Supplementary Information for:

Reaction of phosphinylated nitrosoalkenes with electron-rich heterocycles. Electrophilic aromatic substitution *vs* cycloaddition.

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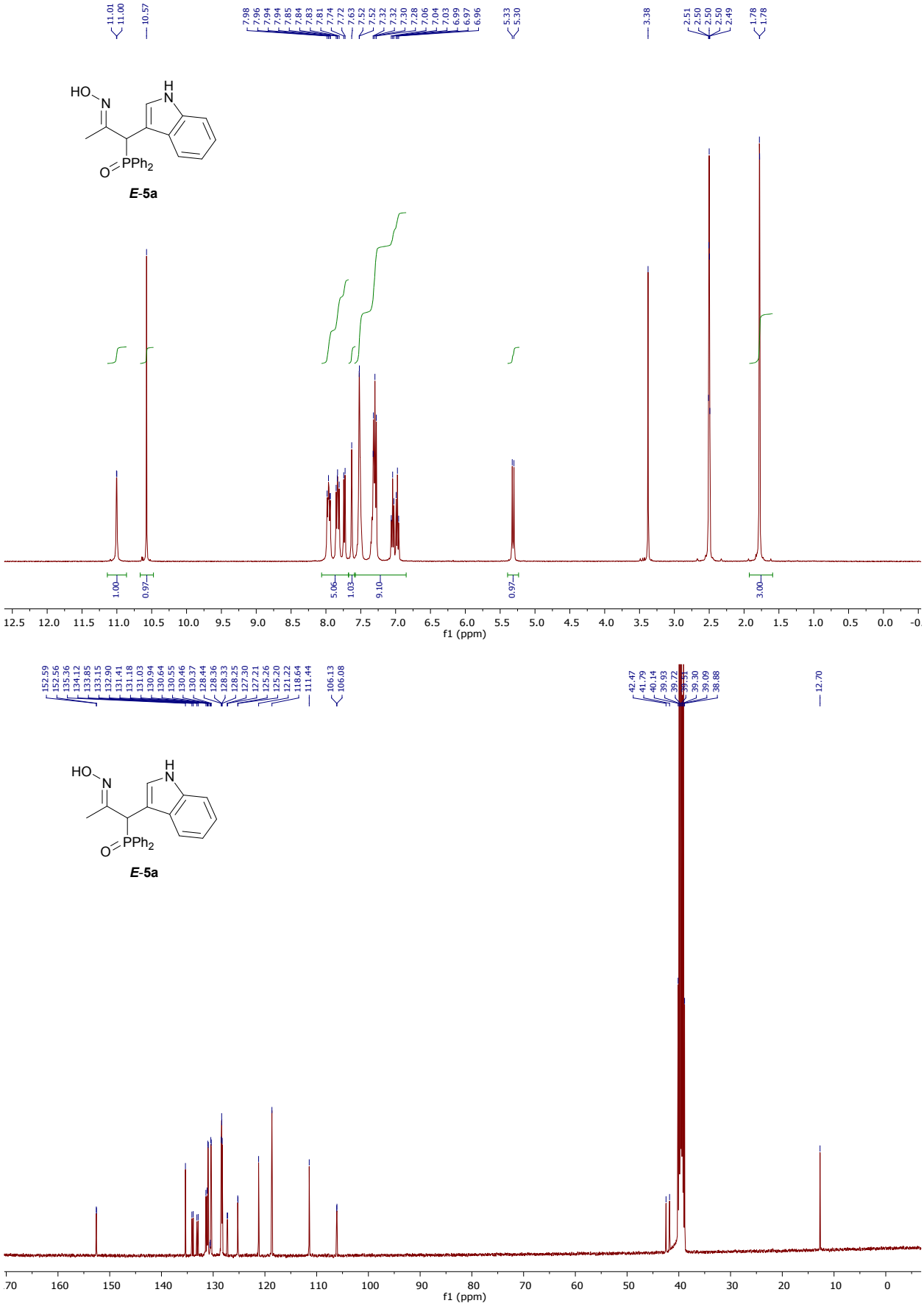


Figure 1. ^{1}H NMR and ^{13}C NMR spectra of compound ***E*-5a** (DMSO-d6).

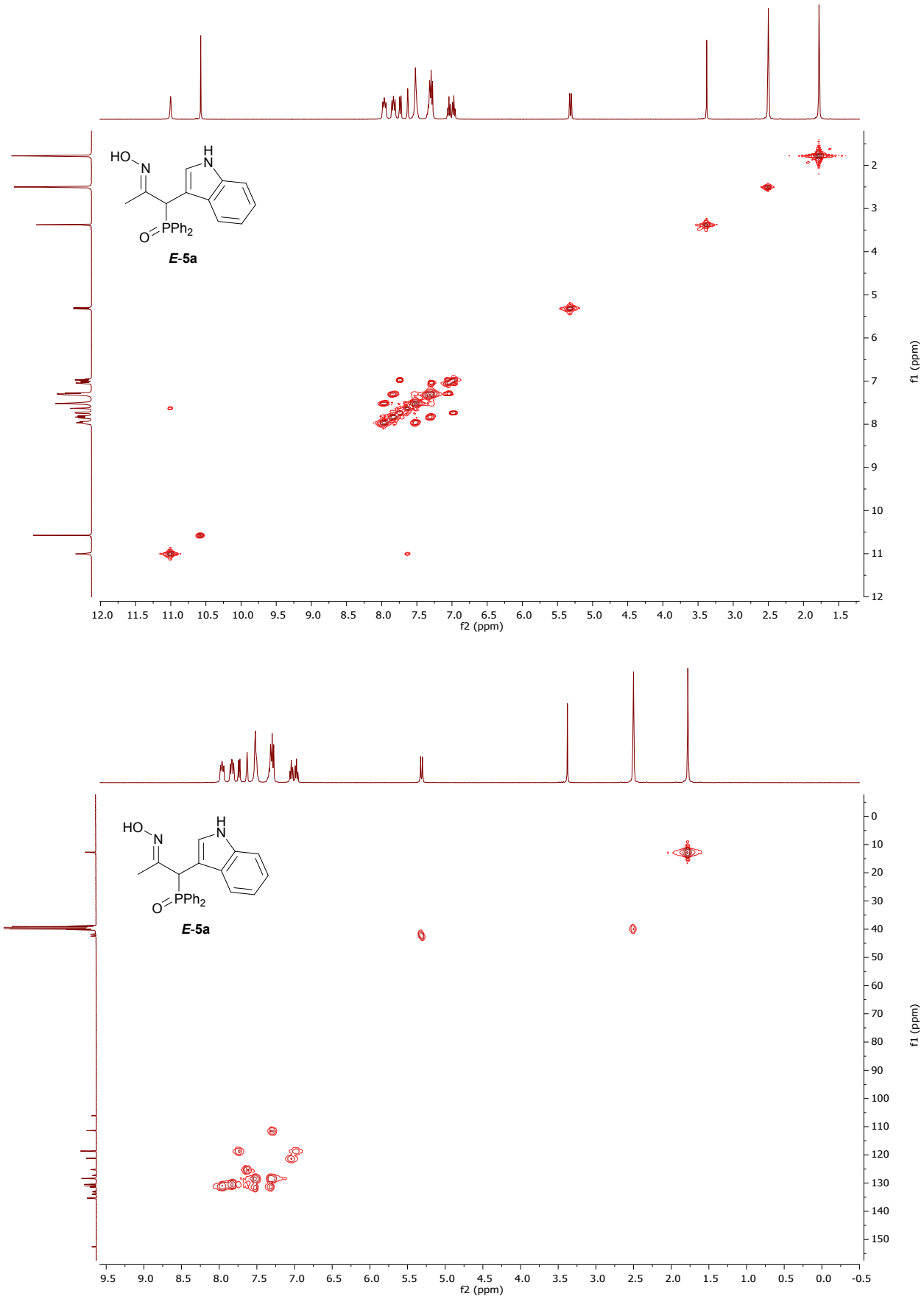


Figure 2. COSY and HMQC spectra of compound ***E*-5a** (DMSO-d6).

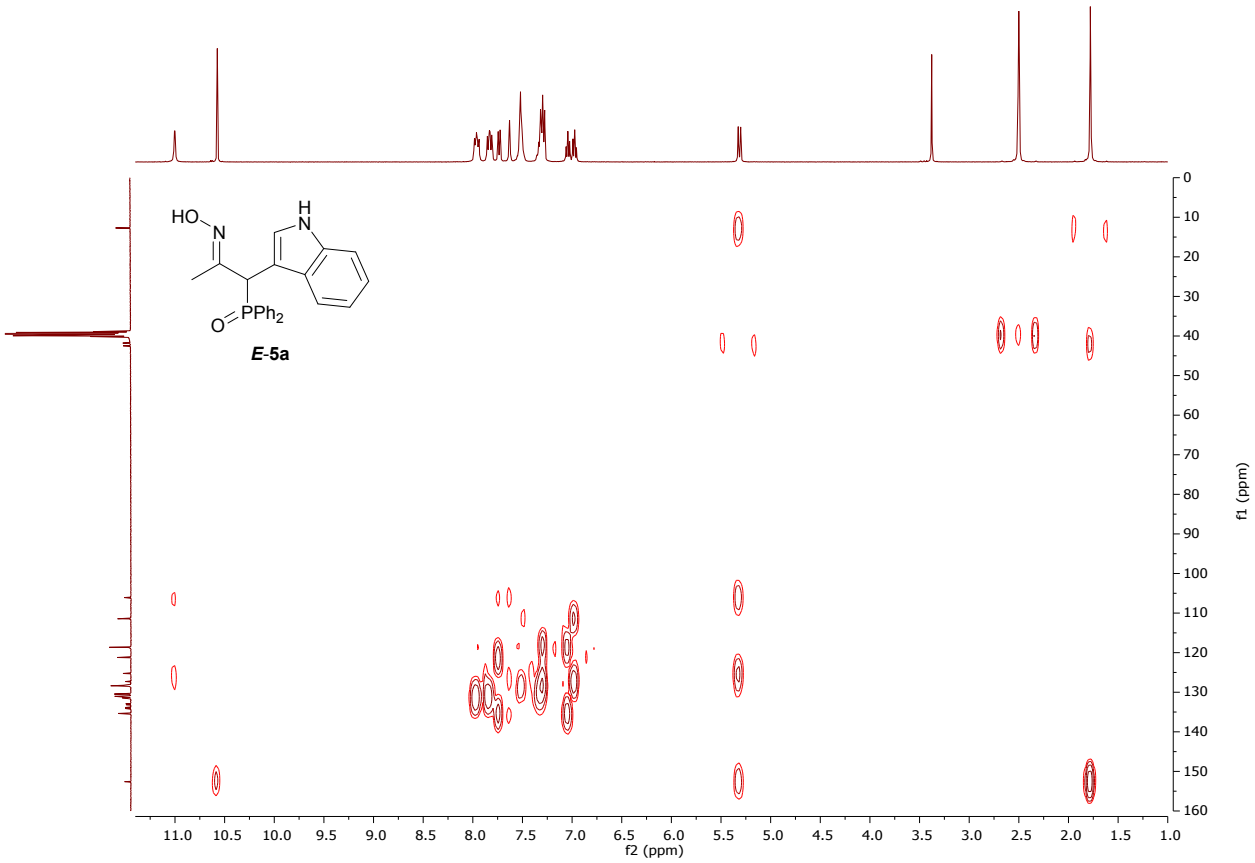


Figure 3. HMBC spectra of compound ***E*-5a** (DMSO-d6).

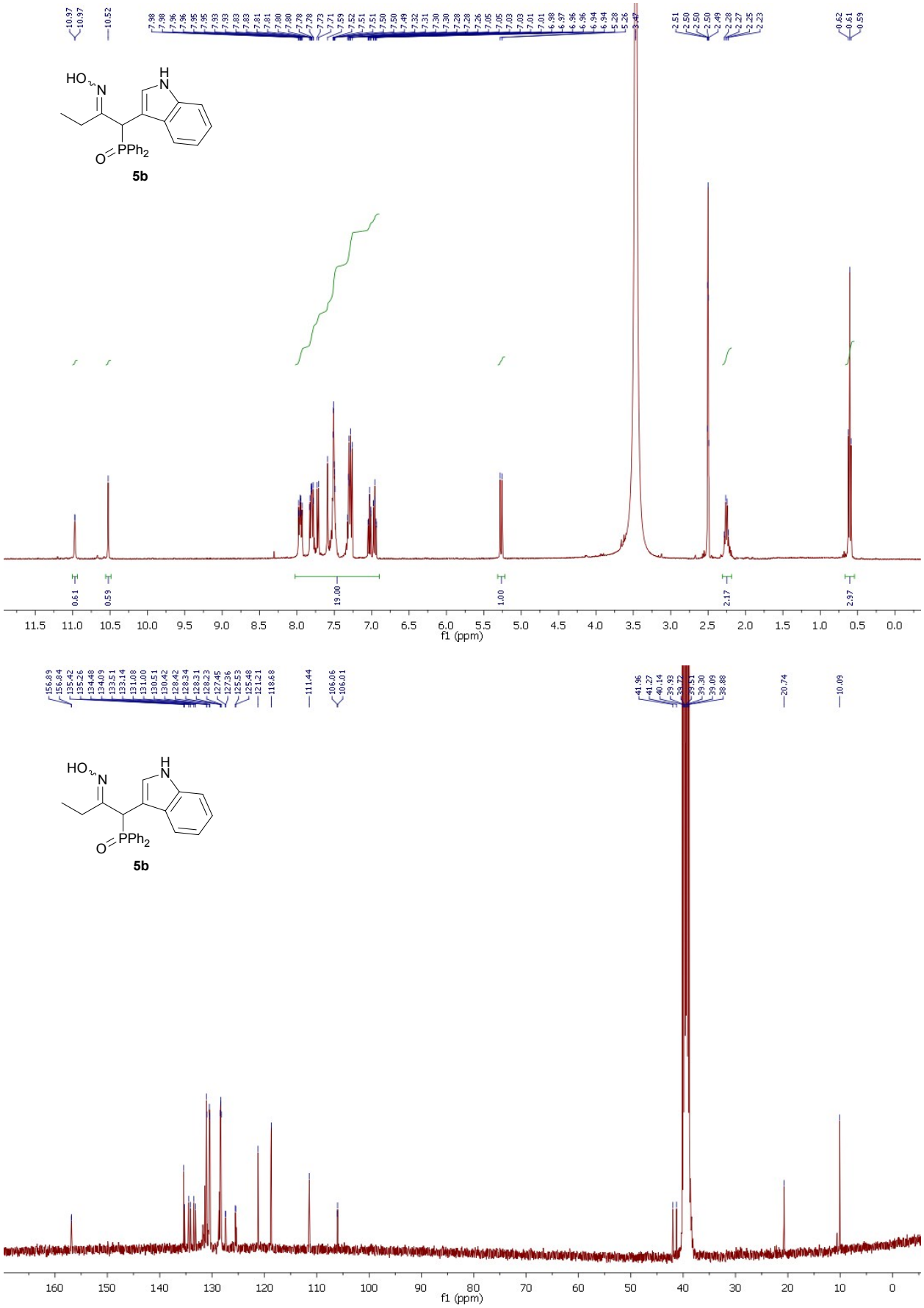


Figure 4. ^{1}H NMR and ^{13}C NMR spectra of compound **5b** (DMSO-d6).

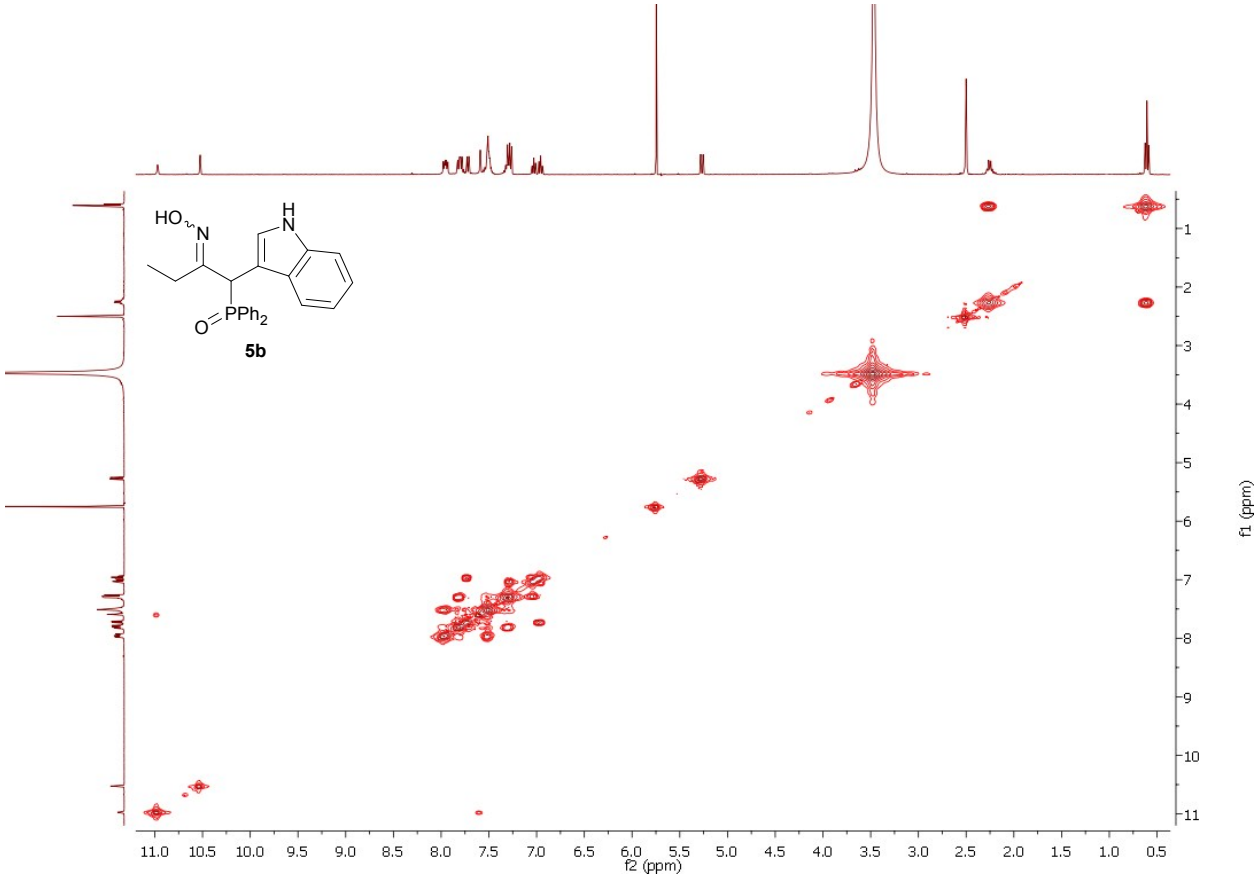


Figure 5. COSY spectra of compound **5b** (DMSO-d6).

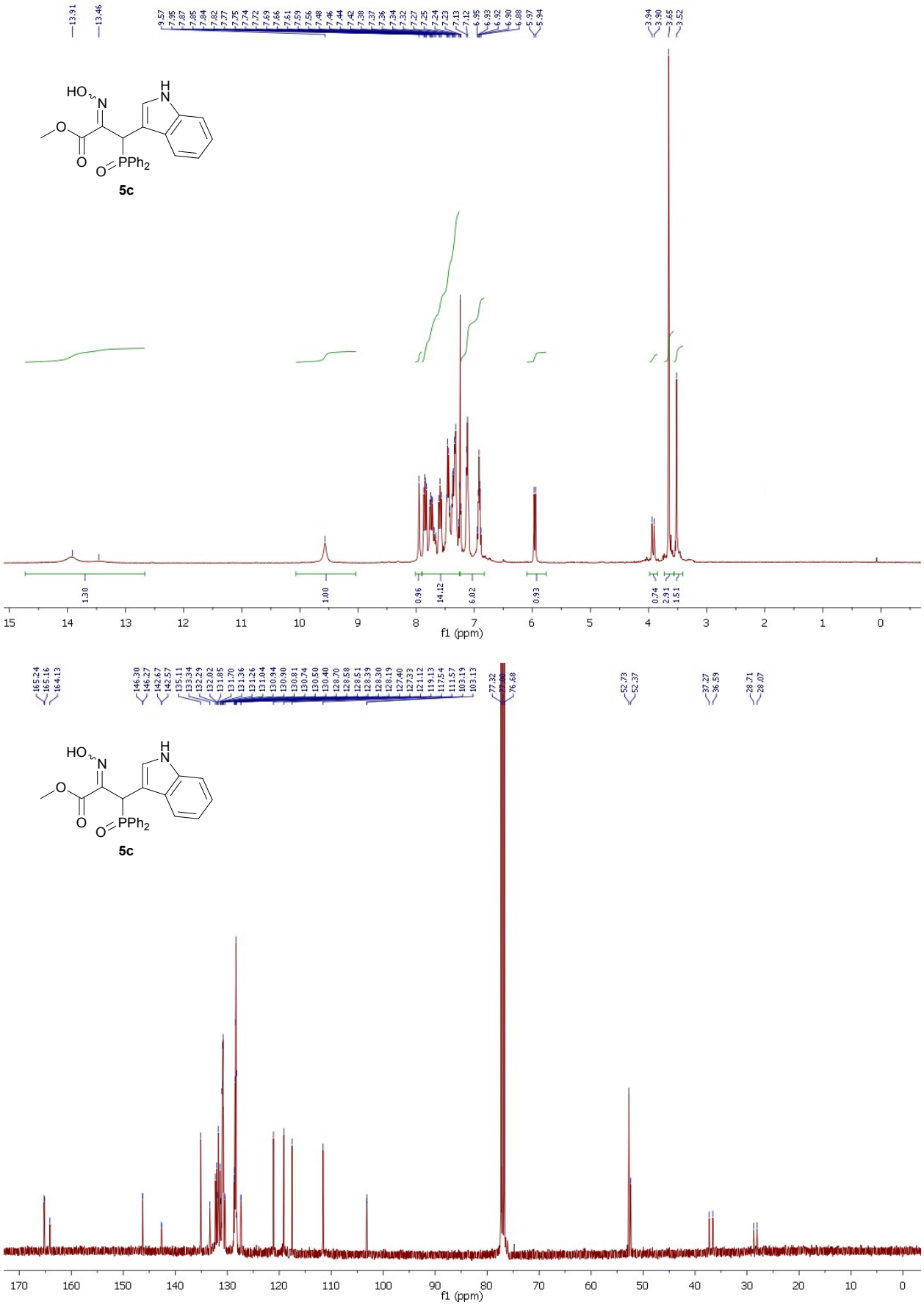


Figure 6. ^{1}H NMR and ^{13}C NMR spectra of compound **5c** ($CDCl_3$).

