0.2236766852	-1.5855386261	1.1501529503
H	0.4866951118	0.7468046181	0.7808320385
O	-1.6209044721	-0.1064430554	-2.2070444060
S	3.2055649317	0.6958233226	-0.0913846187
O	2.6247044378	1.6692860897	0.8668464840

O	3.4322792551	-0.6633991850	0.4239842677
C	4.8898017787	1.3821895156	-0.4693406309
F	5.6248624067	1.4358709021	0.6481327441
F	5.5197060854	0.6122430577	-1.3631424885
F	4.7796443251	2.6207194188	-0.9700878694

**6,8-Ts**      $E_{elec} = -1972.21610716983$

C	0.000491792	-0.0008935135	-0.0001401905
O	0.000370474	0.0002960629	1.9647778444
Re	1.609394090	0.0001910625	1.2626269614
O	2.158414663	1.7314365205	1.6144848772
H	2.014041406	2.5347259789	0.9930877499
O	1.741378959	3.6550791125	-0.0085638194
N	3.664340059	-0.4562784045	1.8779111002
N	2.654676237	-0.1480163725	-0.6393798071
N	1.623961621	-2.2316068800	1.2060705503
N	4.4335604060	-1.4355702154	1.3399228532
N	3.4880306827	-1.1895659261	-0.9383815642
N	2.6116193125	-2.9560889867	0.6227191491
B	3.8806700770	-2.2280494396	0.1298075785
H	4.6877106303	-3.0028546790	-0.2936088185
C	4.3805609447	0.1510561823	2.8369937970
C	2.5850264855	0.6452906324	-1.7234044804
C	0.7794549319	-3.0985551180	1.7835168093
C	5.6285790736	-1.4505857273	1.9631062594
C	3.9412422888	-1.0372349006	-2.1986344366
C	2.3874679616	-4.2725922772	0.8300119152
C	5.6358983291	-0.4569888797	2.9343022364
C	3.3867522361	0.1144025402	-2.7377821225
C	1.2164401973	-4.4104747927	1.5590803870
H	6.4391852438	-0.2004815740	3.6072681292
H	3.5436544518	0.5250491022	-3.7229889995
H	0.7472428158	-5.3253887451	1.8861649548
H	-0.0816778309	-2.7350158419	2.3247541504
H	3.0800427899	-5.0091559269	0.4505517140
H	3.9604556621	0.9889632625	3.3729737783
H	6.3890358134	-2.1580404263	1.6669170653
H	1.9653680972	1.5350216087	-1.7345225525



H	4.6320777540	-1.7550252255	-2.6160776741
C	-1.0944923430	-0.9629287429	-0.2218671885
H	-1.0607520231	-1.8559474530	0.3985066285
H	-2.0630042613	-0.4585095416	-0.1081264008
H	-1.0337138024	-1.2483111329	-1.2845101701
H	-0.1023029932	0.9075419443	-0.6041568947
S	0.3682774996	3.5782190669	-0.6248509029
O	0.3666456357	2.8781910839	-1.9336635103
O	-0.6884779334	3.1537808939	0.3110565154
C	0.0023162640	5.3530817562	-1.0339246340
F	-1.2038994946	5.4427149201	-1.6088061344
F	0.0045692385	6.0961242706	0.0786888867
F	0.9189910863	5.8392257729	-1.8801246616

**8**      $E_{elec} = -1972.28564961107$

C	-0.158100961	-0.1427387820	-0.1511298960
O	-0.217859823	-0.1240890589	1.2139412725
Re	1.682279544	0.0768077521	0.8711653678
O	1.945660259	1.7721979299	0.5972098014
H	2.421773182	2.9601155695	1.3937798637
O	2.809310652	3.7548987154	1.9160362223
N	3.966623042	0.2244041028	1.0331897872
N	2.429766670	-1.8490191151	0.1934638890
N	1.845363848	-0.8206499425	2.7688738911
N	4.6772543575	-0.7257192899	1.6969058035
N	3.3079899106	-2.6171103315	0.9059694391
N	2.8562150557	-1.6452958440	3.1624846957
B	3.9702993579	-2.0161260178	2.1683217315
H	4.7479991553	-2.7830320393	2.6601727245
C	4.8164016709	1.2123364824	0.7278689654
C	2.3062119352	-2.4254190850	-1.0164110948
C	1.0546760064	-0.6088758454	3.8363604522
C	5.9663736155	-0.3379205843	1.7973528316
C	3.7152681097	-3.6524071719	0.1506885155
C	2.7003296173	-1.9434511951	4.4650856524
C	6.1021889043	0.9007814911	1.1863476822
C	3.0857529008	-3.5798265148	-1.0868021863
C	1.5562701774	-1.3072849886	4.9354089457

H	6.9985185700	1.4946799923	1.0939551392
H	3.1840446970	-4.2606335604	-1.9179735432
H	1.1510139261	-1.3408912888	5.9347139792
H	0.1885371042	0.0283484499	3.7415315470
H	3.4121586132	-2.5826177788	4.9669521184
H	4.4570136243	2.0901351553	0.2127131976
H	6.6902863632	-0.9666110148	2.2953636491
H	1.6701528447	-1.9790093955	-1.7627351707
H	4.4333281041	-4.3606158170	0.5381948363
C	-0.7385911837	-1.3482345010	-0.8486786152
H	-0.3959415956	-2.2875512547	-0.4079895419
H	-1.8327380166	-1.3158933955	-0.7615861951
H	-0.4993020407	-1.3390729517	-1.9172770171
H	-0.4149514523	0.8145389871	-0.6217015676
S	2.2441929177	3.8311047973	3.3945567659
O	2.3689215585	5.1979931983	3.8681406749
O	1.0038334869	3.0743085614	3.5264337260
C	3.5390383346	2.8380031832	4.2931379878
F	3.2208749261	2.7819334458	5.5886003359
F	3.5797337564	1.5906106644	3.8013740510
F	4.7415166546	3.3962408578	4.1574029426

**6.9-Ts**  $E_{elec} = -2525.4564140584$

C	-0.000015423	-0.0000792751	-0.0010537924
O	-0.002401926	0.0012162359	2.1057666263
S	1.414452683	0.0000056738	2.7418862874
Re	-1.842539108	0.3798022853	-0.6535012461
N	-3.617306779	1.4814781262	-1.3163509431
N	-1.726727358	2.3588921693	0.5290126814
N	-2.926934761	-0.0642205057	1.2082107529
N	-4.525638450	2.0043901541	-0.4505455782
N	-2.828126062	2.8642298900	1.1499993695
N	-3.9527904330	0.7085542100	1.6499867551
B	-4.1732803012	2.1162409141	1.0556040278
H	-5.0407764030	2.6931415176	1.6468358145
C	-4.0545083694	1.7089248890	-2.5614040834
C	-0.7413498623	3.2570527081	0.6680466684
C	-2.8806051862	-1.1539021913	1.9829590920

C	-5.5342669984	2.5543217963	-1.1551150595
C	-2.5313265576	4.0674888436	1.6825606837
C	-4.5380949404	0.1100348560	2.7067488752
C	-5.2811834003	2.3782938391	-2.5111368649
C	-1.2038160929	4.3570778075	1.4031272244
C	-3.8887381677	-1.0929806968	2.9507677554
H	-5.8941337798	2.6962096558	-3.3403100989
H	-0.6495354090	5.2417516896	1.6769385728
H	-4.1124346528	-1.8181026078	3.7179567120
O	-1.1021893359	1.3246254009	-2.1396618598
H	-2.1308296853	-1.9092394200	1.8063683970
H	-5.3654091007	0.5852227323	3.2127656552
H	-3.4567980090	1.3908190526	-3.4027701331
H	-6.3540329339	3.0397588854	-0.6459296079
H	0.2396487462	3.0827682728	0.2415992365
H	-3.2857500951	4.6296363957	2.2135042895
C	0.7159546772	-1.2876286620	-0.2631174275
H	0.0781122001	-2.1622858221	-0.1230988206
H	1.0089619179	-1.2382126180	-1.3214738266
H	1.6475530349	-1.3805153799	0.3003844960
H	0.6595466845	0.8549702517	0.1029513868
C	1.8893156523	1.7358364424	3.0075121446
H	1.0548081668	2.2727069550	3.4649478811
H	2.7749557209	1.7536116190	3.6491339312
H	2.1322275398	2.1461461165	2.0224075185
C	1.1031840277	-0.4727895894	4.4721228526
H	2.0389156230	-0.4057923168	5.0330414084
H	0.3424424842	0.1875364219	4.8938029960
H	0.7456773555	-1.5035758565	4.4646965004
O	-2.2487806107	-1.1817544878	-1.1439183172
H	-0.1188997362	1.3472336628	-2.2169653986
O	1.6292972094	1.2692693756	-2.2328152898
S	2.7121389910	1.6183601809	-1.2661765622
O	2.2291414518	2.4652086496	-0.1324715158
O	3.5809279940	0.4988771189	-0.8697229482
C	3.7974583159	2.7722020586	-2.2358804831
F	4.8214024625	3.1880890780	-1.4765947433
F	4.2899418536	2.1546713438	-3.3163073752