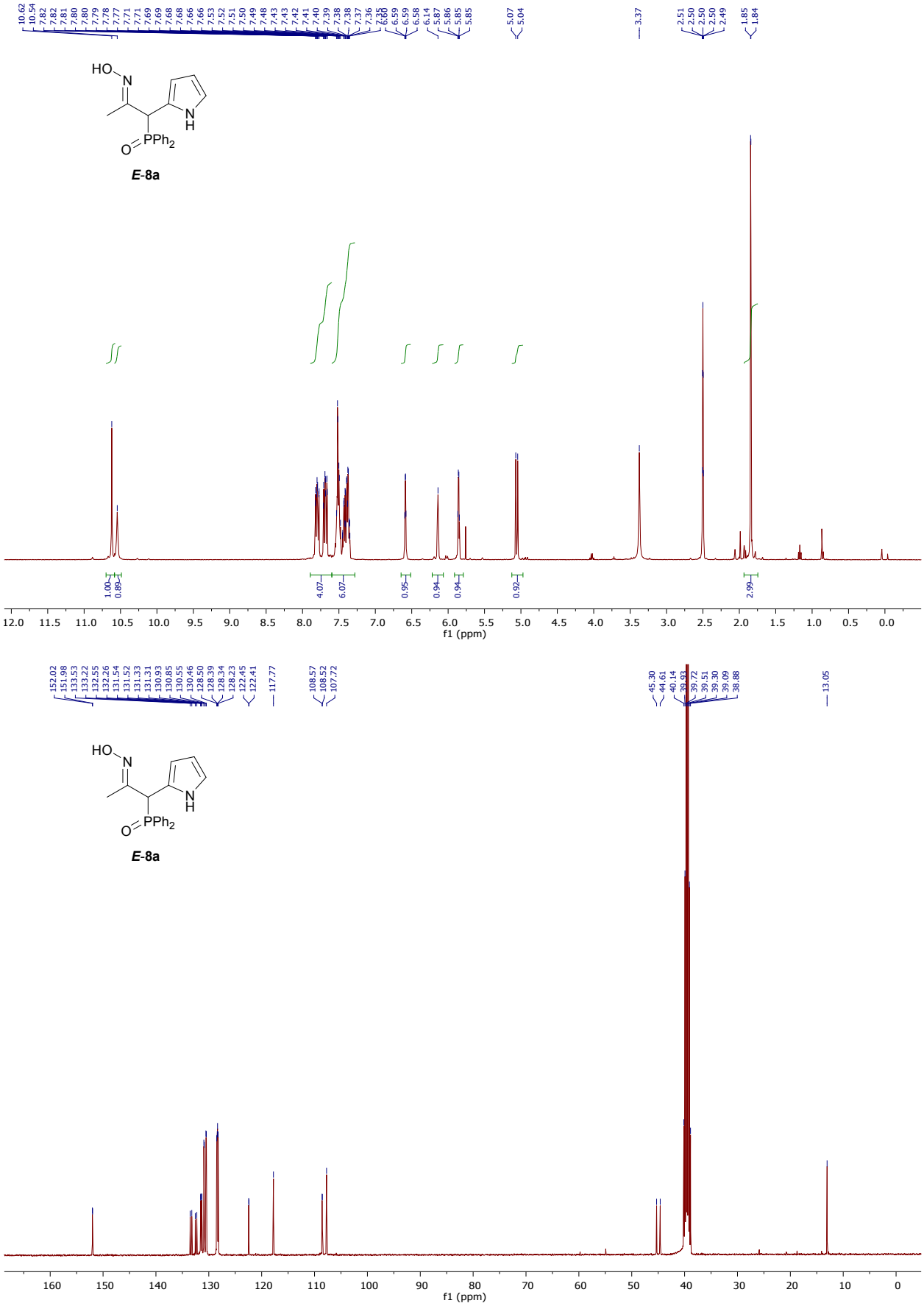


Figure 7. ^{1}H NMR and ^{13}C NMR spectra of compound ***E*-8a** (DMSO-d6).

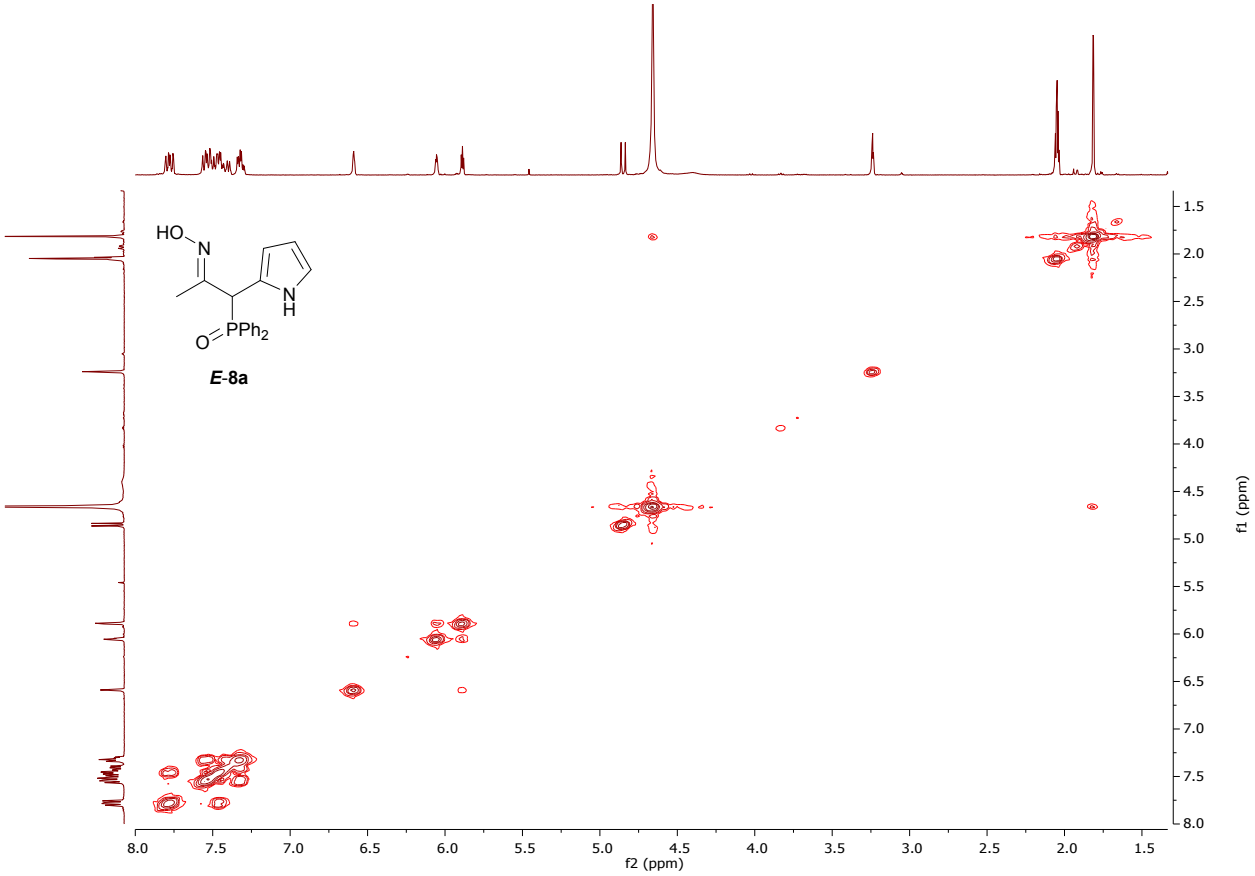


Figure 8. COSY spectra of compound ***E*-8a** (CD_3OD + acetone-d6).

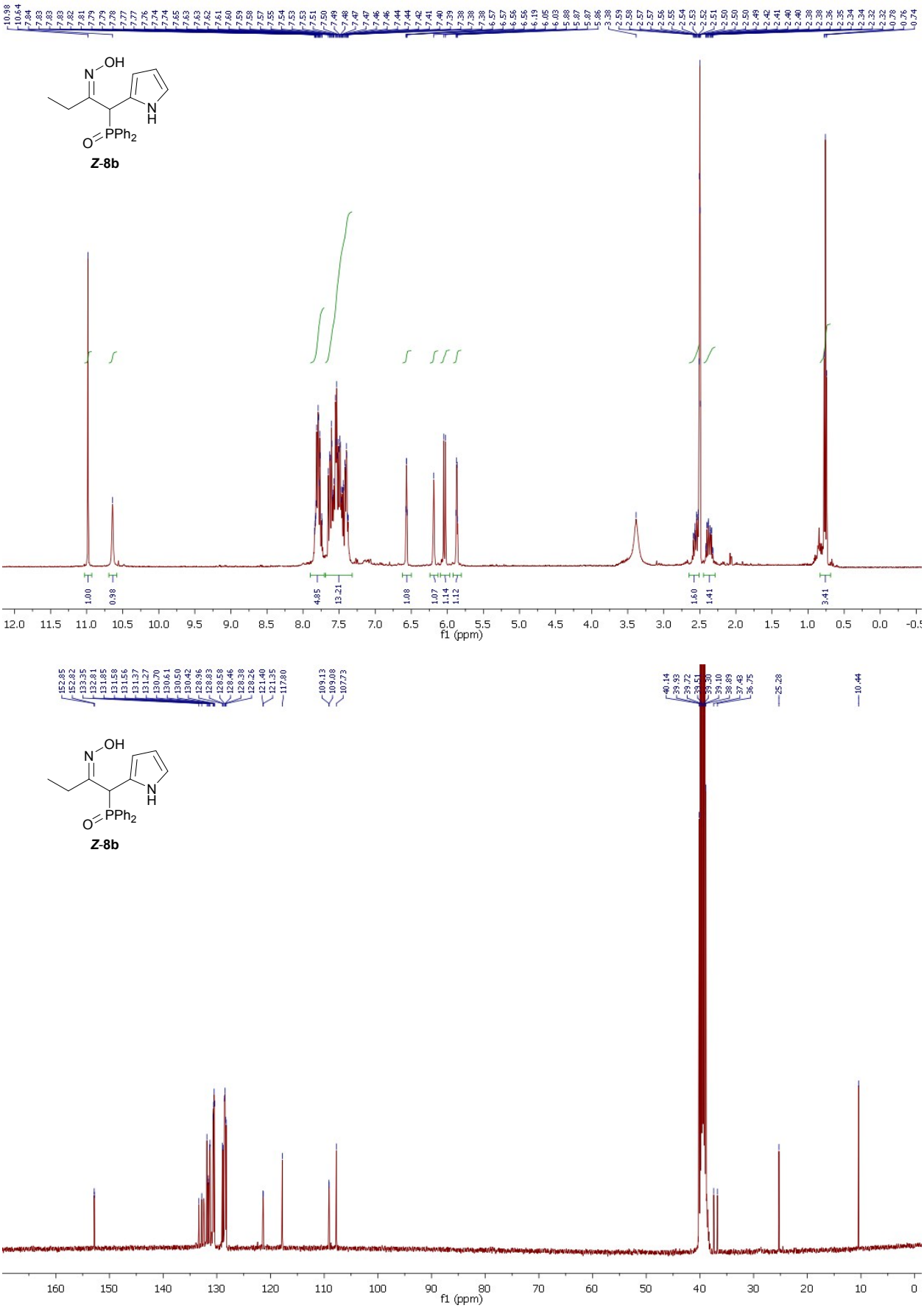


Figure 9. ^{1}H NMR and ^{13}C NMR spectra of compound ***Z*-8b** (DMSO-d6).

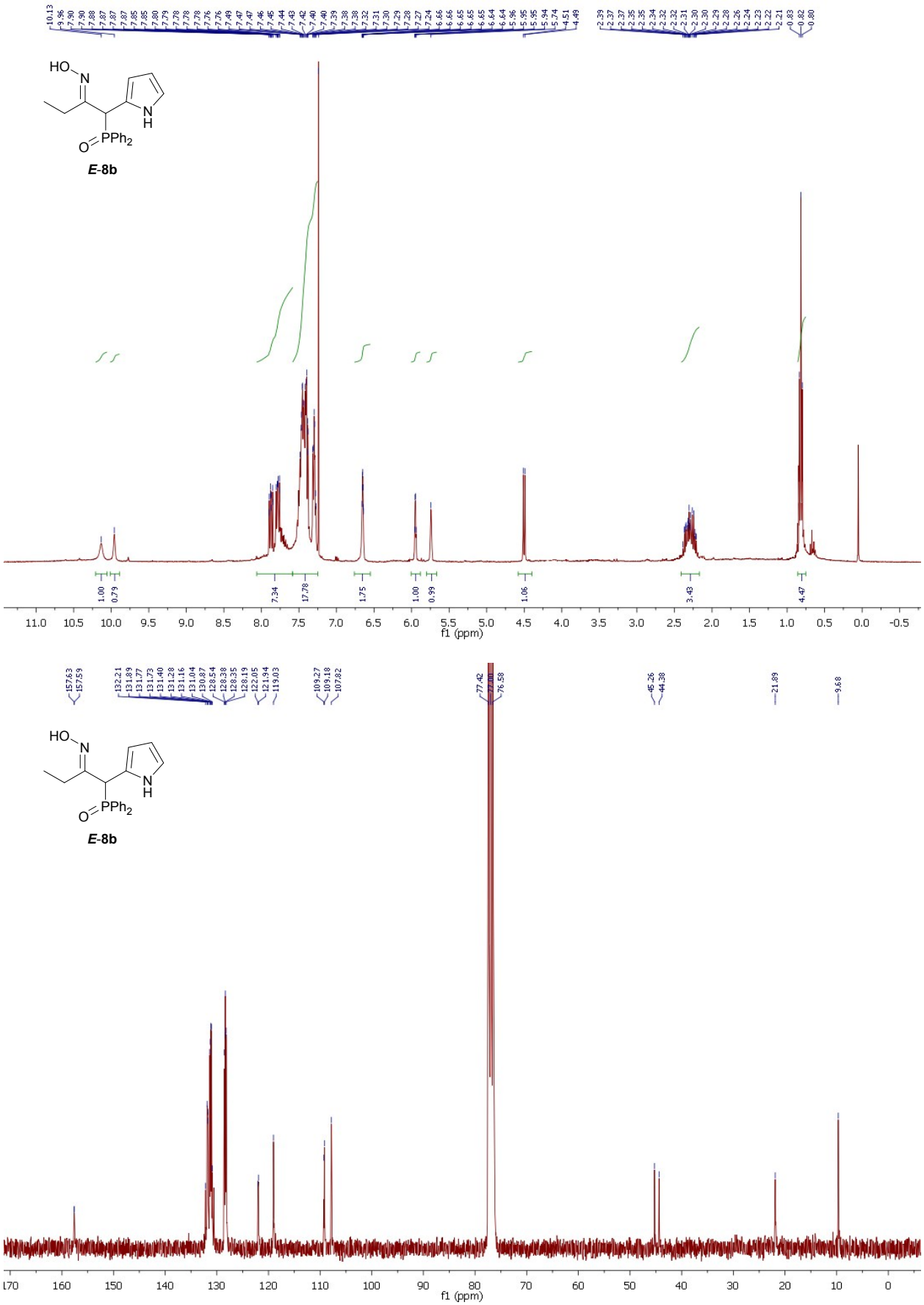


Figure 10. ^{1}H NMR and ^{13}C NMR spectra of compound ***E*-8b** ($CDCl_3$).

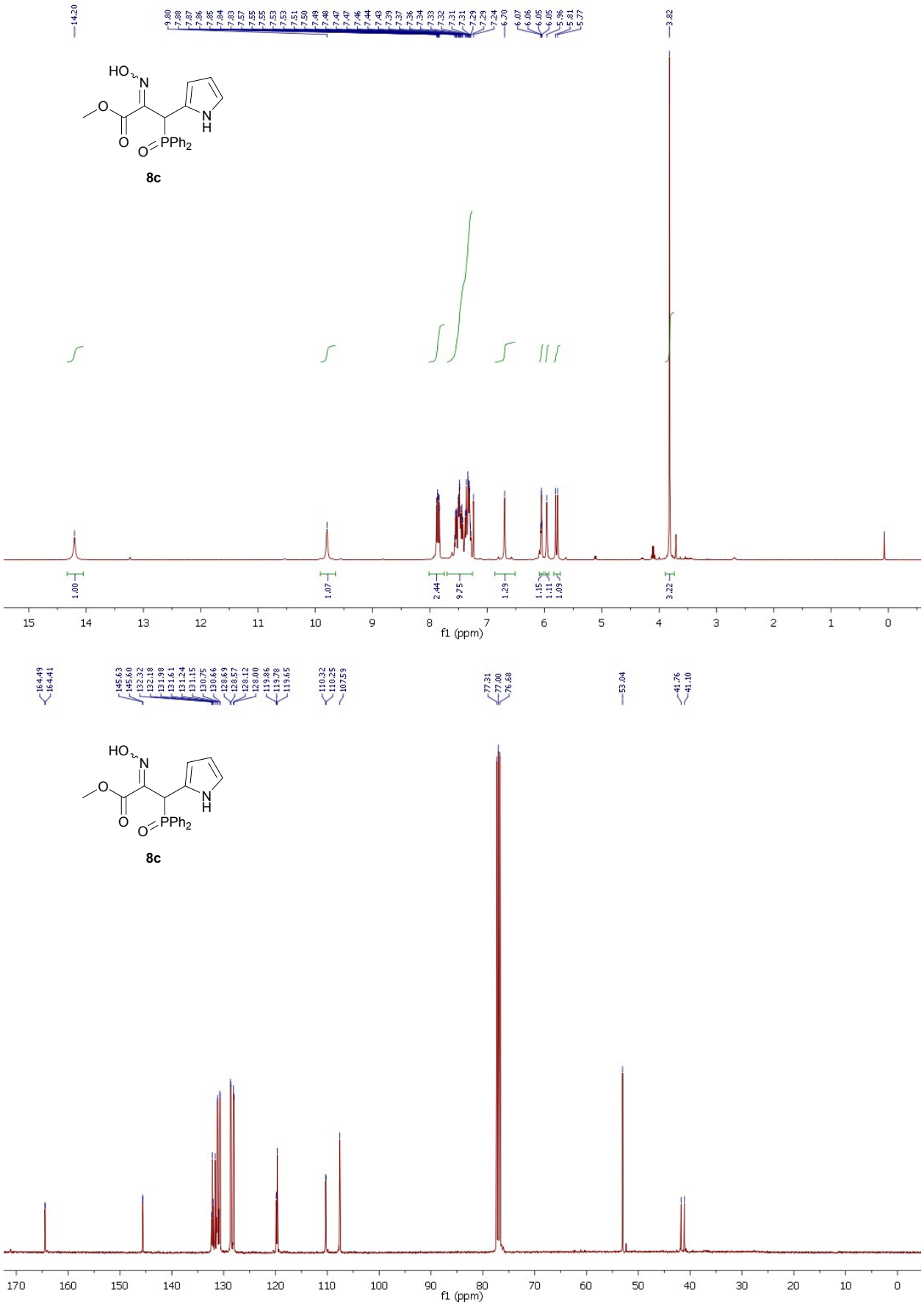


Figure 11. ^{1}H NMR and ^{13}C NMR spectra of compound **8c** ($CDCl_3$).

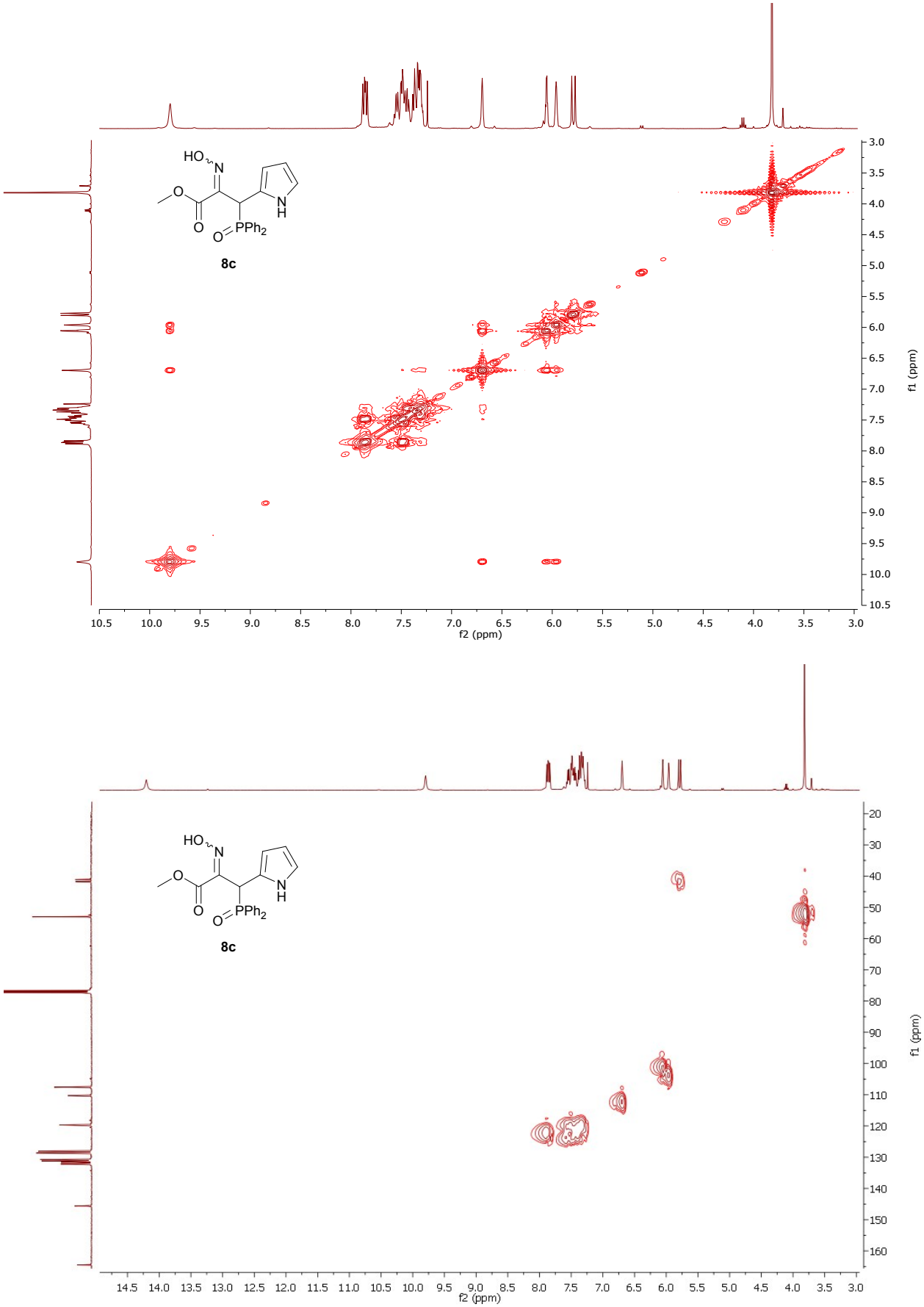


Figure 12. COSY and HMQC spectra of compound **8c** ($CDCl_3$).