F	3.1004678609	3.8448761166	-2.6355981997
<b>9</b>	<b><math>E_{elec} = -2525.46585296618</math></b>		
C	-0.082167655	-0.0047484643	0.0883622559
O	-0.025656100	0.1508389503	1.5975916992
S	1.451896236	0.1648759249	2.3160943334
Re	-2.048756938	0.3959895444	-0.6107640694
N	-3.706225862	1.5528062928	-1.3596154389
N	-1.729690810	2.5098627839	0.3337514602
N	-3.082365672	0.2591600609	1.3164100382
N	-4.560666472	2.2266297936	-0.5407803602
N	-2.774110545	3.1602485803	0.9172905627
N	-4.0251524364	1.1596517015	1.6964774809
B	-4.1653750535	2.4967539939	0.9355473168
H	-4.9814538778	3.1970990749	1.4646813905
C	-4.1691802174	1.6569584816	-2.6120602280
C	-0.7003415411	3.3663726251	0.3011766091
C	-3.0986828795	-0.7361151142	2.2121357500
C	-5.5574605893	2.7470997714	-1.2833620347
C	-2.3958944967	4.4106248035	1.2592678538
C	-4.6163170228	0.7400359495	2.8336915178
C	-5.3559238687	2.3968564033	-2.6139249100
C	-1.0705478009	4.5839109014	0.8906689664
C	-4.0595060807	-0.4791969517	3.1972958127
H	-5.9758739833	2.6498300649	-3.4601559564
H	-0.4589161338	5.4649931173	1.0098279762
H	-4.3173549319	-1.0932055349	4.0466326436
O	-1.1878196685	1.1172359048	-2.1768320440
H	-2.4347597512	-1.5785496546	2.0906705336
H	-5.3818718415	1.3392801043	3.3042000750
H	-3.6166258964	1.2044535402	-3.4222344361
H	-6.3330158896	3.3381794170	-0.8182652830
H	0.2472271878	3.0998729578	-0.1459591029
H	-3.0978231061	5.0836137859	1.7301419744
C	0.4553625521	-1.3738292120	-0.3067162250
H	-0.1463017369	-2.1857960654	0.1117043367
H	0.4249261074	-1.4577613001	-1.3967331493
H	1.5053170148	-1.4862468388	-0.0103817093

H	0.5866712262	0.7516625435	-0.3054539613
C	1.7637031254	1.9188367105	2.6419983312
H	0.8599014540	2.3705491880	3.0547598199
H	2.5959025592	1.9653195035	3.3506817153
H	2.0610422928	2.3863670599	1.6975556939
C	0.8709760773	-0.3522423992	3.9526721026
H	1.6814688678	-0.2041621708	4.6700518104
H	-0.0096447266	0.2329342720	4.2237913839
H	0.6194970353	-1.4114152544	3.8876428576
O	-2.5414802919	-1.1885493460	-0.9085437883
H	-0.2122292646	1.1214953548	-2.2009456939
O	1.8103523466	1.6011754201	-2.0193794963
S	2.7992654911	1.8746546914	-0.9470522879
O	2.6063608503	3.1684807802	-0.2400698881
O	3.0390061219	0.7319576574	-0.0188622861
C	4.4096464092	2.0653340969	-1.8534829772
F	5.4019709171	2.3084333394	-0.9841025307
F	4.6994244922	0.9461500425	-2.5290210701
F	4.3407893544	3.0837996989	-2.7185788539

**9,10-Ts**  $E_{elec} = -2525.44499501224$

C	0.050417337	-0.0674547997	-0.0018209807
O	-0.061466813	-0.0222150999	1.3554001315
S	1.652233262	-0.0544745438	2.4105803960
Re	-2.034100077	0.3874347892	-0.5148545553
N	-3.699852876	1.4338051604	-1.3439455383
N	-1.719414487	2.5151563336	0.3030789893
N	-3.079740080	0.3623450004	1.4170307091
N	-4.555855601	2.1727784931	-0.5844411474
N	-2.776000072	3.2063256770	0.8193049330
N	-4.0396447340	1.2718991454	1.7227053095
B	-4.1701653717	2.5537445081	0.8717694472
H	-4.9886141999	3.2933212147	1.3381194306
C	-4.1511731494	1.4451271711	-2.6068074760
C	-0.6727209557	3.3537886356	0.2770237680
C	-3.0957243696	-0.5744977925	2.3737815278
C	-5.5416600504	2.6395631339	-1.3730566610
C	-2.3867714321	4.4625349191	1.1230775292

C	-4.6433774028	0.9177722233	2.8753252372
C	-5.3314039916	2.1882883416	-2.6727931432
C	-1.0459458162	4.5991724809	0.7986369973
C	-4.0760747831	-0.2673840294	3.3248901014
H	-5.9429330848	2.3802810200	-3.5407900861
H	-0.4220624211	5.4728395740	0.9062074103
H	-4.3373162094	-0.8273896493	4.2096054390
O	-1.2320575219	1.0014876811	-2.1507385160
H	-2.4152962024	-1.4103017635	2.3156947146
H	-5.4233376713	1.5356037138	3.2953483841
H	-3.5936325200	0.9323659288	-3.3761661525
H	-6.3169402852	3.2691966013	-0.9610985043
H	0.2870501229	3.0565887637	-0.1203483551
H	-3.0929779033	5.1653801155	1.5407161993
C	0.5414089782	-1.3759895910	-0.5907612405
H	-0.0194106019	-2.2294189544	-0.1993236449
H	0.4541550599	-1.3627330556	-1.6803842483
H	1.6072648977	-1.4828512706	-0.3494549186
H	0.5920771349	0.7787395497	-0.4161687072
C	1.7549126499	1.7243065998	2.7357549389
H	0.7466332066	2.1130520421	2.8932197780
H	2.3787852295	1.8807475533	3.6201572405
H	2.2143998970	2.1899247173	1.8598023221
C	0.7388815384	-0.6047269437	3.8749875428
H	1.2940933693	-0.3372938737	4.7770046443
H	-0.2500904142	-0.1406094014	3.8750757469
H	0.6420422423	-1.6898548576	3.8120587134
O	-2.5284017514	-1.2161106447	-0.6726045575
H	-0.2588507664	1.0708595432	-2.1955312784
O	1.7034973361	1.8162319183	-1.9577711831
S	2.7713984589	1.9735800392	-0.9324507015
O	2.6568894003	3.2090251220	-0.1179993358
O	3.0397783624	0.7491986065	-0.1288392813
C	4.3135546156	2.2037816435	-1.9415941099
F	5.3743449682	2.3613772923	-1.1366548768
F	4.5251067355	1.1347747140	-2.7209767985
F	4.2031006132	3.2869243581	-2.7212380680

**10**      $E_{elec} = -2525.50956007869$

C	0.482147875	-0.8807315354	-0.3112788876
O	-0.439711953	-0.1528082597	0.1353025564
S	2.712676115	0.5260110076	3.7939968987
Re	-2.136862444	0.6606691058	-0.8698471049
N	-3.676081006	1.8912875784	-1.4733589522
N	-1.937516379	2.2756600150	0.7007749054
N	-3.348092931	-0.0736897577	0.8069676349
N	-4.620135398	2.3445394899	-0.5936797112
N	-3.053071527	2.7693678506	1.3070076887
N	-4.3685071535	0.6732022976	1.3018354258
B	-4.4294749556	2.1717467620	0.9471252459
H	-5.3192823178	2.7204666286	1.5302458166
C	-3.9522875357	2.4092530351	-2.6844390277
C	-0.8852745038	2.9733334532	1.1537063071
C	-3.4116533100	-1.2764843309	1.3895522482
C	-5.4786142905	3.1336178484	-1.2600893258
C	-2.6995876276	3.7650862653	2.1451349469
C	-5.0592182571	-0.0538249936	2.2043716397
C	-5.1019439236	3.1908590103	-2.6013481179
C	-1.3221336641	3.9273358747	2.0820881366
C	-4.4865031700	-1.3157808760	2.2857505925
H	-5.5900986315	3.7331840996	-3.3960973972
H	-0.7192145882	4.6445120870	2.6174399748
H	-4.8002634005	-2.1423287250	2.9042728769
O	-1.0936551871	1.7687348638	-2.0019228720
H	-2.6996018381	-2.0447996633	1.1275168427
H	-5.8990470734	0.3785070920	2.7280671363
H	-3.3014921680	2.1904153421	-3.5173963045
H	-6.2919966611	3.6151014147	-0.7369897646
H	0.1135134509	2.7806468382	0.7806515504
H	-3.4504142911	4.2883256157	2.7192719982
C	1.1447300450	-1.8548419005	0.6014728844
H	1.2985394091	-1.4033435654	1.5847434474
H	0.4703389057	-2.7170145263	0.7064754605
H	2.0927057120	-2.1926164061	0.1846707829
H	0.6356996435	-0.9545421644	-1.3923285744
C	3.6848373810	1.5772730958	2.6603695681

H	3.0343687688	2.1658546167	2.0108364262
H	4.3597151469	2.2293292748	3.2221292925
H	4.2719398957	0.9080953673	2.0291589469
C	1.7413798473	1.8087555195	4.6549622187
H	2.3954980909	2.5182722479	5.1702878744
H	1.0912294966	2.3457226953	3.9585094360
H	1.1209574853	1.3006367186	5.3971690421
O	-2.6153540898	-0.7501688407	-1.6681930604
H	-0.1136610825	1.6384754897	-2.0623691546
O	1.5469320053	1.4037830590	-2.3233921381
S	2.3551700852	1.5484459842	-1.0805695722
O	2.0626646886	2.7443257366	-0.2668866931
O	2.4411331683	0.2699232863	-0.3054474041
C	4.0929927525	1.7911421287	-1.6938785536
F	4.9320085765	1.8868747631	-0.6524351196
F	4.4675605522	0.7562395694	-2.4542393828
F	4.1729482645	2.9118818266	-2.4170302980

***II*  $E_{elec} = -1010.59633886752$**

H	0.232643002	-0.0547874083	-1.3150728722
C	0.077218916	-0.0780007537	1.5782710670
O	1.056101809	0.4236656506	-1.1508713159
Re	1.452485658	0.9308224836	0.6571426842
N	3.335177853	1.4671225421	-0.2595344037
N	2.688899374	-1.0102118259	0.7224322068
N	2.526083624	1.1889308834	2.5315954668
N	4.556763490	1.2202699386	0.2872728125
N	3.979828725	-1.0242906983	1.1591578424
N	3.8580471781	0.9554093366	2.6751323281
B	4.6676411879	0.3079948895	1.5341576426
H	5.8059657409	0.1454514871	1.8518095586
C	3.5227795456	2.1347169082	-1.4159597845
C	2.4445274245	-2.2211776237	0.1883464922
C	2.0772669332	1.7031133499	3.6942058986
C	5.5028730970	1.7398935153	-0.5155535997
C	4.5249792767	-2.2320006230	0.9134708437
C	4.2370391263	1.3124119020	3.9151695726
C	4.8867420667	2.3408476234	-1.6104705725