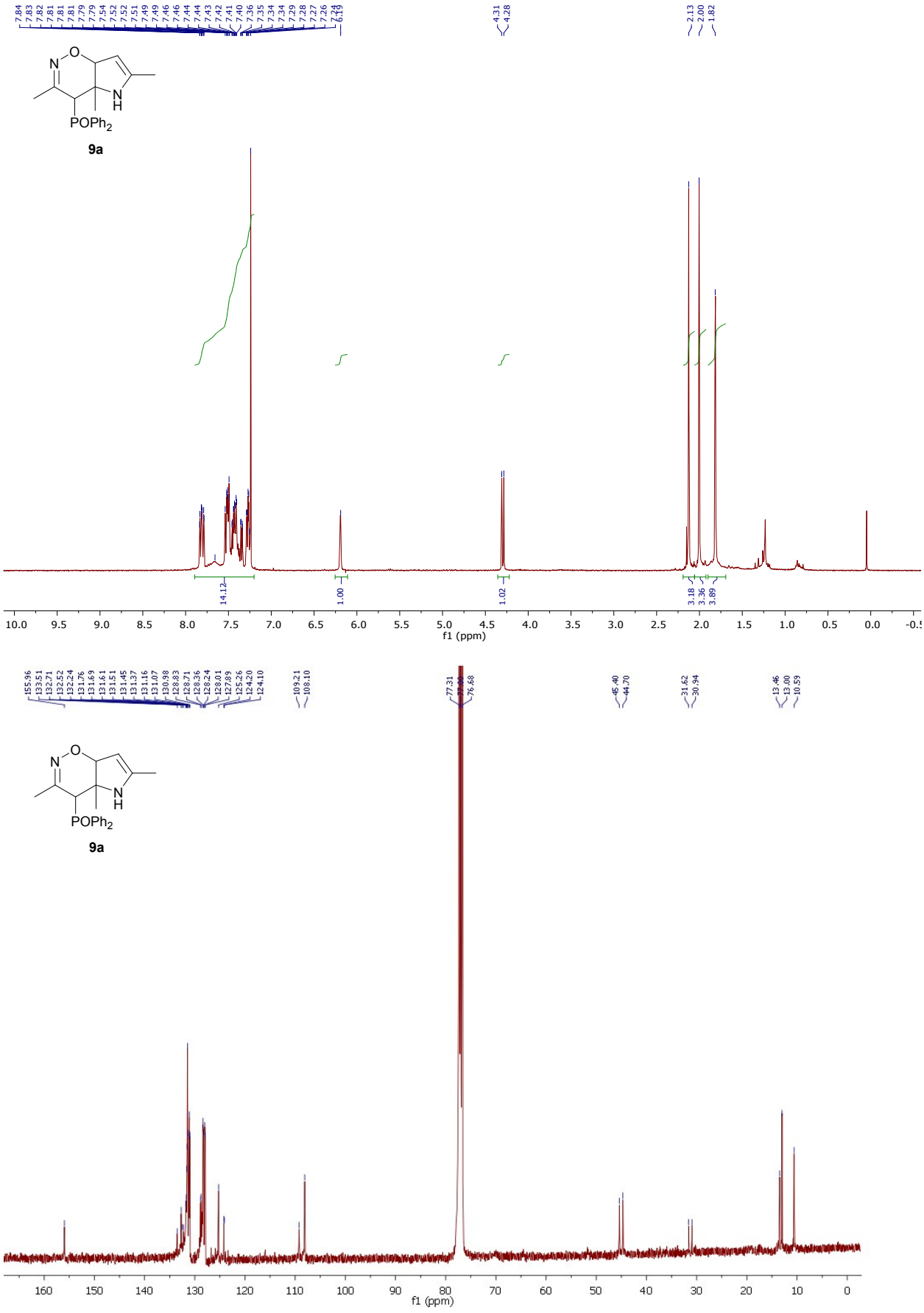


Figure 13. ^{1}H NMR and ^{13}C NMR spectra of compound **9a** ($CDCl_3$).

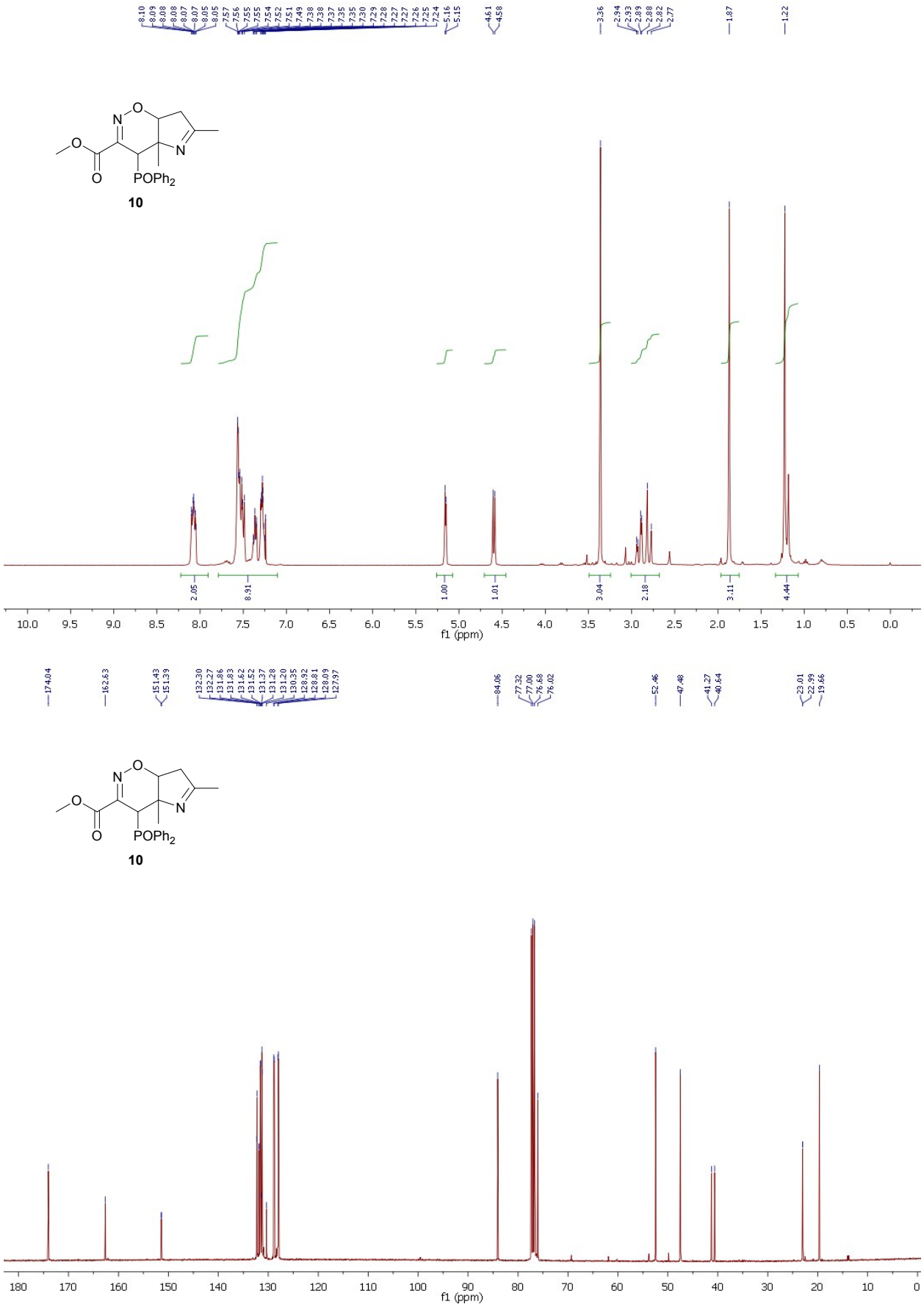


Figure 14. ^{1}H NMR and ^{13}C NMR spectra of compound **10** ($CDCl_3$).

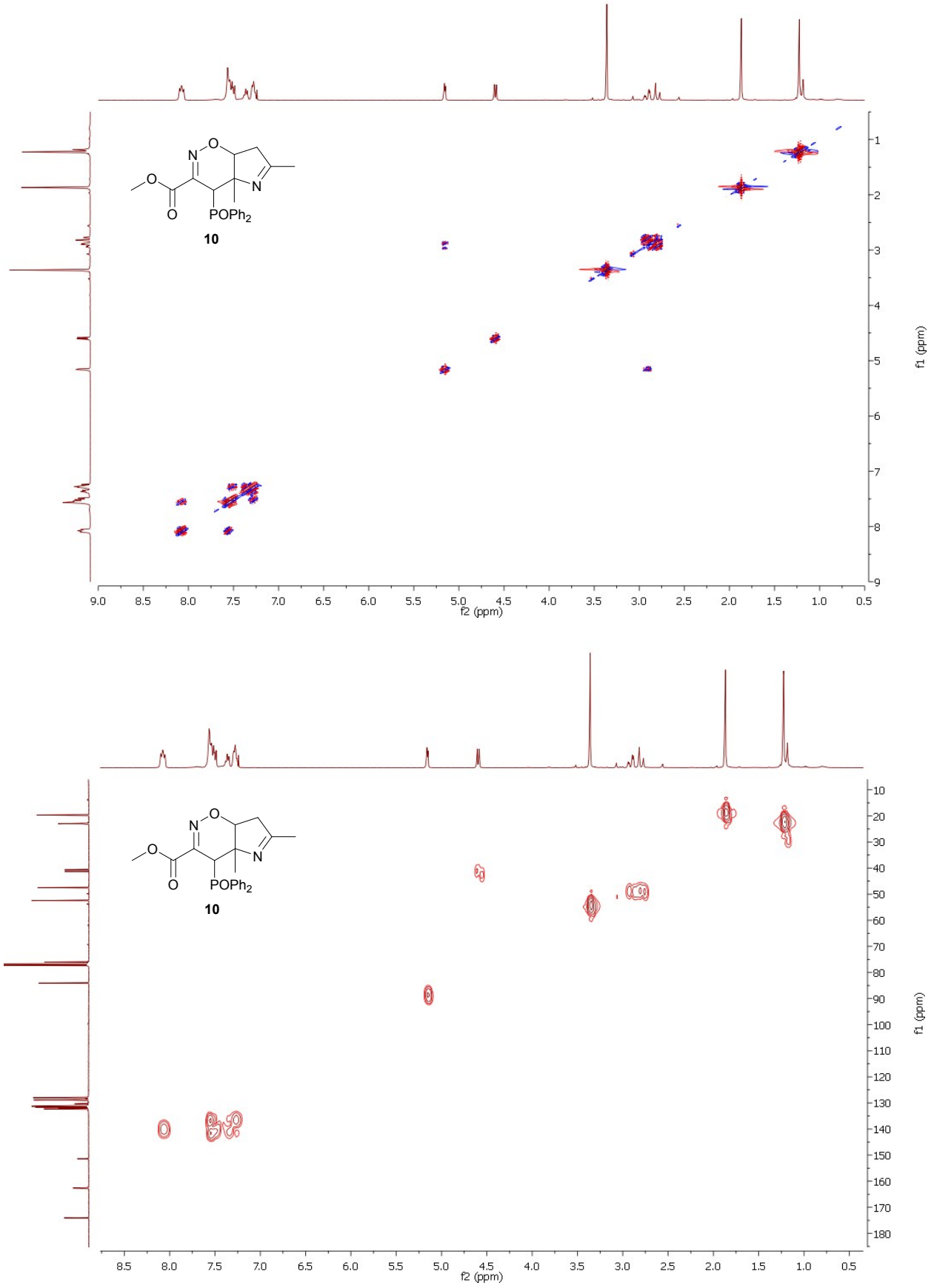


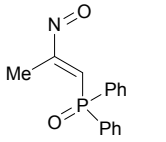
Figure 15. COSY and HMQC spectra of compound **10** ($CDCl_3$).

Theoretical Calculations

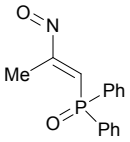
Computational Methodology

All calculations included in this paper were carried out with Gaussian 09[1] program within the density functional theory (DFT) framework[2] using the B3LYP,[3] and we also performed single-point energy calculations with the M06-2X[4] hybrid functional were used along with the standard 6-31G* basis set, and in some cases with 6-311+G** basis set.[5] The accuracy of both methods has been extensively tested for stable molecules and pericyclic reactions.[6] Activation energies (ΔEa) were computed including zero-point vibrational energy (ZPVE) corrections and ΔG corrections. All transition structures and minima were fully characterized by harmonic frequency analysis.[7] For each located transition structure, only one imaginary frequency was obtained in the diagonalized Hessian matrix, and the corresponding vibration was found to be associated with nuclear motion along the reaction coordinate. The solvent effect in DFT calculations was evaluated by means of the Polarizable Continuum Model (PCM)[8] using methylene chloride and/or water as solvents.

Experimental results indicate that nitrosoalkenes **2** are obtained mainly as *E*-stereoisomers for the carbon-carbon double bond, and we computationally examined which of either conformations *s-cis* or *s-trans*, was the most stable. Thus, computational results indicate that for both nitrosoalkenes **2a** (R = Me) or **2c** (R = CO_2Me) in the gas phase, in the presence of dichloromethane, or in water, the *s-trans* conformation is favoured about 2 kcal/mol. M06-2X(PCM)/6-31G*, B3LYP/6-311+G**//B3LYP/6-31G* and M06-2X(PCM)/6-311+G** calculated energetics also predicted similar results (for a full comparison of energetics see Figure 16).

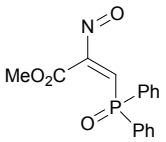


2'a

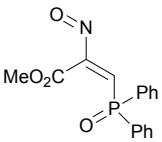


2a

	ΔG° (gas phase)	ΔG° (CH_2Cl_2)	ΔG° (H_2O)
B3LYP/6-31G*	– 2.46	– 2.91	– 2.99
M06-2X/6-31G*//B3LYP/6-31G*	– 2.30	– 2.66	– 2.73
B3LYP/6-311+G**//B3LYP/6-31G*	– 2.81	– 3.35	– 3.45
M06-2X/6-311+G**//B3LYP/6-31G*	– 2.62	– 3.04	– 3.12



2'b



2b

	ΔG° (gas phase)	ΔG° (CH_2Cl_2)	ΔG° (H_2O)
B3LYP/6-31G*	– 2.05	– 2.08	– 2.06
M06-2X/6-31G*//B3LYP/6-31G*	– 1.47	– 1.48	– 1.45
B3LYP/6-311+G**//B3LYP/6-31G*	– 2.23	– 2.14	– 2.09
M06-2X/6-311+G**//B3LYP/6-31G*	– 1.79	– 1.66	– 1.59

Figure 16. Free energy differences computed at different levels of theory.

The molecular DFT-based parameters such as, electronic chemical potential (μ), chemical hardness (η), global electrophilicity (ω) and maximum number of accepted electrons (ΔN_{max}) for nitrosoalkenes **2a**,**c** and electron-rich heterocycles **3**, **6a** and **6b** are reported in Table 1. These parameters indicate that nitrosoalkenes (entries 1–4) are more electrophilic than heterocylic compounds (entries 5–7). However, heterocycles **3**, **6a** and **6b** are harder than

nitrosoalkenes **2a**,**c**, which have chemicals potentials lower than those observed for heterocycles **3**, **6a,b**, and the ΔN_{max} values for **2'a**,**c** are the largest. The *s-trans* conformations (**2a** and **2c**) exhibit higher chemical hardness (η) and chemical potential (μ), but lower global electrophilicity (ω) than *s-cis* conformations (**2'a** and **2'b**). The maximum number of accepted electrons values (ΔN_{max}) for **2'a,** and **2'c** are the largest. Moreover, the presence of a carboxylate group at the 3-position of nitrosoalkenes (**2c** and **2'c**) decreases the hardness and the chemical potential and increases the electrophilicity and maximum number of accepted electrons, compared with dienes (**2a** and **2'a**), respectively.

On the other hand, pyrrole **6a** is harder than 2,5-dimethylpyrrole **6b**, and the former harder than indole **3**. But the presence of two methyl groups in 2,5-dimethylpyrrole **6b** increases the electronic chemical potential and decreases electrophilicity and the ΔN_{max} towards **3** and **6a**.

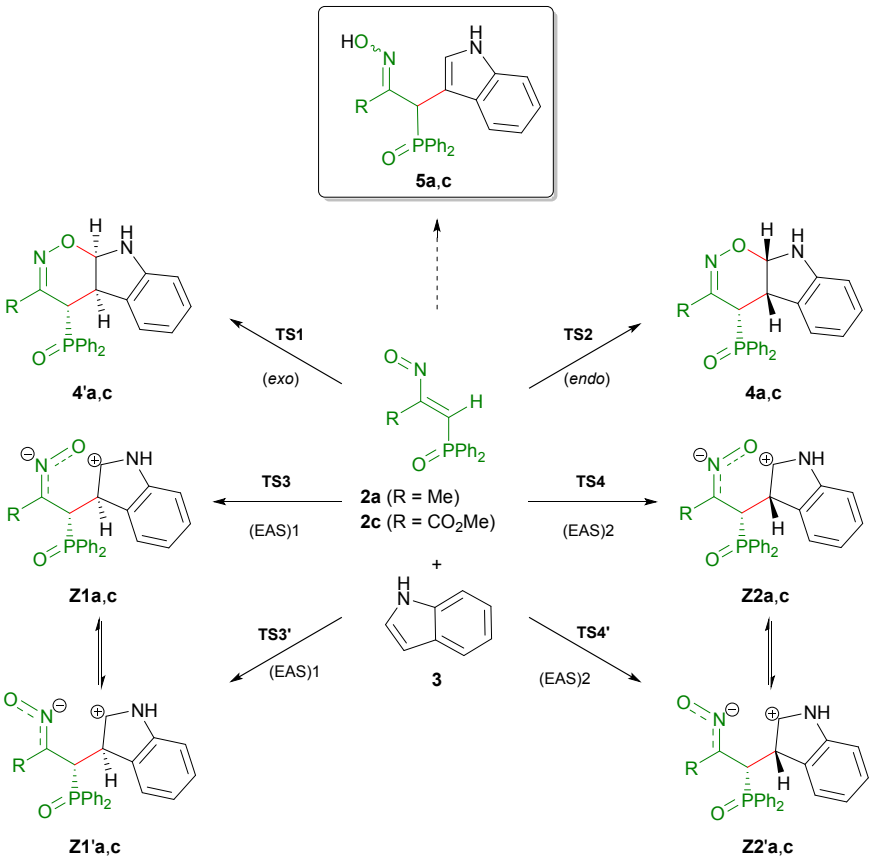
Table 1. Hardnesses[a] (η, in a.u.), Chemical Potentials[a] (μ, in a.u.), Global Electrophilicities[a] (ω, in eV) and Maximun Number of Accepted Electrons[a] (ΔNmax, in a.u.) for Compounds **2a**,**c** and Heterocycles **3, 6a,b**.

Entry	Compound	η	μ	ω	ΔN_{max}
1	**2'a**	0.11528	– 0.17024	0.125701	1.476752
2	**2a**	0.11868	– 0.16266	0.111469	1.370576
3	**2'c**	0.11321	– 0.18080	0.144364	1.596988
4	**2c**	0.11847	– 0.17312	0.126483	1.461256
5	**3**	0.19604	– 0.10044	0.025730	0.512344
6	**6a**	0.25248	– 0.07529	0.011226	0.298202
7	**6b**	0.23373	– 0.06749	0.009742	0.288731

[a] Computed at the B3LYP/6-31G* level according to the approach and equations described previously.[9]

*1. Reactivity of indole (**3**) towards nitrosoalkenes **2a** and **2c.***

Experimentally, the reaction of **2a** (R = Me) or **2c** (R = CO_2Me) with indole (**3)** in methylene chloride at room temperature, gave the corresponding oximes **5a** or **5c**, respectively in good yields. The formation of these oximes can be explained *via* six pathways depicted in Scheme 1. The process may be initiated by an electrophilic aromatic substitution from nitrosoalkenes **2a**,**c** to the C–3 of indole (**3**), by means of transition structures **TS3**, **TS3'**, **TS4** or **TS4'**, affording zwitterionic intermediates **Z1**, **Z1'**, **Z2** or **Z2'**, respectively. Subsequent 1,5-*H*-shift would give oxime derivatives **5**. However, another pathways involving a concerted [4+2] cycloaddition reaction through transition structures **TS1** or **TS2** between the nitrosoalkenes **2a**,**c** and indole (**3)** could also explain the formation of oxazines **4'a**,**c** or **4a**,**c** respectively. Further rearomatization of these cycloadducts would afford oximes **5** in a similar process to that previously described.[10]



Scheme 1. Possible pathways for the formation of oximes **5a,c**.