C	3.5717509564	-3.0360086532	0.3010307287
C	3.1302592006	1.8029886013	4.6002010118
H	5.3631664356	2.8547670369	-2.4309600038
H	3.6826538095	-4.0587455152	-0.0243769240
H	3.0960324095	2.1810900430	5.6101595862
O	0.7641483762	2.4588723994	0.8128462080
H	1.0420334995	1.9907901334	3.8055306092
H	5.2638284397	1.1900992319	4.2274383573
H	2.6782910830	2.4194923707	-2.0254571839
H	6.5481801209	1.6464114149	-0.2586397546
H	1.4860438425	-2.4449653400	-0.2564489036
H	5.5521226382	-2.4333942567	1.1810573241
H	-0.7326857631	0.6019959247	1.8701737157
C	-0.1538388121	-1.4359467490	2.1134711333
H	-1.1005341655	-1.8186061564	1.6999169502
H	0.6462126215	-2.1477604918	1.9259446958
H	-0.3346498285	-1.3640359448	3.1965290901

**12**      $E_{elec} = -1087.04741390915$

H	1.174214461	0.0850127864	-1.7457572782
C	-0.034207200	-0.2665415136	1.5794219089
O	0.589190778	0.3947273958	-1.0385398015
Re	1.451598105	1.0947262678	0.7366836209
N	3.199571532	1.5881147350	-0.3656714876
N	2.626617243	-0.9409654873	0.6184225718
N	2.545968947	1.1383396880	2.5033872486
N	4.460402396	1.3571124518	0.0902627374
N	3.961193303	-0.9333441050	0.9029748797
N	3.9041772638	0.9666947659	2.5147955250
B	4.6528508288	0.3907743328	1.2812732936
H	5.8099413425	0.2359778954	1.5295859932
C	3.3030128311	2.3470312444	-1.4788729014
C	2.2952622474	-2.2203032089	0.3608545306
C	2.1681314558	1.4363102028	3.7652410071
C	5.3431939035	1.9528335634	-0.7294168894
C	4.4518364718	-2.1862104851	0.8217833414
C	4.3535293729	1.1413563704	3.7690619720
C	4.6461109322	2.6069660108	-1.7424231735

C	3.4179443723	-3.0444795759	0.4715623011
C	3.2814736738	1.4609563494	4.5980789315
H	5.0577873051	3.1907072899	-2.5511080390
H	3.4710390093	-4.1120012024	0.3233159470
H	3.3095980032	1.6800311914	5.6541853701
O	0.7280836658	2.5919236855	0.9402267828
H	1.1339508779	1.6450356777	3.9917609405
H	5.4028081677	1.0157788655	3.9937650050
H	2.4171351634	2.6816787837	-2.0004643071
H	6.4046133655	1.8702527179	-0.5449193524
H	1.2717135346	-2.4787196289	0.1321529600
H	5.4960476404	-2.3805462928	1.0198970232
H	0.4477504810	-0.9629323068	2.2703401479
C	-1.1783966274	0.4748678267	2.2713759326
H	-0.8250462579	1.0368349597	3.1389205342
H	-1.6783233987	1.1783110538	1.5998641827
H	-1.9218542459	-0.2450784181	2.6436713877
H	-1.5175897152	-1.2793579228	0.6404487570
H	-0.0662223799	-0.3271852837	-0.7156624461
O	-0.5855230070	-1.0745102921	0.4760891968

**12,13-Ts**  $E_{elec} = -1086.98294504749$

C	0.003692703	-0.0008071646	-0.0041453531
H	-0.002107874	-0.0016498557	1.4501898717
O	0.591128776	-0.0018151233	2.5209933347
Re	1.382049168	1.5076902862	1.3193902499
H	0.128088446	0.3289299194	3.3069955498
N	1.670865563	2.7637646924	2.9482749832
N	-0.753967573	2.4147382274	1.7527391932
N	1.330393440	3.0835269857	-0.0090780721
N	1.374619917	4.0940818698	2.8998404290
N	-0.8508367088	3.7667938794	1.8803307417
N	1.0659727637	4.3610922763	0.4026408505
B	0.4304264003	4.6229138465	1.7925743027
H	0.2033616024	5.7849346342	1.9400124667
C	2.3466051235	2.5343743294	4.0919155193
C	-1.9858551142	1.9201415116	1.9785641691
C	1.7042235349	3.1414937590	-1.3078910024

C	1.8384666908	4.6828875893	4.0161207678
C	-2.1199577771	4.1103261721	2.1758312497
C	1.2594739016	5.1962664039	-0.6296783821
C	2.4747517538	3.7251525901	4.8022309918
C	-2.8854169288	2.9533942619	2.2485770332
C	1.6802493242	4.4622958404	-1.7386714261
H	2.9637245278	3.8750353539	5.7522271152
H	-3.9402517728	2.8733871682	2.4614483169
H	1.9334824153	4.8403712095	-2.7170005738
O	3.0542877361	1.2726901183	1.2886401441
H	1.9785113644	2.2379943315	-1.8307834843
H	1.0779851458	6.2553858025	-0.5164249919
H	2.7220292844	1.5460295856	4.3161872845
H	1.6794815334	5.7382656011	4.1837548009
H	-2.1750492004	0.8571012446	1.9313300605
H	-2.3911288518	5.1470856921	2.3130446466
H	-0.1752539097	-1.0759849164	0.1460543970
C	-1.0003548847	0.5730155927	-0.9736174327
H	-2.0110784306	0.4291771126	-0.5812958138
H	-0.8546874717	1.6415970798	-1.1406325994
H	-0.9416707585	0.0540131431	-1.9373421525
H	1.8980131387	-0.6419070297	-0.3682170194
O	1.3744407760	0.1649752968	-0.5009941423

**13**  $E_{elec} = -1087.07289371846$

O	1.269710458	-0.2516256468	-1.0283364398
Re	1.498928082	0.6733492972	0.3608758893
N	3.146415891	1.7177526038	-0.2766586065
N	2.786616646	-0.8974477407	1.0939588408
N	2.190883586	1.4738001583	2.3586427919
N	4.362642817	1.5904532186	0.3419074365
N	4.062264284	-0.6361674834	1.4893385855
N	3.510916754	1.4596840138	2.6887920067
B	4.507832553	0.8265421868	1.6963341488
H	5.6337155425	0.8904397419	2.0865767214
C	3.3162734492	2.5270635021	-1.3491428788
C	2.6332425272	-2.2337912429	1.0923327970
C	1.5354083236	2.0833364194	3.3623226643

C	5.2655699721	2.3154208613	-0.3334175636
C	4.6933084947	-1.7974241807	1.7524342483
C	3.6801486273	2.0479430262	3.8885115306
C	4.6452377939	2.9213232754	-1.4278955309
C	3.8171413637	-2.8474725949	1.5052995177
C	2.4375096794	2.4598417321	4.3593863420
H	5.1028263631	3.5543640146	-2.1721744620
H	4.0129531771	-3.9040159132	1.6031927716
H	2.2232980741	2.9652827004	5.2883511304
H	0.4661111067	2.2229048936	3.3043186210
H	4.6652945986	2.1378929766	4.3229804268
H	2.4844415406	2.7452570435	-2.0039304232
H	6.2901053417	2.3643597276	0.0063837148
H	1.7055276437	-2.6804990187	0.7633698116
H	5.7161684771	-1.7987983244	2.0998968423
O	0.3933410227	2.2450949657	0.3505461157
H	0.8392875259	3.0865645117	0.1713932653
C	-1.5948299243	0.1008135679	0.9835886023
H	-1.7541389775	-0.6154314883	0.1718396094
H	-1.6270569282	1.1148754120	0.5884232550
C	-2.5400554612	-0.1090903622	2.1466085052
H	-3.5688798854	0.0195189388	1.7963963483
H	-2.4623108644	-1.1212417414	2.5600545615
H	-2.3591706911	0.6168658606	2.9438534409
O	-0.1926889653	-0.0533266915	1.4311624670
H	-0.0776177743	-0.8559692122	1.9601344102

**14**  $E_{elec} = -1067.19251416734$

H	1.375565068	0.2970850419	-1.8225494127
C	-0.169240667	-0.2924367716	1.3814797879
O	0.782261066	0.2198917181	-1.0626699910
Re	1.440543222	0.9812410815	0.6359160397
N	3.235130535	1.5387174728	-0.3679829103
N	2.696200110	-0.9756826422	0.7058006017
N	2.495806313	1.1945163706	2.4999822861
N	4.474034728	1.3272656679	0.1601222308
N	4.005358274	-0.9396266383	1.0706971412
N	3.8473880805	1.0323380980	2.5806646974

B	4.6454244476	0.4197074437	1.4111255722
H	5.8006201242	0.3095110249	1.6931512903
C	3.3949339174	2.2749417012	-1.4889391878
C	2.4286767929	-2.2440066798	0.3518843857
C	2.0872083338	1.6974152789	3.6801347655
C	5.3928088916	1.9192263865	-0.6217062925
C	4.5464385317	-2.1687596125	0.9574393591
C	4.2692398829	1.4069693933	3.8040303969
C	4.7468601859	2.5459510857	-1.6852805408
C	3.5662880382	-3.0413193818	0.5017320118
C	3.1764136244	1.8486448821	4.5385280430
H	5.1970650266	3.1195612379	-2.4805885882
H	3.6657386133	-4.0969636553	0.3016774921
H	3.1716784399	2.2284566202	5.5484582432
O	0.6665159957	2.4499333306	0.8995816816
H	1.0504375824	1.9509290673	3.8372333988
H	5.3133589073	1.3273398939	4.0690339272
H	2.5355112033	2.5898875454	-2.0644737629
H	6.4430170178	1.8563365756	-0.3756650113
H	1.4488193439	-2.5192621876	-0.0093517934
H	5.5850454166	-2.3365937189	1.2028086309
H	0.1958211743	-1.3197085657	1.4210591728
C	-0.8215624523	0.0599566294	2.7140959805
H	-0.0912910806	-0.0599923261	3.5165518239
H	-1.1815019240	1.0945368302	2.7357627944
H	-1.6653300317	-0.6037810674	2.9483644401
N	-1.2614120209	-0.3261301737	0.2945077361
H	-1.8257673020	0.5260305834	0.3355271569
H	-0.7349827422	-0.3193540361	-0.6152235236
H	-1.8934926426	-1.1274279350	0.3639018866