In order to explain the experimental results, we computationally calculated the energy of optimized transition structures energies at different levels of theory. Thus, in the case of nitrosoalkene **2a** (R = Me), computational results indicate that the activation barriers associated with a concerted process to form **4a**, through a transition structure *endo* **TS2a**, are lower than the activation barriers associated with the formation of **4'a** through a transition structure *exo* **TS1a** (Table 2a and 2b, entries 1–2). Moreover, these activation barriers are lower than those associated with an electrophilic aromatic substitution process *via* transition structures **TS3a**, **TS3'a**, **TS4a**, and **TS4'a**, which could lead to zwitterionic intermediates **Z1a**, **Z1'a**, **Z2a**, and **Z2'a**, respectively (Table 2a and 2b, entries 3–6). Similar results have been achieved when M06-2X/6-31G*, B3LYP/6-311+G**//B3LYP/6-31G*, and M06-2X/6-311+G**//B3LYP/6-31G* levels of theory have been used, in gas phase and in the presence of methylene chloride as the solvent (for a full comparison of energetics see Table 2a and 2b, and Figure 17). Since the *endo* process is slight asynchronous, it can be assume that the formation of oxime **5a** takes place through a [4+2] concerted asynchronous process kinetically favored to give oxazine **4a**, whose opening and subsequent rearomatization would give oxime **5a**.

Table 2a. Activation Energies (ΔE_a, kcal/mol) Associated with the Formation of **4a,c**, **4'a,c** and Zwitterionic Intermediates **Z1–2a,c and Z'1–2a,c** for the Reaction of Nitrosoalkenes **2a,c** with Indole (**3**) using ΔZPVE correction. Synchronicities Associated with the Formation of **4** and **4'**.

Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]	*Sy*[i]
1	**2a + 3→4'a**	**TS1a**	20.21	20.51	13.30	13.70	23.43	23.69	14.08	14.45	0.910
2	**2a + 3→4a**	**TS2a**	16.98	17.61	11.60	12.31	20.55	21.22	12.61	11.07	0.910
3	**2a + 3→Z1a**	**TS3a**	26.31	21.07	20.48	14.28	28.31	22.25	20.10	12.97	–
4	**2a + 3→Z'1a**	**TS3'a**	30.20	23.81	24.80	16.21	31.22	23.39	23.25	13.22	–
5	**2a + 3→Z2a**	**TS4a**	24.06	20.86	16.34	12.78	26.68	22.90	16.33	12.17	–
6	**2a + 3→Z'2a**	**TS4'a**	29.03	24.48	23.46	17.15	29.01	24.08	21.58	14.23	–
7	**2c + 3**→C1→**4'c**	**TS1c**	22.58	18.36	16.91	12.73	24.19	19.09	17.27	12.35	0.860
8	**2c + 3**→C1→**4c**	**TS2c**	13.88	10.39	6.64	2.93	15.21	11.07	6.58	2.45	0.796
9	**2c + 3**→C1→**Z1c**	**TS3c**	13.68	9.85	6.59	2.75	14.79	10.40	6.54	2.15	–
10	**2c + 3**→C1→**Z1'c**	**TS3'c**	17.97	12.67	10.73	5.20	18.36	12.36	10.06	3.85	–
11	**2c + 3**→C1→**Z2c**	**TS4c**	14.92	12.00	9.22	6.28	16.27	12.78	9.23	5.72	–
12	**2c + 3**→C1→**Z2'c**	**TS4'c**	19.17	14.58	13.93	9.13	20.19	14.97	13.81	8.40	–

[a] Computed at the B3LYP/6-31G* + ΔZPVE level. [b] Computed a B3LYP(PCM)/6-31G* +ΔZPVE level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔZPVE level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔZPVE level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [g] Computed at the M06-2X /6-311+G**// B3LYP/6-31G* + ΔZPVE level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [i] Computed at the B3LYP/6–31G* level according to approach and equations described previously.[11]

Table 2b. Activation Energies (ΔE_a, kcal/mol) Associated with the Formation of **4a,c**, **4'a,c** and Zwitterionic Intermediates **Z1–2a,c and Z'1–2a,c** for the Reaction of Nitrosoalkenes **2a,c** with Indole (**3**) using ΔG correction.

Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]
1	**2a + 3→4'a**	**TS1a**	35.14	35.44	28.23	28.64	38.36	38.62	29.02	29.39
2	**2a + 3→4a**	**TS2a**	31.12	31.75	26.54	27.24	35.48	36.15	27.54	26.01
3	**2a + 3→Z1a**	**TS3a**	43.21	35.32	34.74	28.54	42.57	36.50	37.87	27.23
4	**2a + 3→Z'1a**	**TS3'a**	44.81	38.42	39.41	30.83	45.83	38.01	34.35	27.84
5	**2a + 3→Z2a**	**TS4a**	38.91	35.71	31.20	27.63	41.53	37.76	31.18	27.02
6	**2a + 3→Z'2a**	**TS4'a**	43.21	38.65	37.63	31.32	43.18	38.25	35.76	28.40
7	**2c + 3→4'c**	**TS1c**	33.88	31.46	25.65	23.46	37.09	34.17	26.66	24.08
8	**2c + 3→4c**	**TS2c**	24.42	22.74	14.42	12.90	27.35	25.39	15.21	13.43
9	**2c + 3→Z1c**	**TS3c**	24.13	22.10	14.47	12.63	26.83	24.62	15.08	13.03
10	**2c + 3→Z1'c**	**TS3'c**	28.54	25.04	18.74	15.20	30.53	26.71	18.74	14.85
11	**2c + 3→ Z2c**	**TS4c**	25.33	24.21	17.07	16.13	28.28	26.97	17.74	16.57
12	**2c + 3→Z2'c**	**TS4'c**	29.90	27.12	22.10	19.30	32.52	29.48	22.64	19.57

[a] Computed at the B3LYP/6-31G* + ΔG correction level. [b] Computed a B3LYP(PCM)/6-31G* + ΔG level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔG correction level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔG correction level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [g] Computed at the M06-2X /6-311+G**// B3LYP/6-31G* + ΔG correction level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent.

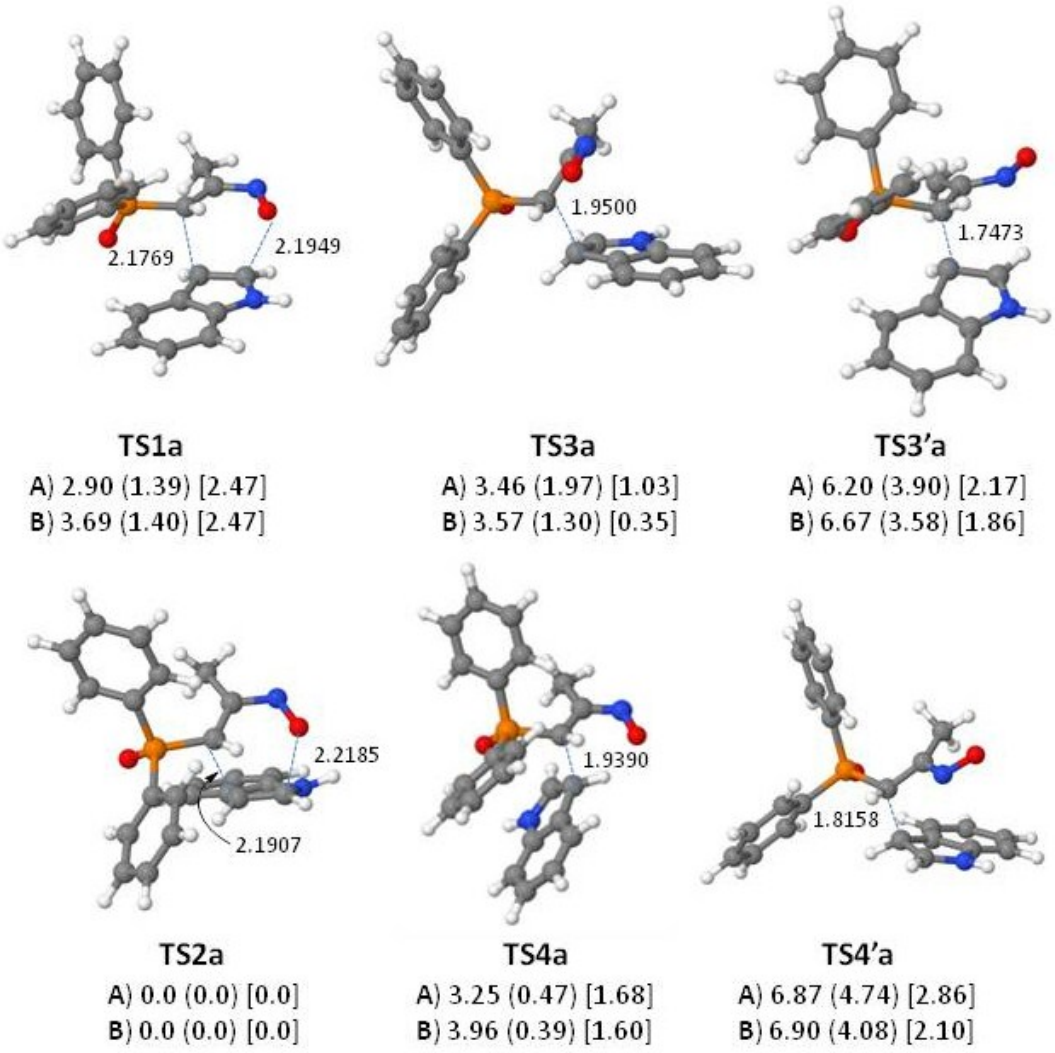


Figure 17. Fully optimized transition structures for the reaction of nitrosoalkene **1a** and indole (**2a**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS2a** computed at B3LYP(PCM)/6-31G* level using CH_2Cl_2 as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent.

Conversely, with nitrosoalkene **2c** (R = CO_2Me) the formation of an earlier molecular complex **C1** had to be taken into account when ΔZPVE was used, since the transition structures associated with the transformation were located below the separated reagents **2c**/**2'c** and **3**. In this case, computational results indicate that the activation barriers associated with an electrophilic aromatic substitution process to afford **Z1c**, through a transition structure **TS3c**, are very similar to those associated with a concerted process through a transition structure **TS2c** to form **4c**, and thus both mechanisms are predicted to be competitive (Table 2a and 2b, entries 8 and 9 and Figure 18). Analogous results have been obtained when M06-2X/6-311+G**//B3LYP/6-31G* level, both in gas phase and in the presence of methylene chloride as the solvent has been used (Table 2a and 2b, entries 7–12). As expected, for all levels of theory tested in the presence of methylene chloride as the solvent, the activation energy values corresponding to the approach of nitrosoalkene **2c** to indole (**3**) *via* transition structures **TS2c** or **TS3c** decrease relative to those observed in gas phase (Table 2). These results suggest that the formation of oxime **5c** would start with an electrophilic attack from nitrosoalkene **2c** to the C–3 of indole (**3**), to furnish zwitterionic intermediate **Z1c**, and subsequent 1,5-*H*-shift, or *via* a concerted [4+2] process to afford oxazine **4c** followed by rearomatization.

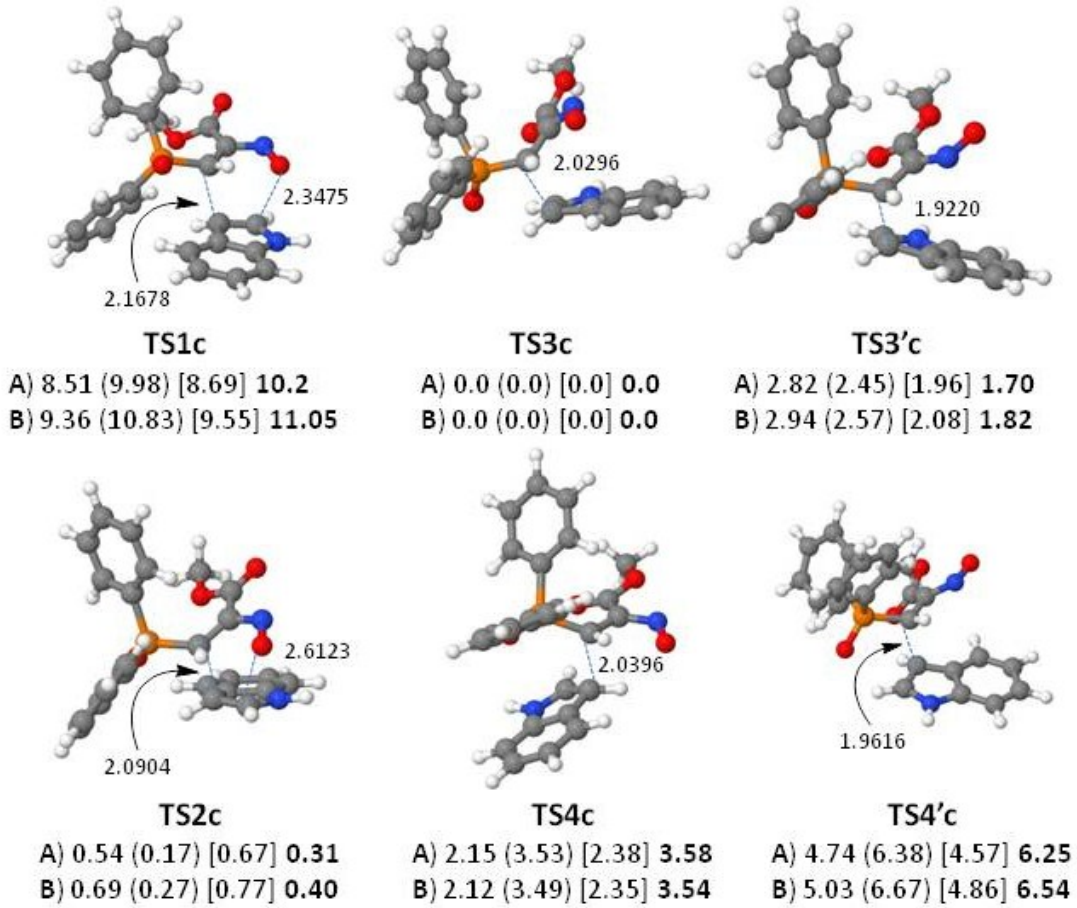


Figure 18. Fully optimized transition structures for the reaction of nitrosoalkene **2c** and indole (**3**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS3c** computed at B3LYP(PCM)/6-31G* level using CH_2Cl_2 as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Bold numbers are the relative energies differences calculated at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent.

In order to know which process is thermodynamically favoured the reaction energies associated with the formation of zwitterionic intermediate **Z1c** and oxazine **4c** was calculated. Both processes in the presence of methylene chloride are exothermic or slightly endothermic processes (Tables 3a and 3b, and Figure 19). However, for all levels of theory tested in the presence of methylene chloride as the solvent or in gas phase, the formation of **4c** is thermodynamically favoured suggesting that in thermodynamic conditions the formation of oxazine **4c**, through a [4+2] cycloaddition process, is favoured.

Table 3a. Reaction Energies (ΔE_{rxn}, kcal/mol) Associated with the Formation of **4c**, and Zwitterionic Intermediate **Z1c** using ΔZPVE correction.

Entry	Reaction	TS	ΔE_{rxn}[a]	ΔE_{rxn}[b]	ΔE_{rxn}[c]	ΔE_{rxn}[d]	ΔE_{rxn}[e]	ΔE_{rxn}[f]	ΔE_{rxn}[g]	ΔE_{rxn}[h]
1	**2c + 3**→C1→**4c**	**TS2c**	– 18.05	– 18.73	– 32.00	– 32.75	– 13.09	– 14.09	– 28.90	– 30.04
2	**2c + 3**→C1→**Z1c**	**TS3c**	12.56	0.81	4.37	– 8.10	12.91	0.21	3.48	– 9.71

[a] Computed at the B3LYP/6-31G* + ΔZPVE level. [b] Computed a B3LYP(PCM)/6-31G* +ΔZPVE level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔZPVE level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔZPVE level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [g] Computed at the M06-2X /6-311+G**// B3LYP/6-31G* + ΔZPVE level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent.

Table 3b. Reaction Energies (ΔE_{rxn}, kcal/mol) Associated with the Formation of **4c**, and Zwitterionic Intermediate **Z1c** using ΔG correction.

Entry	Reaction	TS	ΔE_{rxn}[a]	ΔE_{rxn}[b]	ΔE_{rxn}[c]	ΔE_{rxn}[d]	ΔE_{rxn}[e]	ΔE_{rxn}[f]	ΔE_{rxn}[g]	ΔE_{rxn}[h]
1	**2c + 3→4c**	**TS2c**	– 6.39	– 5.24	– 22.88	– 21.62	0.20	1.38	– 19.12	– 17.91
2	**2c + 3→Z1c**	**TS3c**	23.45	13.51	12.69	2.22	25.40	14.88	12.47	1.62

[a] Computed at the B3LYP/6-31G* + ΔG correction level. [b] Computed a B3LYP(PCM)/6-31G* + ΔG correction level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔG correction level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔG correction level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [g] Computed at the M06-2X /6-311+G**// B3LYP/6-31G* + ΔG correction level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent.

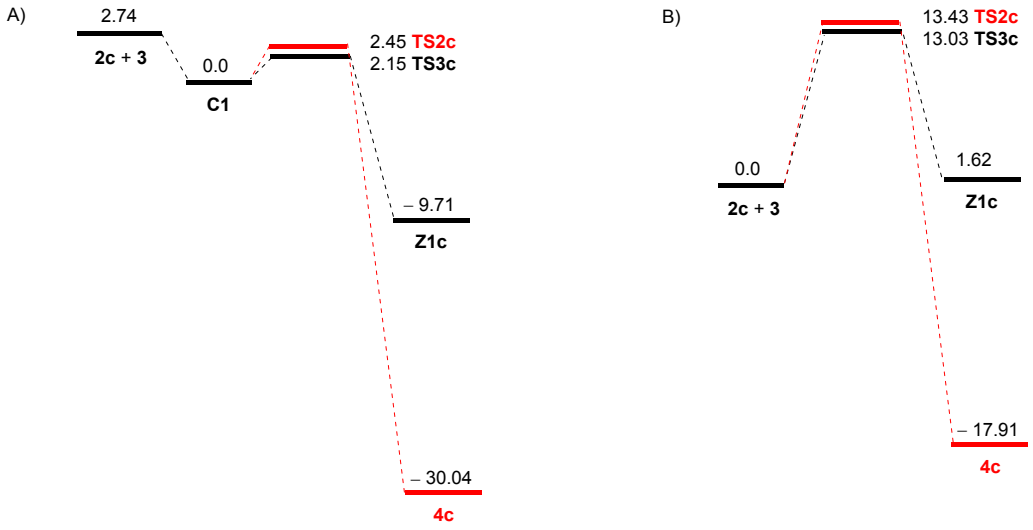


Figure 19. A) Energy profile for transformation from reactants **2c** and **3** through molecular complex **C1** to oxazine **4c** and zwitterionic intermediate **Z1c** at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* + ΔZPVE level (unit: kcal/mol) using methylene chloride as solvent. B) Energy profile for transformation from reactants **2c** and **3** to oxazine **4c** and zwitterionic intermediate **Z1c** at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* + ΔG correction level (unit: kcal/mol) using methylene chloride as solvent.

To establish the stability of both isomers, oxazines **4** and oxime **5**, we next computationally examined the tautomeric equilibrium between both compounds.[12] Free energy differences computed at different levels of theory (for a full comparison of energetics see Figure 20), using methylene chloride as the solvent, indicate that oximes **5a**,**c** are more stable than oxazines **4a**,**b**. Furthermore, for oxime **5a** the *E*-configuration, where the hydroxyl group is in the opposite side of the heterocyclic ring, is slightly more stable than the *Z*-configuration, where the hydroxyl group is placed toward the heterocyclic substituent (Figure 20a), confirming the experimental results. Nevertheless, in the case of oxime **5c** the *Z*-isomer is more stable than the *E*-isomer (Figure 20b). Consequently, these results indicated that the formation of the open chain tautomeric oximes **5**,**c** is favored over cyclic tautomeric oxazines **4a**,**c** and confirms the *E*-stereochemistry for the C-N double bond in oxime **5a**.