**14,15-Ts**  $E_{elec} = -1067.13192162962$

N	0.003667792	0.0989063776	-0.0220569034
H	0.049123241	-0.0627890961	1.3982210047
O	0.687870923	-0.2308700510	2.2962681535
Re	2.372242703	0.2168874429	1.7531376343
H	1.741436154	2.1051482598	0.1836621439
C	1.435790714	-0.3388172430	-0.1676941398

O	2.271552077	1.9614064866	0.9820312062
N	3.632557630	1.3446517819	3.0431126145
N	4.239618518	-0.4310381010	0.9589718383
N	2.7492393652	-1.4325524066	3.0955782036
N	4.7249233469	0.7982505117	3.6517382822
N	5.3092978743	-0.7029403892	1.7645944436
N	3.9825203138	-1.5987898192	3.6615768125
B	5.1423563028	-0.6426789740	3.3012850422
H	6.1494668557	-0.9552404234	3.8608753191
C	3.5061925311	2.6092847826	3.4976494154
C	4.6584208010	-0.6063274003	-0.3176059836
C	1.9444932260	-2.3907781222	3.6094308217
C	5.2607119304	1.7019103886	4.4892648538
C	6.3631522405	-1.0450203955	1.0101473601
C	3.9493819234	-2.6498878271	4.4953463006
C	4.5117652473	2.8757563099	4.4221683295
C	5.9944470124	-0.9854439374	-0.3333969358
C	2.6618786805	-3.1891714559	4.4909912432
H	4.6777093072	3.7895909004	4.9713614483
H	6.6127828100	-1.1876475741	-1.1941331181
H	2.3051192277	-4.0347002287	5.0586129083
H	0.9041650278	-2.4207107652	3.3260210727
H	4.8347429475	-2.9450816955	5.0403629365
H	2.7131263922	3.2385687070	3.1242600796
H	6.1321109993	1.4543904665	5.0786320882
H	3.9909858922	-0.4338697257	-1.1466602526
H	7.3031436876	-1.3118895353	1.4715392162
H	1.9036664710	0.1838704679	-1.0094676218
C	1.4459525889	-1.8473697060	-0.4049094427
H	2.4624876706	-2.2427281637	-0.4420167944
H	0.9145944890	-2.3755856352	0.3929025197
H	0.9572331022	-2.0974818867	-1.3578314050
H	-0.1585371429	1.0697218973	-0.2802001159
H	-0.6312658020	-0.4703018244	-0.5811647457

**15**  $E_{elec} = -1067.18913576917$

H	0.133521130	-0.0920154313	-1.4480412283
C	-0.081084966	-0.5142873515	1.2123363418

O	1.011151522	0.2841824193	-1.2642119494
Re	1.410889870	0.8851781118	0.5172729129
N	3.249146683	1.5116953271	-0.3212642726
N	2.666486478	-0.9009371049	0.7981621717
N	2.202877948	1.2867651073	2.4907691557
N	4.426621089	1.4572932053	0.3623961147
N	3.932544464	-0.7793093987	1.2857761356
N	3.5469623548	1.2183746308	2.7203728079
B	4.4908897035	0.6153252734	1.6585746465
H	5.6084128255	0.5425103593	2.0724553994
C	3.5029551079	2.0496669824	-1.5293137972
C	2.4997240625	-2.1903146924	0.4486971116
C	1.6489483121	1.8125041639	3.6019780243
C	5.4091462589	1.9545307472	-0.4147114932
C	4.5420274825	-1.9787166910	1.2511463857
C	3.8187570669	1.6751610023	3.9551123810
C	4.8607646009	2.3615828302	-1.6258194119
C	3.6605023542	-2.9134953554	0.7203641996
C	2.6294398570	2.0761068863	4.5557765722
H	5.3761812217	2.8074982863	-2.4623621040
H	3.8378602585	-3.9644835077	0.5521999561
H	2.4987564644	2.4998513011	5.5394111817
H	0.5873207143	2.0039245223	3.6574216845
H	4.8333675865	1.6822519628	4.3260286396
H	2.7055730010	2.1621566269	-2.2493982659
H	6.4296050817	1.9755430445	-0.0602665057
H	1.5732370437	-2.5272011437	0.0092866496
H	5.5572358683	-2.0856306621	1.6046442519
H	-0.4360823816	-1.1427347502	0.3927128963
C	-0.0345097204	-1.2155256911	2.5471201644
H	0.6548272354	-2.0609296676	2.5036096805
H	0.3018714624	-0.5561257778	3.3496802335
H	-1.0261165947	-1.6078295893	2.8048924996
N	-0.6315343949	0.7914396253	1.1588541598
H	-1.2935639581	1.0187281544	0.4194697074
H	-0.8814099814	1.2504253677	2.0308666668
O	0.8973898429	2.7127263251	0.4315806846
H	1.6289085134	3.2789308651	0.1363843998