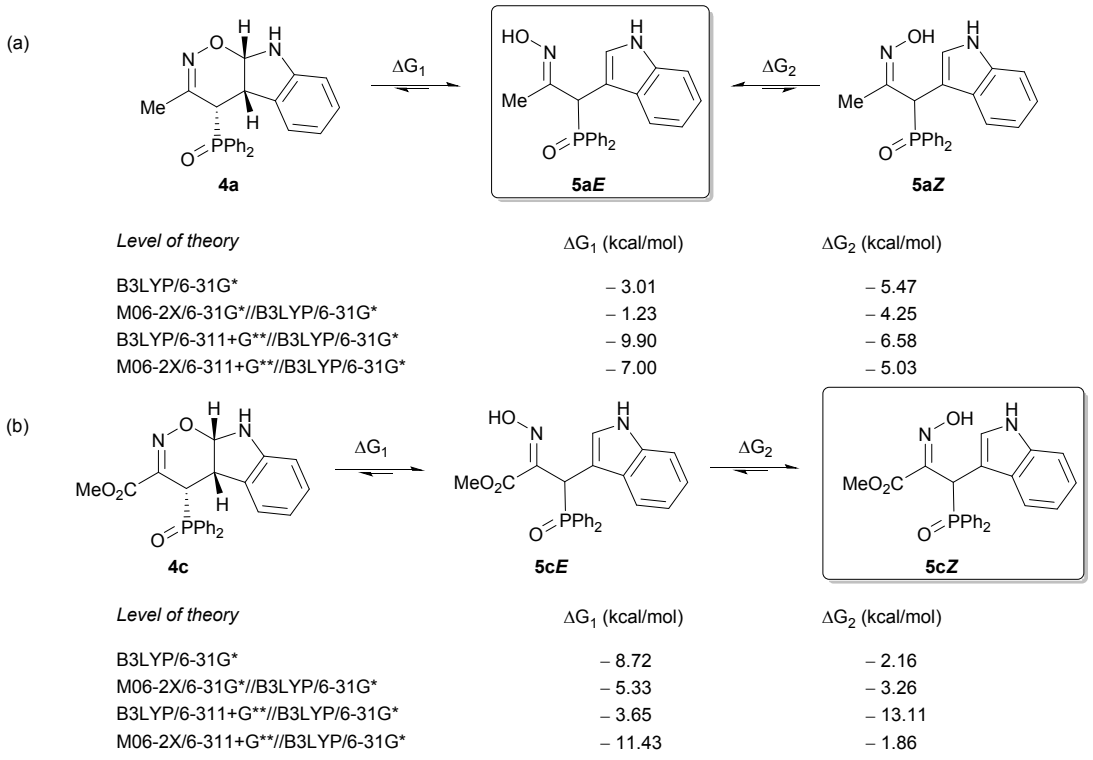


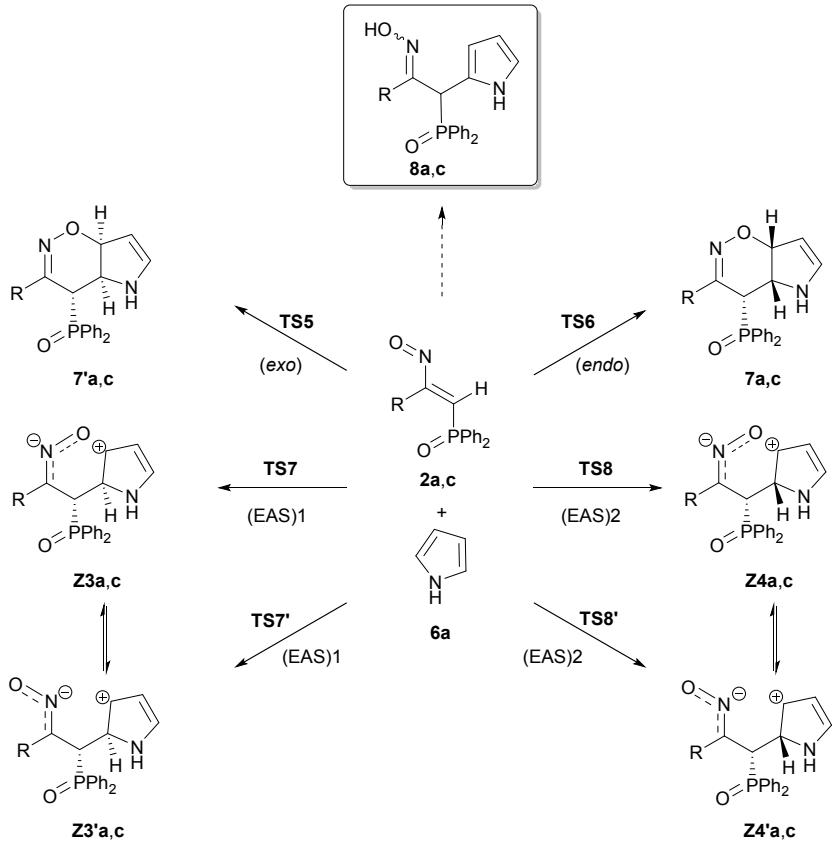
Figure 20. (a) Tautomeric equilibria between oxazine **4a** and oxime **5a**, and oximes **5a*E*** and **5a*Z***. (b) Tautomeric equilibria between oxazine **4c** and oxime **5c**, and oximes **5c*E*** and **5c*Z***.

*2. Reactivity of pyrrole (**6a**) towards nitrosoalkenes **2a** and **2c.***

Experimentally, the reaction of **2a**,**c** with pyrrole (**6a**) in the presence of aqueous $NaHCO_3$ at room temperature, gave to the formation of the corresponding oximes **8a**,**c** in good yields. As previously reported for indole (**3**), these compounds could be formed *via* six pathways depicted in Scheme 2. The process may start through an electrophilic aromatic substitution from nitrosoalkenes **2a**,**c** to the C–2 of pyrrole (**6a**), by means of transition structures **TS7**, **TS7'**, **TS8** or **TS8'**, to give zwitterionic intermediates **Z3**, **Z3'**, **Z4** or **Z4'**, respectively. Subsequent 1,5-*H*-shift would give oxime derivatives **8a**,**c**. However, another pathways involving a concerted [4+2] cycloaddition reaction through transition structures **TS5** or **TS6** (Scheme 2) between nitrosoalkenes **2a**,**c** and pyrrole (**6a**) could also explain the formation of oxazines **7'a**,**c** or **7a**,**c**, respectively. Further rearomatization of these cycloadducts would afford oxime **8a**,**c**.

In order to explain experimental results, the optimized transition structures energy was calculated computationally at different levels of theory. Therefore, when using nitrosoalkenes **2a,c**, computational results indicate that the activation barriers associated with a concerted process to form **7a** or **7c**, through a transition structure *endo* **TS6a** or **TS6c**, respectively, are lower than the activation barriers associated with the formation of **7'a** or **7'c**, through a transition structure *exo* **TS5a** or **TS5c**, respectively (Table 4a and 4b, compare entry 1 with 2, and entry 7 with 8). In addition, these activation barriers are lower than those associated with an electrophilic aromatic substitution process, through transition structures **TS7a**,**c**, **TS7'a**,**c**, **TS8a**,**c** and **TS8'a**,**c** (for a full comparison of energetics see Table 4a and 4b, entries 1–6 and 7–12, and Figure 21) which could lead to zwitterionic intermediates **Z3a**,**c**, **Z3'a**,**c**, **Z4a**,**c** and **Z4'a**,**c**, respectively. In the case of nitrosoalkene **2c** (R = CO_2Me) the formation of an earlier molecular complex **C2** had to be taken into account when ΔZPVE was used, since the transition structure associated with the transformation were located below the separated reagents **2c**/**2'c** and **6a**. Analogous results have been achieve when M06-2X/6-31G*//B3LYP/6-31G*, B3LYP/6-311+G**//B3LYP/6-31G* and M06-2X/6-311+G**//B3LYP/6-31G* levels of theory have been used, both in gas phase and in the presence of water as the solvent (Table 4a and 4b, entries 1–12, and Figure

22). Since the *endo* process is very asynchronous, especially in the case of nitrosoalkene **2c**, it can be assume that the formation of oximes **8a**,**c** takes place through a concerted asynchronous [4+2] cycloaddition process, kinetically favoured, to give oxazines **7a**,**c** whose opening and subsequent rearomatization give oximes **8a**,**c**.



Scheme 2. Possible pathways for the formation of oximes **8a,c**.

Table 4a. Activation energies (ΔE_a, kcal/mol) associated with the formation of **7**, **7'** and zwitterionic intermediates **Z3–4a**,**c** and **Z'3–4a**,**c** of the reaction between nitrosoalkenes **2a**,**c** and pyrrole (**6a**) using ΔZPVE correction. Synchronicities associated with the formation of **7** and **7'**.

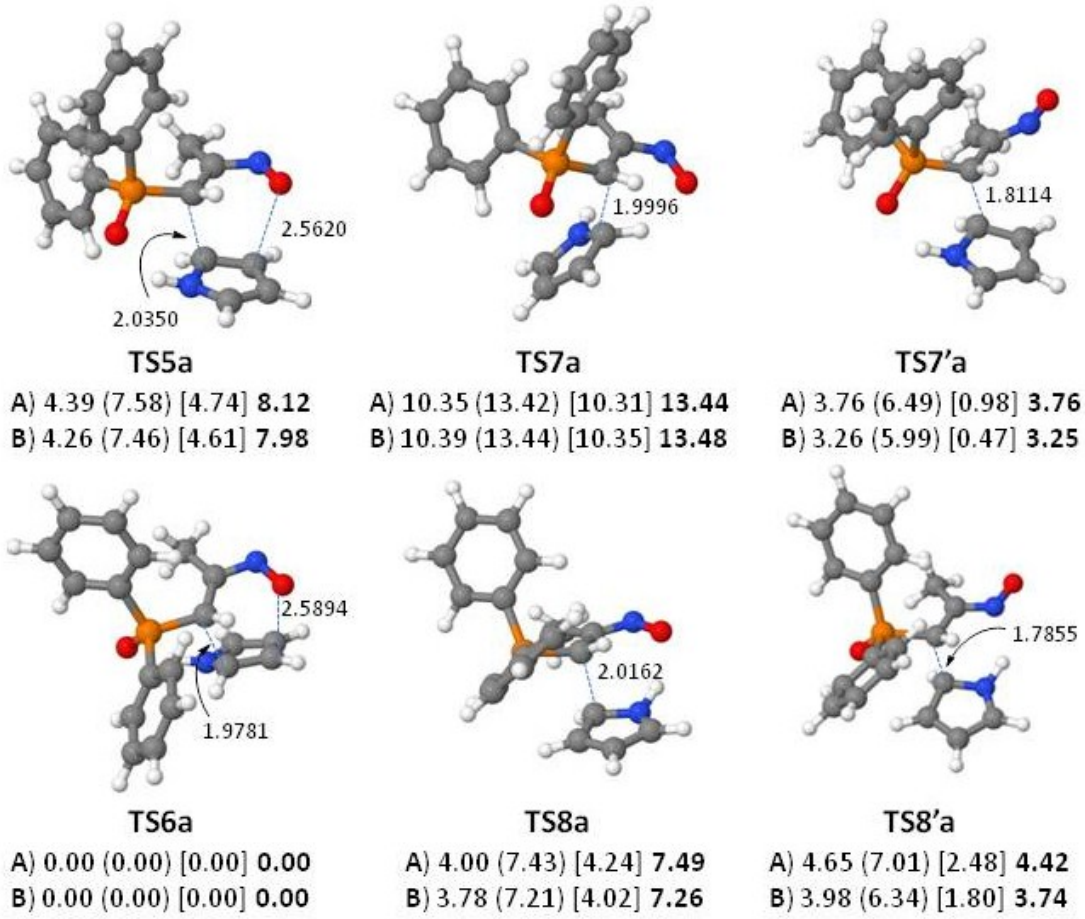
Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]	*Sy*[i]
1	**2a + 6a→7'**	**TS5a**	16.32	14.34	9.72	10.50	17.93	18.01	11.70	12.07	0.814
2	**2a + 6a→7**	**TS6a**	12.22	9.95	2.61	2.92	13.52	13.27	4.15	3.95	0.808
3	**2a + 6a→Z3a**	**TS7a**	25.30	20.30	18.72	16.34	26.77	23.58	20.42	17.39	–
4	**2a + 6a→Z3'a**	**TS7'a**	19.62	13.71	13.92	9.41	19.14	14.25	13.82	7.71	–
5	**2a + 6a→Z4a**	**TS8a**	16.53	13.95	10.49	10.35	18.25	17.51	12.28	11.44	–
6	**2a + 6a→Z4'a**	**TS8'a**	20.56	14.60	15.05	9.93	20.74	15.75	15.16	8.37	–
7	**2c + 6a**→C2→**7'c**	**TS5c**	9.12	7.43	12.58	11.30	9.81	7.76	13.06	11.54	0.708
8	**2c + 6a**→C2→**7c**	**TS6c**	5.47	2.85	4.39	1.96	6.45	3.34	5.03	2.16	0.695
9	**2c + 6a**→C2→**Z3c**	**TS7c**	18.24	15.63	21.93	19.73	19.34	16.16	22.42	11.73	–
10	**2c + 6a**→C2→**Z3'c**	**TS7'c**	13.15	10.69	15.28	13.07	14.53	11.47	16.65	13.94	–
11	**2c + 6a**→C2→**Z4c**	**TS8c**	13.24	10.04	16.97	13.95	14.47	10.75	17.78	14.33	–
12	**2c + 6a**→C2→**Z4'c**	**TS8'c**	12.45	7.56	9.76	4.69	14.00	8.25	11.22	5.31	–

[a] Computed at the B3LYP/6-31G* + ΔZPVE level. [b] Computed a B3LYP(PCM)/6-31G* +ΔZPVE level using water as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔZPVE level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔZPVE level using water as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔZPVE level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using water as solvent. [g] Computed at the M06-2X/6-311+G**//B3LYP/6-31G* + ΔZPVE level. [h] Computed at the M06-2X(PCM)/6-311+G**//B3LYP/6-31G* + ΔZPVE level using water as solvent. [i] Computed at the B3LYP/6–31G* level according to approach and equations described previously.[11]

Table 4b. Activation energies (ΔE_a, kcal/mol) associated with the formation of **7**, **7'** and zwitterionic intermediates **Z3–4a**,**c** and **Z'3–4a**,**c** of the reaction between nitrosoalkenes **2a**,**c** and pyrrole (**6a**) using ΔG correction.

Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]
1	**2a + 6a→7'**	**TS5a**	30.62	31.15	26.54	27.32	34.74	34.82	28.51	28.88
2	**2a + 6a→7**	**TS6a**	26.66	26.89	19.56	19.86	30.47	30.21	21.09	20.90
3	**2a + 6a→Z3a**	**TS7a**	39.77	37.29	35.71	33.30	43.76	40.57	37.41	34.38
4	**2a + 6a→Z3'a**	**TS7'a**	33.55	30.15	30.37	25.85	35.58	30.69	30.26	24.15
5	**2a + 6a→Z4a**	**TS8a**	30.74	30.67	27.21	27.07	34.97	34.23	29.00	28.16
6	**2a + 6a→Z4'a**	**TS8'a**	34.32	30.87	31.32	26.20	37.01	32.02	31.43	24.64
7	**2c + 6a→7'c**	**TS5c**	17.27	18.62	12.24	14.10	21.42	22.63	14.48	16.28
8	**2c + 6a→7c**	**TS6c**	14.67	15.10	5.11	5.82	19.11	19.27	7.51	7.96
9	**2c + 6a→Z3c**	**TS7c**	26.92	27.36	22.13	23.06	31.48	31.57	24.37	17.01
10	**2c + 6a→Z3'c**	**TS7'c**	21.93	22.46	17.23	18.09	25.64	25.92	19.10	19.77
11	**2c + 6a→Z4c**	**TS8c**	21.29	21.14	16.53	16.65	25.98	25.52	19.11	18.98
12	**2c + 6a→Z4'c**	**TS8'c**	21.71	19.81	12.20	10.19	25.59	23.18	14.15	11.63

[a] Computed at the B3LYP/6-31G* + ΔG correction level. [b] Computed a B3LYP(PCM)/6-31G* + ΔG correction level using water as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔG correction level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔG correction level using water as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔG correction level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using water as solvent. [g] Computed at the M06-2X/6-311+G**//B3LYP/6-31G* + ΔG correction level. [h] Computed at the M06-2X(PCM)/6-311+G**//B3LYP/6-31G* + ΔG correction level using water as solvent.



TS5a
A) 4.39 (7.58) [4.74] **8.12**
B) 4.26 (7.46) [4.61] **7.98**

TS7a
A) 10.35 (13.42) [10.31] **13.44**
B) 10.39 (13.44) [10.35] **13.48**

TS7'a
A) 3.76 (6.49) [0.98] **3.76**
B) 3.26 (5.99) [0.47] **3.25**

TS6a
A) 0.00 (0.00) [0.00] **0.00**
B) 0.00 (0.00) [0.00] **0.00**

TS8a
A) 4.00 (7.43) [4.24] **7.49**
B) 3.78 (7.21) [4.02] **7.26**

TS8'a
A) 4.65 (7.01) [2.48] **4.42**
B) 3.98 (6.34) [1.80] **3.74**

Figure 21. Fully optimized transition structures for the reaction of nitrosoalkene **2a** and pyrrole (**6a**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS6a** computed at B3LYP(PCM)/6-31G* level using water as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using water as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using water as solvent. Bold numbers are the relative energies differences calculated at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* level using water as solvent.

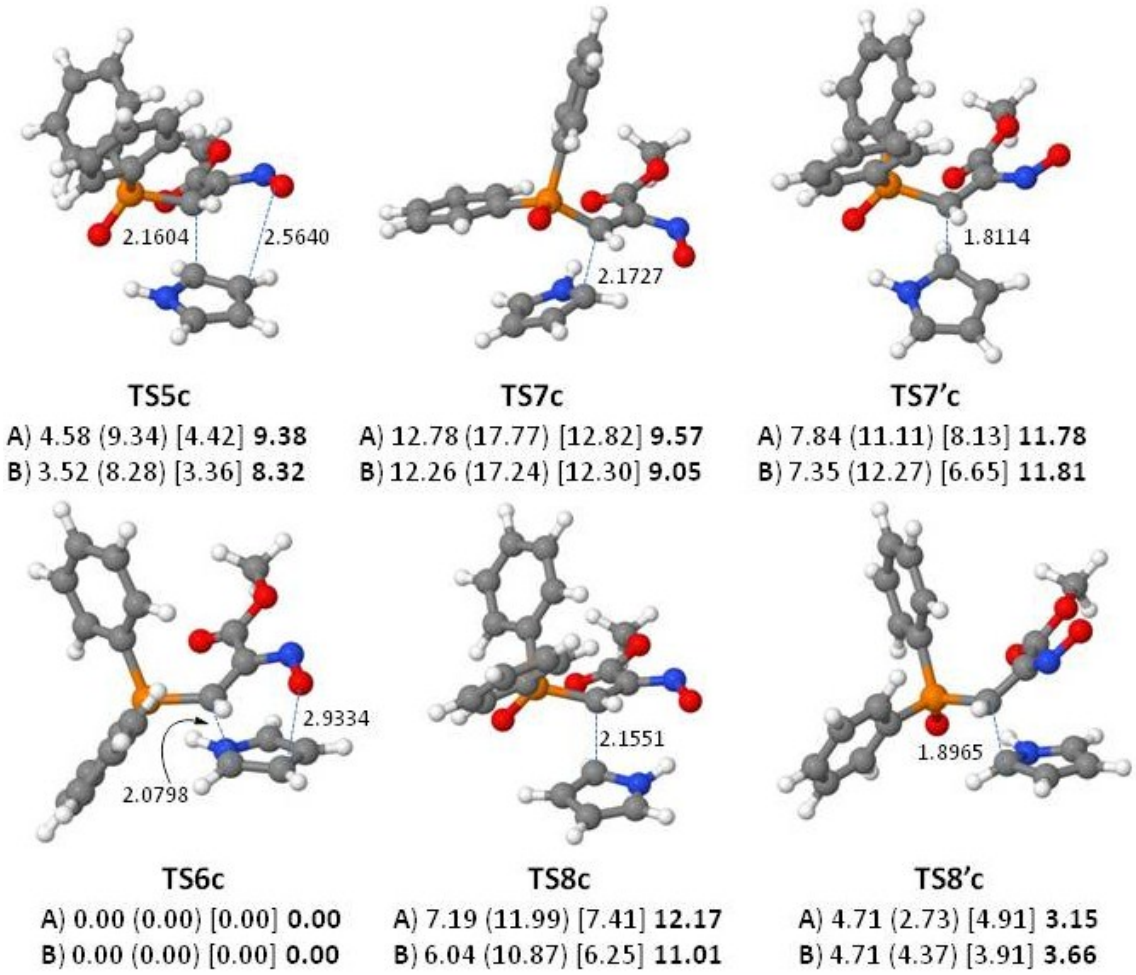


Figure 22. Fully optimized transition structures for the reaction of nitrosoalkene **2c** and pyrrole (**6a**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS6c** computed at B3LYP(PCM)/6-31G* level using water as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using water as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using water as solvent. Bold numbers are the relative energies differences calculated at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* level using water as solvent.

We also studied the tautomeric equilibrium between oxazines **7** and the corresponding oximes **8**[12] in order to study the stability of both isomers. Free energy differences computed at different levels of theory (for a full comparison of energetics see Figure 23), using water as the solvent, indicate that oximes **8a**,**c** are more stable than oxazines **7a**,**c** (this stability difference is in the range of 20 kcal/mol). Therefore, these results indicated that the formation of the open chain tautomeric oximes **8a**,**c** is favoured over cyclic tautomeric oxazines **7a**,**c** and confirms the experimental results. Moreover, in the case of oxime **8a**, the *E*-configuration is more stable than the *Z*-configuration (Figure 23a), while for oxime **8c** the *Z*-configuration is more stable than *E*-configuration (Figure 23b), most likely in order to avoid steric repulsions between both oxygen atoms in the ester and the hydroxyimino groups. In addition, free energy differences computed at different levels of theory, using water as the solvent, indicate similar stability for the *Z* and *E*-configuration of oxime **8b** (Figure 23c), and this confirm the experimental results where a mixture of *Z* and *E* oximes **8b** were obtained.

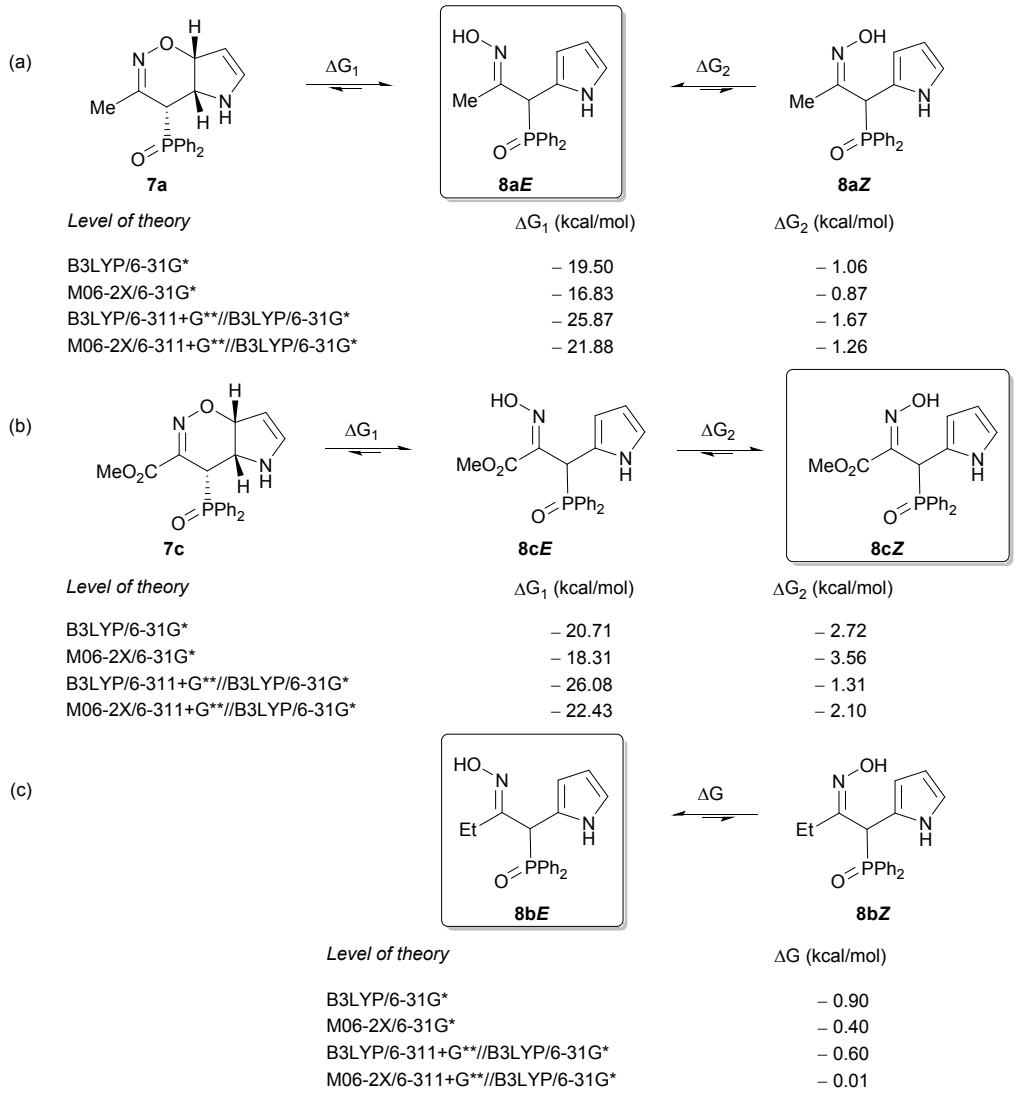


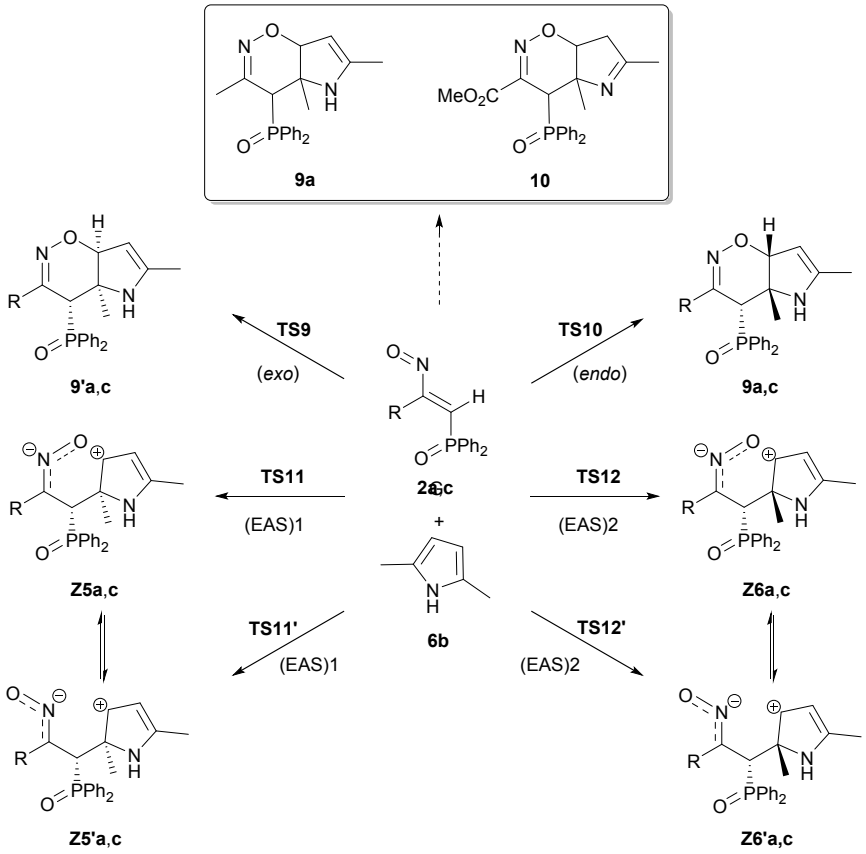
Figure 23. (a) Tautomeric equilibria between oxazine **7a** and oxime **8a**, and oximes **8a*E*** and **8a*Z***. (b) Tautomeric equilibria between oxazine **7c** and oxime **8c**, and oximes **8c*E*** and **8c*Z***. (c) Tautomeric equilibrium between oximes **8b*E*** and **8b*Z***.

*3. Reactivity of 2,5-dimethylpyrrole (**6b**) towards nitrosoalkenes **2a** and **2c**.*

Finally the reaction of nitrosoalkenes **2a**,**c** with 2,5-dimethylpyrrole (**6b**) was also studied. Experimentally, the reaction of **2a**,**c** with **6b** in methylene chloride at room temperature, gave the corresponding oxazines **9a** or **10** in good yields. Similarly to the previous reaction with indole (**3**) and pyrrole (**6a**), oxazines **9** and **10** may be formed *via* six pathways depicted in Scheme 3. The process may be begun by an electrophilic aromatic substitution from nitrosoalkenes **2a**,**c** to the C–2 of **6b**, *via* transition structures **TS11**, **TS11'**, **TS12** or **TS12'**, to give zwitterionic intermediates **Z5**, **Z5'**, **Z6** or **Z6'**, respectively, followed by a cyclization reaction to give oxazines **9'a,c** or **9a**,**c**. However, another pathways involving a concerted [4+2] cycloaddition reaction through transition structures **TS9** or **TS10** between the nitrosoalkenes **2a**,**c** and 2,5-dimethylpyrrole (**6b**) could also explain the formation of oxazines **9'** and **9** (Scheme 3).

We computationally calculated the optimized transition structures energies at different levels of theory. Thus, when using both nitrosoalkenes **2a** or **2c**, computational results indicate that the activation barriers associated with a concerted process to form **9a** or **9c**, through transition structures *endo* **TS10a** or **TS10c**, are lower than the activation barriers associated with the formation of **9'a**,**c** through transition structures *exo* **TS9a** or **TS9c** (Table 5a and 5b, compare entry 1 with 2, and entry 7 with 8). Moreover, these activation barriers are lower than those associated with

an electrophilic aromatic substitution process by means transition structures **TS11a**,**c**, **TS11'a,c**, **TS12a**,**c** or **TS12'a**,**c** (for a full comparison of energetics see Table 5a and 5b, entries 1–6 and 7–12, and Figure 24 and 25), which could lead to the formation of zwitterionic intermediates **Z5a**,**c**, **Z5'a**,**c**, **Z6a**,**c** and **Z6'a**,**c**, respectively. As in previous studies, in the case of nitrosoalkene **2c** (R = CO_2Me) the formation of an earlier molecular complex **C3** had to be assumed when ΔZPVE was used, since the transition structure associated with the transformation were located below the separated reagents **2c**/**2'c** and **6b**. Comparable results has been obtained when M06-2X/6-31G*//B3LYP/6-31G*, B3LYP/6-311+G**//B3LYP/6-31G* and M06-2X/6-311+G**//B3LYP/6-31G* levels of theory have been used, both in gas phase and in the presence of methylene chloride as the solvent (Table 5a and 5b, entries 1–12, and Figure 24 and 25). Moreover, the *endo* processes are asynchronous, especially in the case of nitrosoalkene **2c**. Under these premises, it can be presumed that the formation of oxazines **9** takes place through a concerted asynchronous [4+2] cycloaddition process kinetically favoured.



Scheme 3. Possible pathways for the formation of oxazines **9** and **10**.

Table 5a. Activation energies (ΔE_a, kcal/mol) associated with the formation of **9**, **9'** and zwitterionic intermediates **Z5**,**6a**,**c** and **Z5'**,**6'a**,**c** of the reaction between nitrosoalkenes **2a**,**c** and 2,5-dimethylpyrrole (**6b**) using ΔZPVE correction. Synchronicities associated with the formation of **9** and **9'**.

Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]	*Sy*[i]
1	**2a + 6b→9'a**	**TS9a**	18.32	18.35	10.75	10.81	21.46	21.10	11.46	11.14	0.829
2	**2a + 6b→9a**	**TS10a**	15.98	15.88	4.70	4.62	18.52	18.02	4.87	4.36	0.811
3	**2a + 6b→Z5a**	**TS11a**	31.66	28.02	24.64	20.84	34.25	29.75	24.70	20.07	–
4	**2a + 6b→Z5'a**	**TS11'a**	28.71	23.49	20.68	14.73	29.83	20.88	19.21	12.03	–
5	**2a + 6b→Z6a**	**TS12a**	16.77	16.62	9.01	8.82	19.76	19.18	9.38	8.73	–
6	**2a + 6b→Z6'a**	**TS12'a**	20.79	18.13	13.80	10.09	22.23	18.48	12.63	7.74	–
7	**2c + 6b→**C3**→9'c**	**TS9c**	10.36	7.39	11.01	8.26	10.70	7.15	11.07	7.82	0.726
8	**2c + 6b→**C3**→9c**	**TS10c**	6.22	4.20	3.23	1.39	6.75	4.24	3.56	1.26	0.705
9	**2c + 6b→**C3**→Z5c**	**TS11c**	12.52	11.48	15.48	14.77	12.47	11.13	15.37	14.41	–
10	**2c + 6b→**C3**→Z5'c**	**TS11'c**	15.69	13.41	17.90	15.73	14.84	12.06	17.06	14.40	–
11	**2c + 6b→**C3**→Z6c**	**TS12c**	13.05	9.30	12.72	9.21	13.43	8.82	12.79	8.54	–
12	**2c + 6b→**C3**→Z6'c**	**TS12'c**	24.21	20.06	28.19	23.73	23.29	18.09	26.87	21.46	–

[a] Computed at the B3LYP/6-31G* + ΔZPVE level. [b] Computed a B3LYP(PCM)/6-31G* +ΔZPVE level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔZPVE. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔZPVE level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [g] Computed at the M06-2X/6-311+G**// B3LYP/6-31G* + ΔZPVE level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔZPVE level using methylene chloride as solvent. [i] Computed at the B3LYP/6–31G* level according to approach and equations described previously.[11]

Table 5b. Activation energies (ΔE_a, kcal/mol) associated with the formation of **9**, **9'** and zwitterionic intermediates **Z5**,**6a**,**c** and **Z5'**,**6'a**,**c** of the reaction between nitrosoalkenes **2a**,**c** and 2,5-dimethylpyrrole (**6b**) using ΔG correction.

Entry	Reaction	TS	ΔE_a[a]	ΔE_a[b]	ΔE_a[c]	ΔE_a[d]	ΔE_a[e]	ΔE_a[f]	ΔE_a[g]	ΔE_a[h]
1	**2a + 6b→9'a**	**TS9a**	33.52	33.54	25.94	26.01	36.65	36.29	26.66	26.34
2	**2a + 6b→9a**	**TS10a**	31.87	31.77	20.59	20.50	34.41	33.90	20.75	20.25
3	**2a + 6b→Z5a**	**TS11a**	46.40	42.76	39.38	35.59	48.99	44.49	39.44	34.81
4	**2a + 6b→Z5'a**	**TS11'a**	43.89	38.67	35.86	29.91	45.01	36.06	34.39	27.21
5	**2a + 6b→Z6a**	**TS12a**	32.05	31.91	24.30	24.10	35.04	34.46	24.66	24.02
6	**2a + 6b→Z6'a**	**TS12'a**	35.95	33.28	28.96	25.25	37.38	33.64	27.79	22.89
7	**2c + 6b→9'c**	**TS9c**	20.38	22.30	11.21	13.66	23.90	25.85	12.37	14.86
8	**2c + 6b→9c**	**TS10c**	17.33	20.19	4.53	7.89	21.04	24.03	5.96	9.39
9	**2c + 6b→Z5c**	**TS11c**	22.25	26.10	15.39	19.89	25.38	29.53	16.38	21.16
10	**2c + 6b→Z5'c**	**TS11'c**	25.62	28.22	18.01	21.04	27.94	30.66	18.26	21.35
11	**2c + 6b→Z6c**	**TS12c**	22.99	24.13	12.85	14.54	26.55	27.44	14.01	15.51
12	**2c + 6b→Z6'c**	**TS12'c**	34.70	35.43	28.85	29.59	36.90	37.24	28.64	28.96

[a] Computed at the B3LYP/6-31G* + ΔG correction level. [b] Computed a B3LYP(PCM)/6-31G* + ΔG correction level using methylene chloride as solvent. [c] Computed at the M06-2X/6-31G*// B3LYP/6-31G* + ΔG correction level. [d] Computed at the M06-2X(PCM)/6-31G*//B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [e] Computed at the B3LYP/6-311+G**// B3LYP/6-31G* + ΔG correction level. [f] Computed at the B3LYP (PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent. [g] Computed at the M06-2X/6-311+G**// B3LYP/6-31G* + ΔG correction level. [h] Computed at the M06-2X(PCM)/6-311+G**// B3LYP/6-31G* + ΔG correction level using methylene chloride as solvent.

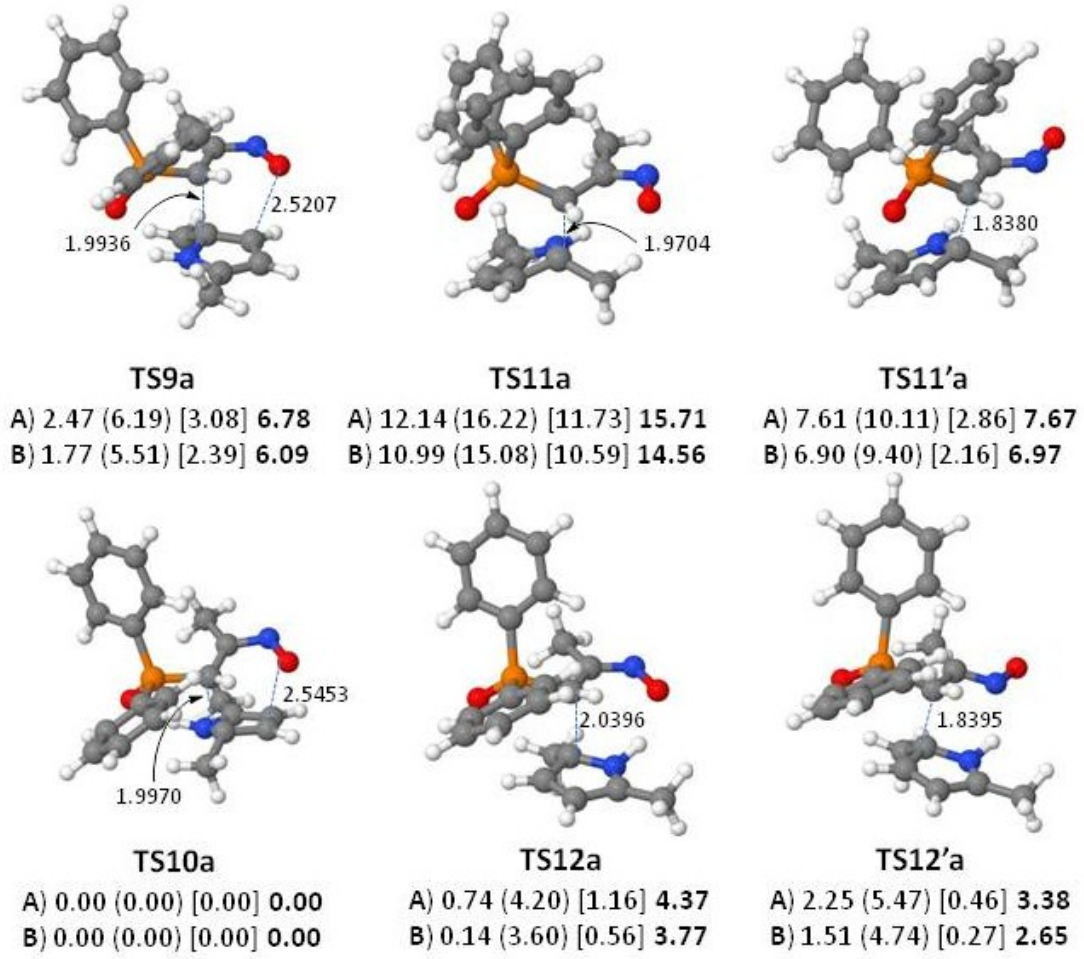


Figure 24. Fully optimized transition structures for the reaction of nitrosoalkene **2a** and 2,5-dimethylpyrrole (**6b**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS10a** computed at B3LYP(PCM)/6-31G* level using CH_2Cl_2 as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Bold numbers are the relative energies differences calculated a M06-2X(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent.

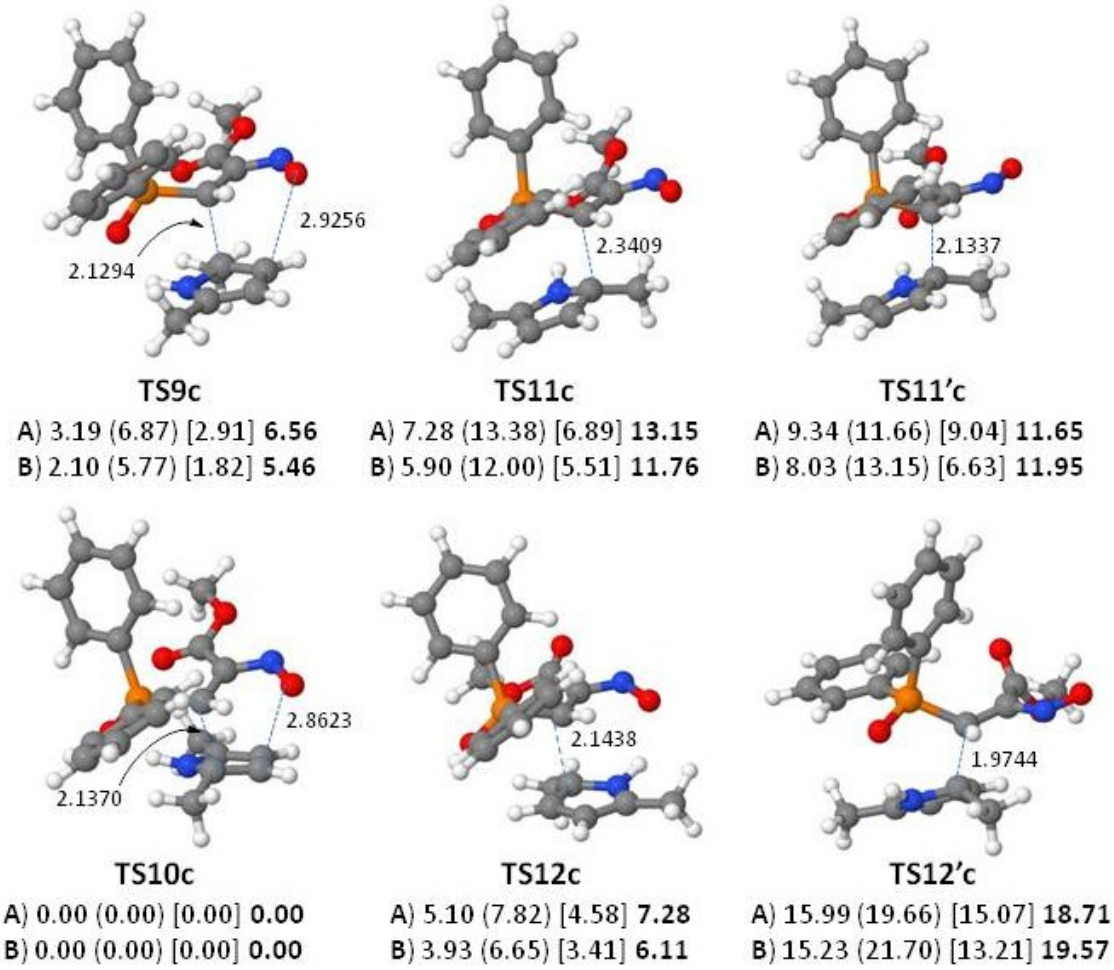
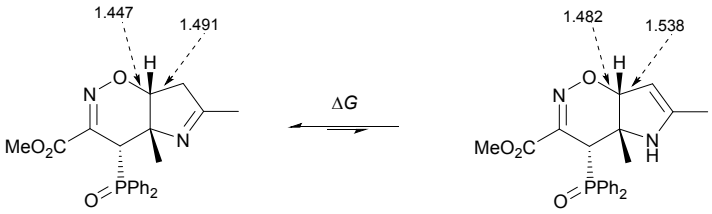


Figure 25. Fully optimized transition structures for the reaction of nitrosoalkene **2c** and 2,5-dimethylpyrrole (**6b**). Selected bond lengths are given in Å. The numbers correspond to the relative energy differences (in kcal/mol) **A**) using ΔZPVE correction and **B**) using ΔG correction, with respect to **TS10c** computed at B3LYP(PCM)/6-31G* level using CH_2Cl_2 as solvent. Numbers within parentheses correspond to relative energy differences computed at M06-2X(PCM)/6-31G*//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Numbers in square brackets are the relative energies differences calculated at B3LYP(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent. Bold numbers are the relative energies differences calculated at M06-2X(PCM)/6-311+G**//B3LYP/6-31G* level using CH_2Cl_2 as solvent.

Since experimentally oxazine **9c** was obtained as iminic tautomer **10**, we investigated the tautomeric equilibrium between iminic **10** and enaminic oxazine **9c**. Free energy differences computed at different levels of theory using CH_2Cl_2 as solvent indicate that iminic oxazine **10** are more stable than enaminic oxazine **9c** (for a full comparison of energetics see Figure 26). Moreover, the O–C and C–C bond distances in compounds **9c** are higher than in compounds **10** (Figure 26). These structural differences could explain the preferential formation of iminic tautomeric oxazine **10** in order to increase its stability.



	ΔG (kcal/mol)
B3LYP/6-31G*	– 5.31
M06-2X/6-31G*	– 4.69
B3LYP/6-311+G**//B3LYP/6-31G*	– 2.46
M06-2X/6-311+G**//B3LYP/6-31G*	– 2.04

Figure 26. Tautomeric equilibrium for compounds **9c** and**10** (distances are given in Å).

Computational data of the stationary points discussed.