15,16-Ts

$E_{elec} = -1067.1189723782$

C	0.043242892	0.0041522642	0.0204682484
H	0.003195194	-0.0218818281	1.4896039725
O	0.484837384	-0.0160003387	2.7028144999
Re	1.761346294	0.4250742327	1.4978535010
N	2.934277768	0.4193187270	3.2845276465
N	1.573361300	2.5375136035	1.7045307963
N	3.779586212	1.0329221466	0.8051628522
N	3.684992870	1.4861621053	3.6754594105
N	2.541149501	3.2761130105	2.3287342114
N	4.4807077510	2.0309913161	1.4025944734
B	3.9112732203	2.6546859178	2.6960563437
H	4.6424761415	3.4793563835	3.1533749755
C	2.9620161229	-0.4849350707	4.2778461399
C	0.5249706678	3.3664544518	1.5010406881
C	4.5457617049	0.5446430840	-0.1903682721
C	4.1955277294	1.2396522287	4.8989299740
C	2.1045534960	4.5335502184	2.4970157602
C	5.6685538366	2.1738739988	0.7876075540
C	3.7537020294	-0.0070958217	5.3242025056
C	0.8127210850	4.6364538239	1.9871496730
C	5.7496144028	1.2457365816	-0.2459769333
H	3.9725334899	-0.4970949643	6.2602076242
H	0.1758673210	5.5073063981	1.9792236768
H	6.5688357450	1.0952354587	-0.9319472461
H	4.2051278128	-0.2909029440	-0.7835192451
H	6.3760247186	2.9157851295	1.1285628732
H	2.3924037914	-1.3992265227	4.1992954880
H	4.8392032417	1.9625884961	5.3787338966
H	-0.3867410253	3.0006410034	1.0571566599
H	2.7379560244	5.2736134974	2.9643324117
H	0.0210587607	-1.0729471765	-0.1571293851
C	-1.2550630696	0.7017913512	-0.3543024963
H	-2.0590567112	0.4089545084	0.3271895587
H	-1.1727138869	1.7913319510	-0.3262092978
H	-1.5612248199	0.4145301083	-1.3667018464
N	1.2756114860	0.5464516812	-0.5650222155



H	1.7860718523	-0.1145070085	-1.1512085940
H	1.1933747041	1.4622446906	-1.0037303182
O	2.3730971565	-1.2955197265	0.8120627259
H	3.1345686146	-1.6475435245	1.2966011128

**16**  $E_{elec} = -1067.21726715633$

O	1.025854291	-0.0487835170	-0.9841815384
Re	1.466793446	0.8026027638	0.3977337743
N	3.211474691	1.7028207792	-0.2659172682
N	2.619691379	-0.9000344100	1.0411552528
N	2.330640902	1.4992436109	2.4027966045
N	4.428631530	1.4359534503	0.3004858033
N	3.932987766	-0.7837954403	1.3831017551
N	3.651927751	1.3149626677	2.6728231361
B	4.537177888	0.6124500414	1.6192991613
H	5.6755285747	0.5429582651	1.9712432062
C	3.4242076965	2.5312782598	-1.3153123995
C	2.3300952102	-2.2138231344	1.0173888726
C	1.8160766687	2.2051966678	3.4266385651
C	5.3774087016	2.0918028045	-0.3842915836
C	4.4510862652	-2.0100468140	1.5888445045
C	3.9567463420	1.8874886509	3.8532301343
C	4.7831318334	2.7954473799	-1.4330832503
C	3.4611948291	-2.9571702497	1.3570282023
C	2.8053503512	2.4648852348	4.3770090689
H	5.2751053783	3.4071338602	-2.1734546281
H	3.5501778623	-4.0306184192	1.4206436309
H	2.7043352973	3.0032636152	5.3066920237
H	0.7780566164	2.5058099820	3.4195793576
H	4.9661931125	1.8522100486	4.2367592357
H	2.5964089781	2.8561149131	-1.9300610885
H	6.4129395677	2.0261587838	-0.0824623659
H	1.3463776906	-2.5545256438	0.7301207459
H	5.4814919976	-2.1251031726	1.8921772266
N	-0.3289193588	0.3378257842	1.5710641807
H	-0.7714958843	1.2575047877	1.6678428672
H	-0.0764461695	0.0265046659	2.5104582729
O	0.5512627155	2.5017038617	0.4956639530

H	1.0812034525	3.2845660248	0.2843174438
C	-1.3327474954	-0.6207046594	0.9907564878
H	-0.8326684220	-1.5855928199	0.8790391963
H	-1.5729215397	-0.2581194222	-0.0109705424
C	-2.5801166293	-0.7433067671	1.8575052236
H	-3.2785798557	-1.4480474960	1.3968389889
H	-2.3427926403	-1.1175605037	2.8593027406
H	-3.0955733935	0.2175742926	1.9576089564