Total electronic and thermal free energies, zero-point vibrational energies (ΔZPVE, in a.u.), and Cartesian coordinates and number of imaginary frequencies (NIMAG) of all the stationary points discussed. If NIMAG = 1, the imaginary frequency ν (in parentheses) is given in cm^{-1}. Values of HF in parenthesis correspond to energies (E, in a.u.) calculated using water as the solvent

2a

HF=-1126.5041888 NIMAG = 0
Zero-point correction= 0.256250 (Hartree/Particle)
Thermal correction to Energy= 0.273998
Thermal correction to Enthalpy= 0.274942
Thermal correction to Gibbs Free Energy= 0.207658
Sum of electronic and zero-point Energies= -1126.247939
Sum of electronic and thermal Energies= -1126.230191
Sum of electronic and thermal Enthalpies= -1126.229246
Sum of electronic and thermal Free Energies= -1126.296531

B3LYP (PCM)/6-31G* HF=-1126.5142519 (-1126.51626)	M06-2X/6-31G* HF=-1126.1307727	B3LYP/6-311+G** HF=-1126.740841	M06-2X/6-311+G** HF=-1126.371686
	M06-2X(PCM)/6-31G* HF=-1126.141359 (-1126.143498)	B3LYP(PCM)/6-311+G** HF=-1126.75252 (-1126.754868)	M06-2X(PCM)/6-311+G** HF=-1126.38372 (-1126.386159)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.685535	-0.480209	-1.305051
2	6	0	-2.828659	-0.410831	-0.127314
3	6	0	-1.544549	-0.190280	-0.474273
4	8	0	-4.859930	-0.687903	-1.046306
5	1	0	-1.360839	-0.088162	-1.544335
6	6	0	-3.437389	-0.584618	1.227402
7	1	0	-2.686149	-0.469696	2.008714
8	1	0	-4.242080	0.145832	1.368241
9	1	0	-3.905218	-1.573420	1.300365
10	15	0	-0.115558	-0.006374	0.641625
11	8	0	-0.432544	-0.018997	2.110333
12	6	0	2.822084	-3.421040	-0.414294
13	6	0	2.081417	-2.839170	-1.445417
14	6	0	1.180940	-1.811378	-1.165308
15	6	0	1.019118	-1.354359	0.151766
16	6	0	1.757110	-1.951460	1.184146
17	6	0	2.656844	-2.978810	0.899465
18	1	0	3.521259	-4.223132	-0.634800
19	1	0	2.198844	-3.190062	-2.467011
20	1	0	0.600366	-1.383610	-1.977802
21	1	0	1.607025	-1.611524	2.204392
22	1	0	3.224763	-3.437040	1.704487
23	6	0	1.692813	4.076357	-0.565772
24	6	0	1.711708	3.034911	-1.497219
25	6	0	1.182495	1.789401	-1.162184
26	6	0	0.627781	1.578894	0.108679
27	6	0	0.615834	2.625233	1.041392
28	6	0	1.147790	3.870124	0.702426
29	1	0	2.106706	5.046101	-0.828878
30	1	0	2.141998	3.192019	-2.482508
31	1	0	1.219423	0.982773	-1.889317
32	1	0	0.195731	2.446946	2.026585
33	1	0	1.138063	4.677390	1.429661

2'a

HF=-1126.4981727 NIMAG = 0

Zero-point correction= 0.255546 (Hartree/Particle)

Thermal correction to Energy= 0.273643

Thermal correction to Enthalpy= 0.274588

Thermal correction to Gibbs Free Energy= 0.205568

Sum of electronic and zero-point Energies= -1126.242626

Sum of electronic and thermal Energies= -1126.224529

Sum of electronic and thermal Enthalpies= -1126.223585

Sum of electronic and thermal Free Energies= -1126.292605

B3LYP (PCM)/6-31G* HF=-1126.50753 (-1126.50941)	M06-2X/6-31G* HF=-1126.125012	B3LYP/6-311+G** HF=-1126.73427	M06-2X/6-311+G** HF=-1126.365414
	M06-2X(PCM)/6-31G* HF=-1126.135026 (-1126.13706)	B3LYP(PCM)/6-311+G** HF=-1126.745093 (-1126.74728)	M06-2X(PCM)/6-311+G** HF=-1126.376776 (-1126.379095)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.640697	3.974933	0.868109
2	8	0	-0.708258	3.619122	2.027751
3	6	0	-0.452490	2.887383	-0.125625
4	6	0	-0.274963	1.629602	0.309137
5	6	0	-0.473098	3.423476	-1.523130
6	1	0	-0.309674	1.498530	1.392265
7	1	0	-1.419319	3.947904	-1.706920
8	1	0	0.324705	4.166498	-1.648285
9	1	0	-0.348641	2.625097	-2.255099
10	15	0	-0.021296	0.146453	-0.709931
11	8	0	-0.074733	0.355546	-2.197488
12	6	0	-3.406358	-2.723256	0.599330
13	6	0	-2.495970	-2.279846	1.562276
14	6	0	-1.460562	-1.419635	1.200035
15	6	0	-1.329661	-0.995449	-0.130631
16	6	0	-2.244703	-1.444202	-1.092855
17	6	0	-3.279050	-2.306705	-0.726517
18	1	0	-4.212428	-3.394138	0.884192
19	1	0	-2.591871	-2.605376	2.594503
20	1	0	-0.753961	-1.092049	1.957655
21	1	0	-2.131125	-1.112488	-2.120435
22	1	0	-3.984413	-2.652987	-1.477034
23	6	0	4.093538	-1.584592	0.510137
24	6	0	3.286537	-1.025277	1.503421
25	6	0	2.041864	-0.489495	1.173249
26	6	0	1.592977	-0.513976	-0.156239
27	6	0	2.413024	-1.067075	-1.150216
28	6	0	3.657117	-1.602523	-0.815680
29	1	0	5.063931	-1.999202	0.769635
30	1	0	3.628685	-0.999597	2.534406
31	1	0	1.435989	-0.043052	1.956699
32	1	0	2.069890	-1.059274	-2.180312
33	1	0	4.287258	-2.029111	-1.591315

2c

HF=-1315.0489232 NIMAG = 0

Zero-point correction= 0.270960 (Hartree/Particle)

Thermal correction to Energy= 0.291746

Thermal correction to Enthalpy= 0.292690

Thermal correction to Gibbs Free Energy= 0.218863

Sum of electronic and zero-point Energies= -1314.777963
Sum of electronic and thermal Energies= -1314.757177
Sum of electronic and thermal Enthalpies= -1314.756233
Sum of electronic and thermal Free Energies= -1314.830060

B3LYP (PCM)/6-31G* HF=-1315.061911 (-1315.064524)	M06-2X/6-31G* HF=-1314.612269	B3LYP/6-311+G** HF=-1315.342365	M06-2X/6-311+G** HF=-1314.911832
	M06-2X(PCM)/6-31G* HF=-1315.62604 (-1314.628834)	B3LYP(PCM)/6-311+G** HF=-1315.357023 (-1315.359999)	M06-2X(PCM)/6-311+G** HF=-1314.927081 (-1314.930196)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.198691	2.590025	-0.028613
2	6	0	-0.829029	1.640168	-0.170006
3	6	0	-2.164077	2.067316	-0.220960
4	6	0	-2.469571	3.425151	-0.121156
5	6	0	-1.446862	4.363110	0.027962
6	6	0	-0.114772	3.944521	0.070724
7	15	0	-0.361947	-0.108837	-0.398706
8	6	0	0.679309	-0.469450	1.064857
9	6	0	2.017304	-0.574245	1.025775
10	6	0	2.892971	-0.287715	-0.170694
11	8	0	3.323012	-1.411280	-0.742198
12	6	0	4.122840	-1.230820	-1.928324
13	1	0	5.014488	-0.642469	-1.699461
14	6	0	-1.843191	-1.133151	-0.102529
15	6	0	-2.194977	-2.043401	-1.108084
16	6	0	-3.299184	-2.880137	-0.937862
17	6	0	-4.052426	-2.814666	0.235217
18	6	0	-3.704548	-1.910191	1.242431
19	6	0	-2.603515	-1.071220	1.076015
20	8	0	0.331632	-0.435000	-1.689818
21	7	0	2.643419	-0.903262	2.290649
22	8	0	3.861349	-0.940815	2.244956
23	8	0	3.183331	0.838725	-0.512030
24	1	0	0.204815	-0.645237	2.030175
25	1	0	-4.910504	-3.468138	0.367632
26	1	0	-4.290510	-1.858732	2.155942
27	1	0	-2.347568	-0.364063	1.861582
28	1	0	-1.593441	-2.087166	-2.011102
29	1	0	-3.569032	-3.583934	-1.720333
30	1	0	-1.686945	5.420082	0.106803
31	1	0	-3.505909	3.749113	-0.162618
32	1	0	-2.964724	1.344316	-0.341426
33	1	0	1.238868	2.274130	-0.013838
34	1	0	0.683178	4.673695	0.179590
35	1	0	4.393225	-2.236613	-2.248567
36	1	0	3.530975	-0.724409	-2.694117

2'c

HF=-1315.0432958 NIMAG = 0
Zero-point correction= 0.270313 (Hartree/Particle)
Thermal correction to Energy= 0.291340
Thermal correction to Enthalpy= 0.292284
Thermal correction to Gibbs Free Energy= 0.216498
Sum of electronic and zero-point Energies= -1314.772983
Sum of electronic and thermal Energies= -1314.751956
Sum of electronic and thermal Enthalpies= -1314.751011
Sum of electronic and thermal Free Energies= -1314.826797

B3LYP (PCM)/6-31G* HF=-1315.056227 (-1315.058869)	M06-2X/6-31G* HF=-1314.607567	B3LYP/6-311+G** HF=-1315.336451	M06-2X/6-311+G** HF=-1314.906621
	M06-2X(PCM)/6-31G* HF=-1315.621315 (-1314.624151)	B3LYP(PCM)/6-311+G** HF=-1315.351247 (-1315.354308)	M06-2X(PCM)/6-311+G** HF=-1314.92207 (-1314.925289)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.505084	-1.425057	-1.420003
2	6	0	1.977712	-0.711249	-0.335669
3	6	0	2.761056	-0.508274	0.809840
4	6	0	4.055692	-1.021876	0.871458
5	6	0	4.576006	-1.737424	-0.210386
6	6	0	3.802253	-1.936291	-1.354718
7	15	0	0.262348	-0.099060	-0.498243
8	8	0	-0.276293	-0.298024	-1.885355
9	6	0	0.239676	1.635274	0.069597
10	6	0	0.287280	2.626090	-0.921227
11	6	0	0.299276	3.973916	-0.562533
12	6	0	0.259558	4.340215	0.784403
13	6	0	0.200309	3.357634	1.774803
14	6	0	0.187983	2.008276	1.420418
15	6	0	-0.611211	-1.039848	0.814776
16	6	0	-1.892589	-1.432987	0.780709
17	7	0	-2.433974	-2.359524	1.797346
18	8	0	-1.762853	-2.434880	2.804918
19	6	0	-2.866088	-1.174609	-0.327905
20	8	0	-2.939756	0.134895	-0.608316
21	6	0	-3.678416	0.471537	-1.798422
22	1	0	-3.732928	1.559888	-1.806737
23	8	0	-3.501580	-2.052371	-0.864445
24	1	0	-0.025058	-1.406909	1.659265
25	1	0	5.585697	-2.136107	-0.160560
26	1	0	4.207579	-2.489186	-2.197671
27	1	0	1.891291	-1.567687	-2.304143
28	1	0	2.372709	0.062044	1.650068
29	1	0	4.659753	-0.860795	1.760140
30	1	0	0.266982	5.390613	1.062661
31	1	0	0.155541	3.641082	2.822738
32	1	0	0.119933	1.254158	2.200139
33	1	0	0.298947	2.331717	-1.966543
34	1	0	0.334946	4.737773	-1.334441
35	1	0	-3.133506	0.106806	-2.672092
36	1	0	-4.676930	0.030245	-1.765863

3

HF=-363.8166882 NIMAG = 0

Zero-point correction= 0.129923 (Hartree/Particle)

Thermal correction to Energy= 0.136253

Thermal correction to Enthalpy= 0.137198

Thermal correction to Gibbs Free Energy= 0.099584

Sum of electronic and zero-point Energies= -363.686765

Sum of electronic and thermal Energies= -363.680435

Sum of electronic and thermal Enthalpies= -363.679491

Sum of electronic and thermal Free Energies= -363.717104

B3LYP (PCM)/6-31G* HF=-363.8226804	M06-2X/6-31G* HF=-363.6596427	B3LYP/6-311+G** HF=-363.9138461	M06-2X/6-311+G** HF=-363.7564817
	M06-2X(PCM)/6-31G*	B3LYP(PCM)/6-311+G**	M06-2X(PCM)/6-311+G**

	HF=-363.666382	HF=-363.920169	HF=-363.7635599

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.159219	0.691734	0.000005
2	6	0	0.982434	1.428995	-0.000160
3	6	0	-0.250101	0.751910	-0.000201
4	6	0	-0.247791	-0.671974	-0.000075
5	6	0	0.935260	-1.418785	0.000134
6	6	0	2.135957	-0.718630	0.000209
7	6	0	-1.626087	1.166801	0.000053
8	6	0	-2.390313	0.030278	0.000406
9	7	0	-1.566602	-1.080960	-0.000419
10	1	0	-1.998477	2.182076	0.000083
11	1	0	-3.465221	-0.086962	0.001121
12	1	0	0.918097	-2.505832	0.000037
13	1	0	1.011281	2.515763	-0.000264
14	1	0	3.073371	-1.268193	0.000475
15	1	0	3.116260	1.206467	0.000036
16	1	0	-1.880560	-2.038581	-0.000791

4a

HF=-1490.3611534 NIMAG = 0

Zero-point correction= 0.392713 (Hartree/Particle)

Thermal correction to Energy= 0.416083

Thermal correction to Enthalpy= 0.417027

Thermal correction to Gibbs Free Energy= 0.338309

Sum of electronic and zero-point Energies= -1489.968441

Sum of electronic and thermal Energies= -1489.945071

Sum of electronic and thermal Enthalpies= -1489.944127

Sum of electronic and thermal Free Energies= -1490.022844

B3LYP (PCM)/6-31G* HF=-1490.37485	M06-2X/6-31G* HF=-1489.857570	B3LYP/6-311+G** HF=-1490.685168	M06-2X/6-311+G** HF=-1490.190321
	M06-2X(PCM)/6-31G* HF=-1489.872464	B3LYP(PCM)/6-311+G** HF=-1490.700691	M06-2X(PCM)/6-311+G** HF=-1490.206999

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745470	-1.908340	0.513260
2	6	0	-0.240045	-0.481134	0.605824
3	6	0	-1.508453	0.412339	0.761998
4	6	0	-2.204888	-0.088219	2.065879
5	8	0	-1.727560	-1.384583	2.483199
6	7	0	-1.537319	-2.341349	1.428981
7	6	0	-0.468438	-2.824357	-0.642337
8	15	0	1.006201	0.101001	-0.637619
9	6	0	-2.607171	0.280783	-0.283916
10	7	0	-3.620639	-0.054857	1.765479
11	6	0	-3.810368	-0.017163	0.376703
12	6	0	-2.587455	0.421366	-1.667042
13	6	0	-3.781823	0.259151	-2.384141
14	6	0	-4.971099	-0.039973	-1.716777
15	6	0	-5.002671	-0.181399	-0.325504
16	8	0	0.574940	0.104126	-2.080088
17	6	0	2.491490	-0.937646	-0.367550
18	6	0	1.427995	1.788528	-0.057511

19	6	0	2.916724	-1.413156	0.882884
20	6	0	4.080174	-2.176189	0.986997
21	6	0	4.828680	-2.471749	-0.154094
22	6	0	4.408588	-2.008343	-1.402057
23	6	0	3.244758	-1.246985	-1.510333
24	6	0	1.967534	2.066507	1.207719
25	6	0	2.255070	3.380359	1.575237
26	6	0	2.010064	4.426422	0.681653
27	6	0	1.480596	4.156191	-0.580752
28	6	0	1.190115	2.841960	-0.951002
29	1	0	0.276738	-0.399909	1.574875
30	1	0	-1.206131	1.458677	0.884660
31	1	0	-1.972141	0.524082	2.941827
32	1	0	-1.014893	-3.760206	-0.504855
33	1	0	-0.774387	-2.351026	-1.581747
34	1	0	0.602581	-3.041618	-0.722975
35	1	0	-4.195409	-0.682717	2.315679
36	1	0	-1.654367	0.618039	-2.185811
37	1	0	-3.776751	0.361138	-3.465539
38	1	0	-5.890423	-0.168099	-2.282812
39	1	0	-5.929464	-0.413107	0.192468
40	1	0	2.342969	-1.208568	1.782474
41	1	0	4.397569	-2.544425	1.958696
42	1	0	5.733623	-3.067446	-0.070255
43	1	0	4.984100	-2.243280	-2.293257
44	1	0	2.900044	-0.895708	-2.478268
45	1	0	2.179543	1.262165	1.907039
46	1	0	2.673785	3.587721	2.556263
47	1	0	2.236085	5.449565	0.969795
48	1	0	1.293685	4.967433	-1.279015
49	1	0	0.783448	2.615649	-1.931899

4’a

HF=-1490.360078 NIMAG = 0

Zero-point correction= 0.392617 (Hartree/Particle)

Thermal correction to Energy= 0.416137

Thermal correction to Enthalpy= 0.417081

Thermal correction to Gibbs Free Energy= 0.337442

Sum of electronic and zero-point Energies= -1489.967462

Sum of electronic and thermal Energies= -1489.943942

Sum of electronic and thermal Enthalpies= -1489.942997

Sum of electronic and thermal Free Energies= -1490.022636

B3LYP (PCM)/6-31G* HF= -1490.376006	M06-2X/6-31G* HF=-1489.856419	B3LYP/6-311+G** HF=-1490.684062	M06-2X/6-311+G** HF=-1490.189060
	M06-2X(PCM)/6-31G* HF=-1489.873784	B3LYP(PCM)/6-311+G** HF=-1490.702110	M06-2X(PCM)/6-311+G** HF=-1490.208461

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.039190	-1.064411	1.698025
2	7	0	-1.257315	-2.227213	1.204353
3	8	0	-0.846307	-2.373148	-0.158961
4	6	0	-0.522831	0.103646	0.884264
5	6	0	-1.350482	-0.862891	3.152188
6	6	0	-1.168626	0.094387	-0.523037
7	6	0	-1.244105	-1.360952	-1.084397
8	15	0	1.346692	0.206304	1.027397
9	8	0	1.743771	0.108466	2.476161
10	6	0	1.815316	1.786006	0.218156

11	6	0	2.107195	-1.108188	0.013205
12	6	0	2.201013	-1.060715	-1.386431
13	6	0	2.779117	-2.118715	-2.087336
14	6	0	3.270837	-3.229038	-1.396369
15	6	0	3.191450	-3.276242	-0.004009
16	6	0	2.614323	-2.219497	0.700482
17	6	0	3.124776	1.932704	-0.270417
18	6	0	3.559703	3.153126	-0.785326
19	6	0	2.693820	4.247651	-0.819834
20	6	0	1.394470	4.118905	-0.328365
21	6	0	0.960550	2.898816	0.191313
22	7	0	-2.622359	-1.514719	-1.535303
23	6	0	-3.421050	-0.485308	-1.038899
24	6	0	-2.625707	0.529318	-0.483965
25	6	0	-4.810042	-0.360601	-1.093914
26	6	0	-5.388638	0.808096	-0.588645
27	6	0	-4.605582	1.830192	-0.046655
28	6	0	-3.212146	1.686799	0.008452
29	1	0	-0.838111	1.014373	1.407017
30	1	0	-0.450816	-0.502358	3.663916
31	1	0	-1.682982	-1.801116	3.602202
32	1	0	-2.136976	-0.106904	3.275135
33	1	0	-0.592899	0.725934	-1.209623
34	1	0	-0.550226	-1.531062	-1.910299
35	1	0	1.840022	-0.192620	-1.931663
36	1	0	2.851848	-2.073880	-3.170723
37	1	0	3.721319	-4.052537	-1.944072
38	1	0	3.580503	-4.135297	0.535507
39	1	0	2.559322	-2.239559	1.784430
40	1	0	3.807729	1.088974	-0.247521
41	1	0	4.575552	3.248690	-1.158807
42	1	0	3.031651	5.197972	-1.224135
43	1	0	0.716715	4.967881	-0.346826
44	1	0	-0.050449	2.828930	0.580043
45	1	0	-2.977060	-2.463647	-1.538751
46	1	0	-5.425540	-1.148563	-1.519050
47	1	0	-6.469252	0.920145	-0.622981
48	1	0	-5.074048	2.733066	0.333543
49	1	0	-2.603710	2.479469	0.439852

C1

HF=-1678.8714179 NIMAG = 0

Zero-point correction= 0.401617 (Hartree/Particle)

Thermal correction to Energy= 0.431048

Thermal correction to Enthalpy= 0.431992

Thermal correction to Gibbs Free Energy= 0.333646

Sum of electronic and zero-point Energies= -1678.469801

Sum of electronic and thermal Energies= -1678.440370

Sum of electronic and thermal Enthalpies= -1678.439425

Sum of electronic and thermal Free Energies= -1678.537772

B3LYP (PCM)/6-31G* HF=-1678.887522	M06-2X/6-31G* HF=-1678.2818049	B3LYP/6-311+G** HF=-1679.2594724	M06-2X/6-311+G** HF=-1678.6771579
	M06-2X(PCM)/6-31G* HF=-1678.2991327	B3LYP(PCM)/6-311+G** HF=-1679.2769774	M06-2X(PCM)/6-311+G** HF=-1678.6957479

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.300846	-1.044703	-1.921911

2	6	0	4.425566	-0.347442	-1.070243
3	6	0	4.960943	0.280894	0.091405
4	6	0	6.321170	0.225522	0.413045
5	6	0	7.158184	-0.473269	-0.449830
6	6	0	6.652537	-1.102059	-1.606495
7	6	0	3.012224	-0.084762	-1.072968
8	6	0	2.737328	0.665501	0.040700
9	7	0	3.908206	0.892713	0.743375
10	8	0	0.070007	3.155801	0.453216
11	6	0	0.765856	3.886527	-0.580926
12	6	0	-1.205090	2.868973	0.182069
13	8	0	-1.813576	3.223444	-0.803743
14	6	0	-1.857436	2.087882	1.297912
15	7	0	-2.343708	2.807246	2.458786
16	8	0	-2.131238	4.007313	2.422033
17	6	0	-2.129026	0.772686	1.290099
18	15	0	-1.572034	-0.377670	-0.023323
19	8	0	-0.403056	0.178782	-0.788354
20	6	0	-3.078216	-0.691722	-1.002069
21	6	0	-3.781438	0.411277	-1.518476
22	6	0	-4.893268	0.207128	-2.333899
23	6	0	-5.309948	-1.089913	-2.642920
24	6	0	-4.608855	-2.187690	-2.141372
25	6	0	-3.495423	-1.991962	-1.323773
26	6	0	-1.169715	-1.889888	0.913367
27	6	0	0.148939	-2.358704	0.833314
28	6	0	0.529658	-3.490528	1.556784
29	6	0	-0.398194	-4.153309	2.361241
30	6	0	-1.713103	-3.686445	2.447227
31	6	0	-2.099626	-2.557362	1.726825
32	1	0	1.775504	4.033907	-0.199530
33	1	0	2.280796	-0.394822	-1.805989
34	1	0	-2.677752	0.382549	2.147172
35	1	0	1.791880	1.062355	0.381253
36	1	0	3.975361	1.398250	1.612684
37	1	0	4.921834	-1.531960	-2.816979
38	1	0	7.335162	-1.638756	-2.260103
39	1	0	6.711942	0.711322	1.303943
40	1	0	8.220515	-0.534620	-0.229110
41	1	0	0.867809	-1.827861	0.215881
42	1	0	1.552609	-3.850470	1.492256
43	1	0	-0.098905	-5.033221	2.924383
44	1	0	-2.435504	-4.201585	3.074335
45	1	0	-3.126953	-2.206526	1.791762
46	1	0	-3.450888	1.423585	-1.300445
47	1	0	-5.433061	1.062612	-2.730034
48	1	0	-6.178103	-1.244566	-3.278018
49	1	0	-4.926037	-3.197304	-2.387532
50	1	0	-2.952734	-2.850401	-0.940649
51	1	0	0.782712	3.296252	-1.499253
52	1	0	0.272264	4.844089	-0.761155

4c

HF=-1678.9060511 NIMAG = 0

Zero-point correction= 0.407484 (Hartree/Particle)

Thermal correction to Energy= 0.433899

Thermal correction to Enthalpy= 0.434843

Thermal correction to Gibbs Free Energy= 0.348752

Sum of electronic and zero-point Energies= -1678.498567

Sum of electronic and thermal Energies= -1678.472152

Sum of electronic and thermal Enthalpies= -1678.471208

Sum of electronic and thermal Free Energies= -1678.557299

	M06-2X/6-31G*	B3LYP/6-311+G**	M06-2X/6-311+G**

B3LYP (PCM)/6-31G* HF=-1678.9232429	HF=-1678.338671	HF=-1679.2862035	HF=-1678.7290856
	M06-2X(PCM)/6-31G* HF=-1678.3571845	B3LYP(PCM)/6-311+G** HF=-1679.3053054	M06-2X(PCM)/6-311+G** HF=-1678.7494909

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.492733	-0.565869	1.793652
2	6	0	-2.495144	-0.897110	0.443932
3	6	0	-3.705658	-1.005965	-0.257596
4	6	0	-4.930478	-0.789975	0.367645
5	6	0	-4.919938	-0.455767	1.726849
6	6	0	-3.720999	-0.344316	2.433723
7	6	0	-1.358717	-1.202973	-0.520962
8	6	0	-2.075824	-1.219612	-1.897028
9	7	0	-3.468873	-1.398612	-1.587841
10	6	0	-0.211106	-0.157147	-0.641992
11	6	0	-0.874829	1.152588	-0.989415
12	7	0	-1.690999	1.211283	-1.984773
13	8	0	-1.826354	0.000109	-2.680334
14	15	0	1.095815	-0.326748	0.684046
15	8	0	0.657247	-0.375572	2.119609
16	6	0	-0.724598	2.395107	-0.165741
17	8	0	-0.187622	2.390825	0.923147
18	6	0	1.839176	-1.944442	0.207756
19	6	0	1.755427	-2.976953	1.152569
20	6	0	2.292996	-4.234669	0.872144
21	6	0	2.920965	-4.470621	-0.351373
22	6	0	3.016045	-3.444812	-1.295256
23	6	0	2.479731	-2.188047	-1.016822
24	6	0	2.369568	0.933811	0.326581
25	6	0	2.716546	1.362493	-0.963141
26	6	0	3.730715	2.304536	-1.141779
27	6	0	4.405768	2.823786	-0.035593
28	6	0	4.059027	2.406056	1.250784
29	6	0	3.043590	1.467712	1.433134
30	8	0	-1.246181	3.482429	-0.748609
31	6	0	-1.160554	4.688446	0.030073
32	1	0	-0.116749	4.933298	0.243579
33	1	0	0.331079	-0.447232	-1.556507
34	1	0	-0.930348	-2.192849	-0.324572
35	1	0	-1.708973	-1.986290	-2.582933
36	1	0	-4.121508	-1.105014	-2.305526
37	1	0	-1.552908	-0.463221	2.328161
38	1	0	-3.735842	-0.080027	3.487149
39	1	0	-5.864563	-0.278080	2.234762
40	1	0	-5.864532	-0.874569	-0.181260
41	1	0	2.194602	0.982002	-1.837332
42	1	0	3.989213	2.634699	-2.144304
43	1	0	5.195884	3.556535	-0.176482
44	1	0	4.575216	2.816198	2.114562
45	1	0	2.749796	1.153315	2.429825
46	1	0	2.582996	-1.395414	-1.753081
47	1	0	3.512686	-3.621958	-2.245499
48	1	0	3.340676	-5.449156	-0.569155
49	1	0	2.222918	-5.028354	1.611103
50	1	0	1.273053	-2.775386	2.104085
51	1	0	-1.620829	5.460970	-0.585797
52	1	0	-1.700555	4.573194	0.973447

4'c

HF=-1678.9099639 NIMAG = 0

Zero-point correction= 0.407870 (Hartree/Particle)

Thermal correction to Energy= 0.434333

Thermal correction to Enthalpy= 0.435277

Thermal correction to Gibbs Free Energy= 0.348636

Sum of electronic and zero-point Energies= -1678.502094

Sum of electronic and thermal Energies= -1678.475631

Sum of electronic and thermal Enthalpies= -1678.474687

Sum of electronic and thermal Free Energies= -1678.561328

B3LYP (PCM)/6-31G* HF=-1678.9290503	M06-2X/6-31G* HF=-1678.3421654	B3LYP/6-311+G** HF=-1679.2914133	M06-2X/6-311+G** HF=-1678.7336362
	M06-2X(PCM)/6-31G* HF=-1678.362403	B3LYP(PCM)/6-311+G** HF=-1679.3128615	M06-2X(PCM)/6-311+G** HF=-1678.7560338

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.591451	-0.822517	2.322644
2	6	0	2.254847	-0.703985	1.091029
3	6	0	3.575470	-1.164041	0.976668
4	6	0	4.226393	-1.716951	2.079471
5	6	0	3.564315	-1.821314	3.304129
6	6	0	2.245915	-1.377548	3.423515
7	15	0	1.519673	-0.004758	-0.431929
8	8	0	2.214454	-0.471917	-1.679802
9	6	0	-0.303392	-0.518786	-0.390536
10	6	0	-1.239101	0.392504	0.416131
11	6	0	-1.872177	1.507523	-0.434473
12	8	0	-2.290274	1.055868	-1.763490
13	7	0	-1.674970	0.015106	-2.413683
14	6	0	-0.787710	-0.691179	-1.807459
15	7	0	-3.071841	1.850666	0.290295
16	6	0	-3.521614	0.682758	0.940455
17	6	0	-2.471807	-0.243700	1.039272
18	6	0	-4.774777	0.413960	1.481977
19	6	0	-4.960419	-0.815578	2.126245
20	6	0	-3.922962	-1.744331	2.229525
21	6	0	-2.662896	-1.455553	1.685181
22	6	0	-0.242095	-1.812990	-2.653031
23	8	0	-0.254322	-1.858237	-3.859033
24	8	0	0.237574	-2.799221	-1.858134
25	6	0	0.902921	-3.864420	-2.554204
26	1	0	1.775301	-3.472057	-3.082551
27	6	0	1.572661	1.818174	-0.282025
28	6	0	1.570355	2.509084	0.938892
29	6	0	1.597284	3.904379	0.955956
30	6	0	1.631900	4.618450	-0.243680
31	6	0	1.651431	3.936716	-1.462595
32	6	0	1.625938	2.542008	-1.484615
33	1	0	-0.273131	-1.513509	0.065270
34	1	0	-0.680745	0.905819	1.210397
35	1	0	-1.222562	2.370471	-0.591043
36	1	0	1.568047	1.962410	1.877686
37	1	0	1.598868	4.432571	1.905493
38	1	0	1.654186	5.704798	-0.227935
39	1	0	1.692861	4.489843	-2.396800
40	1	0	1.664748	2.004327	-2.427312
41	1	0	4.073413	-1.099718	0.013872
42	1	0	5.248589	-2.071813	1.980372
43	1	0	4.071194	-2.253846	4.162514
44	1	0	1.723335	-1.466873	4.371998

45	1	0	0.561294	-0.496926	2.435976
46	1	0	-3.755263	2.373986	-0.247516
47	1	0	-5.588374	1.129585	1.401142
48	1	0	-5.934770	-1.049797	2.546734
49	1	0	-4.091902	-2.694044	2.728232
50	1	0	-1.856429	-2.181417	1.761779
51	1	0	1.206926	-4.573057	-1.783040
52	1	0	0.225990	-4.337704	-3.269780

***E*-5a**

HF=-1490.3587103 NIMAG = 0

Zero-point correction= 0.391099 (Hartree/Particle)

Thermal correction to Energy= 0.415857

Thermal correction to Enthalpy= 0.416801

Thermal correction to Gibbs Free Energy= 0.335003

Sum of electronic and zero-point Energies= -1489.967611

Sum of electronic and thermal Energies= -1489.942853

Sum of electronic and thermal Enthalpies= -1489.941909

Sum of electronic and thermal Free Energies= -1490.023707

B3LYP (PCM)/6-31G* HF=-1490.3763373	M06-2X/6-31G* HF=-1489.8517184	B3LYP/6-311+G** HF=-1490.6941713	M06-2X/6-311+G** HF=-1490.1941419
	M06-2X(PCM)/6-31G* HF=-1489.8711112	B3LYP(PCM)/6-311+G** HF=-1490.7131717	M06-2X(PCM)/6-311+G** HF=-1490.2148415

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.134348	-0.380777	-0.288353
2	6	0	-3.870561	-0.418925	0.311010
3	6	0	-2.696414	-0.787925	-0.399544
4	6	0	-2.809191	-1.120322	-1.762548
5	6	0	-4.062693	-1.089717	-2.359330
6	6	0	-5.214410	-0.725310	-1.631584
7	7	0	-3.492886	-0.142697	1.608584
8	6	0	-2.133442	-0.335865	1.741568
9	6	0	-1.593810	-0.733603	0.539629
10	6	0	-0.159318	-1.124694	0.250999
11	6	0	0.598765	-1.617563	1.468802
12	7	0	0.920639	-2.860300	1.415622
13	8	0	1.610163	-3.264740	2.578427
14	15	0	0.681253	0.182537	-0.840628
15	8	0	0.021924	0.181758	-2.194642
16	6	0	0.506659	1.811764	-0.018982
17	6	0	-0.565853	2.606221	-0.452169
18	6	0	-0.796025	3.855055	0.125613
19	6	0	0.045185	4.326059	1.135356
20	6	0	1.121375	3.546823	1.565365
21	6	0	1.351522	2.295189	0.991841
22	6	0	2.475198	-0.185588	-0.912820
23	6	0	3.386386	0.853679	-1.166334
24	6	0	4.737889	0.579269	-1.373593
25	6	0	5.197399	-0.738296	-1.340137
26	6	0	4.298468	-1.780039	-1.107391
27	6	0	2.945696	-1.508940	-0.899950
28	6	0	0.942384	-0.743730	2.647176
29	1	0	-1.923278	-1.353750	-2.342413
30	1	0	-4.158383	-1.341083	-3.412092
31	1	0	-6.179848	-0.707995	-2.130304
32	1	0	-6.018436	-0.094351	0.275835
33	1	0	-4.113526	0.131695	2.353570

34	1	0	-1.665340	-0.188324	2.702864
35	1	0	1.759560	-4.206926	2.404003
36	1	0	-0.189544	-1.976396	-0.440890
37	1	0	0.569397	0.273253	2.530200
38	1	0	0.537241	-1.179675	3.567594
39	1	0	2.030414	-0.710469	2.779391
40	1	0	3.038692	1.881227	-1.208843
41	1	0	5.429972	1.394705	-1.566134
42	1	0	6.250615	-0.952592	-1.501392
43	1	0	4.648835	-2.808510	-1.088423
44	1	0	2.264263	-2.333132	-0.719803
45	1	0	2.200736	1.705388	1.324052
46	1	0	1.786500	3.915088	2.342067
47	1	0	-0.131696	5.301297	1.581546
48	1	0	-1.629228	4.462377	-0.217664
49	1	0	-1.201863	2.238375	-1.251215

_Z_-5a

HF=-1490.3490999 NIMAG = 0

Zero-point correction= 0.390671 (Hartree/Particle)

Thermal correction to Energy= 0.415396

Thermal correction to Enthalpy= 0.416340

Thermal correction to Gibbs Free Energy= 0.334871

Sum of electronic and zero-point Energies= -1489.958429

Sum of electronic and thermal Energies= -1489.933704

Sum of electronic and thermal Enthalpies= -1489.932760

Sum of electronic and thermal Free Energies= -1490.014229

B3LYP (PCM)/6-31G* HF=-1490.3674789	M06-2X/6-31G* HF=-1489.8443333	B3LYP/6-311+G** HF=-1490.682354	M06-2X/6-311+G** HF=-1490.185197
	M06-2X(PCM)/6-31G* HF=-1489.864199	B3LYP(PCM)/6-311+G** HF=-1490.7025613	M06-2X(PCM)/6-311+G** HF=-1490.2067021

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.802826	-0.063256	0.232671
2	6	0	-2.648677	-0.587550	-0.410185
3	6	0	-2.751009	-1.003595	-1.751119
4	6	0	-3.979613	-0.904438	-2.390034
5	6	0	-5.113566	-0.389108	-1.728303
6	6	0	-5.040765	0.043252	-0.410511
7	7	0	-3.438370	0.276103	1.521282
8	6	0	-2.112567	-0.032458	1.719035
9	6	0	-1.576572	-0.566495	0.566978
10	8	0	-0.841291	-3.416922	1.618255
11	7	0	0.103422	-2.635996	2.288704
12	6	0	0.432131	-1.516276	1.741616
13	6	0	-0.150830	-1.062980	0.404076
14	6	0	1.392269	-0.684204	2.551051
15	15	0	0.820186	0.075534	-0.745835
16	8	0	0.180869	0.017904	-2.107670
17	6	0	2.563653	-0.480953	-0.747969
18	6	0	3.561648	0.401149	-1.194659
19	6	0	4.878567	-0.033611	-1.339314
20	6	0	5.214978	-1.356774	-1.046962
21	6	0	4.229063	-2.245492	-0.615738
22	6	0	2.910224	-1.813231	-0.471576
23	6	0	0.780813	1.777616	-0.071248
24	6	0	1.698291	2.301702	0.851685
25	6	0	1.573642	3.617053	1.301526

26	6	0	0.531373	4.420749	0.835396
27	6	0	-0.380967	3.909945	-0.089758
28	6	0	-0.255627	2.597747	-0.545755
29	1	0	-1.872238	-1.352101	-2.281831
30	1	0	-4.068522	-1.219667	-3.425906
31	1	0	-6.058957	-0.322706	-2.259822
32	1	0	-5.910513	0.446873	0.101480
33	1	0	-4.059656	0.636624	2.228692
34	1	0	-1.650360	0.134276	2.681613
35	1	0	-1.448648	-2.818212	1.136169
36	1	0	-0.193398	-1.962368	-0.230437
37	1	0	0.974833	0.306859	2.765007
38	1	0	1.593809	-1.196505	3.494744
39	1	0	2.341384	-0.533028	2.026320
40	1	0	3.307986	1.429641	-1.434174
41	1	0	5.640730	0.660309	-1.683262
42	1	0	6.241407	-1.695391	-1.159265
43	1	0	4.483548	-3.277721	-0.392050
44	1	0	2.159203	-2.522627	-0.137114
45	1	0	2.522572	1.693945	1.210289
46	1	0	2.295055	4.014761	2.010381
47	1	0	0.436763	5.445234	1.185799
48	1	0	-1.186651	4.535585	-0.464252
49	1	0	-0.944928	2.201850	-1.284879

***E*-5c**

HF=-1678.9152011 NIMAG = 0

Zero-point correction= 0.405160 (Hartree/Particle)

Thermal correction to Energy= 0.433325

Thermal correction to Enthalpy= 0.434269

Thermal correction to Gibbs Free Energy= 0.342658

Sum of electronic and zero-point Energies= -1678.510041

Sum of electronic and thermal Energies= -1678.481876

Sum of electronic and thermal Enthalpies= -1678.480932

Sum of electronic and thermal Free Energies= -1678.572543

B3LYP (PCM)/6-31G* HF=-1678.933844	M06-2X/6-31G* HF=-1678.3417583	B3LYP/6-311+G** HF=-1679.3078237	M06-2X/6-311+G** HF=-1678.742526
	M06-2X(PCM)/6-31G* HF=-1678.362372	B3LYP(PCM)/6-311+G** HF=-1679.307824	M06-2X(PCM)/6-311+G** HF=-1678.764395

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.222536	-0.691272	0.120980
2	6	0	-3.873154	-0.654126	0.483893
3	6	0	-2.828172	-0.584295	-0.477859
4	6	0	-3.164663	-0.562796	-1.841946
5	6	0	-4.504582	-0.600064	-2.207884
6	6	0	-5.523922	-0.662059	-1.236173
7	7	0	-3.276367	-0.672234	1.729284
8	6	0	-1.908211	-0.617452	1.588971
9	6	0	-1.584761	-0.554629	0.253762
10	6	0	-0.208582	-0.503430	-0.362578
11	6	0	0.433088	-1.871882	-0.519349
12	7	0	0.589621	-2.301192	-1.714917
13	8	0	1.162473	-3.582334	-1.744741
14	15	0	0.904655	0.659653	0.589390
15	8	0	1.093205	0.260727	2.030977
16	6	0	2.492027	0.724171	-0.317771
17	6	0	2.597448	0.778081	-1.715303

18	6	0	3.850606	0.856232	-2.322279
19	6	0	5.007364	0.880626	-1.540064
20	6	0	4.909804	0.818787	-0.149092
21	6	0	3.657832	0.737483	0.460617
22	6	0	0.122844	2.306628	0.427050
23	6	0	-0.223626	2.885296	-0.802333
24	6	0	-0.809156	4.149779	-0.842941
25	6	0	-1.048465	4.848144	0.343176
26	6	0	-0.702485	4.279155	1.569475
27	6	0	-0.119934	3.011718	1.613197
28	6	0	0.800137	-2.664448	0.718379
29	8	0	-0.006338	-3.189790	1.450967
30	8	0	2.128384	-2.668126	0.900079
31	6	0	2.576685	-3.278320	2.123884
32	1	0	3.664955	-3.226807	2.090532
33	1	0	-2.388186	-0.532066	-2.602428
34	1	0	-4.774460	-0.586454	-3.260458
35	1	0	-6.562998	-0.691409	-1.552578
36	1	0	-6.007915	-0.743470	0.870764
37	1	0	-3.761963	-0.743421	2.609699
38	1	0	-1.251474	-0.629435	2.445764
39	1	0	1.181621	-3.777983	-2.694666
40	1	0	-0.297606	-0.104222	-1.380147
41	1	0	0.150208	2.554008	2.559980
42	1	0	-0.887843	4.820628	2.493326
43	1	0	-1.504284	5.834149	0.309283
44	1	0	-1.079260	4.589630	-1.799109
45	1	0	-0.039915	2.357641	-1.734388
46	1	0	1.710375	0.742594	-2.341172
47	1	0	3.923954	0.892312	-3.405869
48	1	0	5.982714	0.941721	-2.015635
49	1	0	5.808654	0.829645	0.461636
50	1	0	3.567004	0.673186	1.540573
51	1	0	2.189263	-2.716838	2.977593
52	1	0	2.239245	-4.315999	2.180752

_Z_-5c

HF=-1678.9183093 NIMAG = 0

Zero-point correction= 0.406188 (Hartree/Particle)

Thermal correction to Energy= 0.433933

Thermal correction to Enthalpy= 0.434877

Thermal correction to Gibbs Free Energy= 0.345154

Sum of electronic and zero-point Energies= -1678.512121

Sum of electronic and thermal Energies= -1678.484376

Sum of electronic and thermal Enthalpies= -1678.483432

Sum of electronic and thermal Free Energies= -1678.573156

B3LYP (PCM)/6-31G* HF=-1678.936782	M06-2X/6-31G* HF=-1678.3470467	B3LYP/6-311+G** HF=-1679.3083904	M06-2X/6-311+G** HF=-1678.7455068
	M06-2X(PCM)/6-31G* HF=-1678.3670622	B3LYP(PCM)/6-311+G** HF=-1679.3282143	M06-2X(PCM)/6-311+G** HF=-1678.76686

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.287599	0.116818	-0.489505
2	6	0	3.925598	-0.012745	-0.776808
3	6	0	2.933325	-0.048998	0.240001
4	6	0	3.336112	0.040090	1.583712
5	6	0	4.688962	0.169488	1.873778
6	6	0	5.655275	0.208775	0.848280
7	7	0	3.269562	-0.130857	-1.986875

8	6	0	1.912259	-0.233056	-1.772630
9	6	0	1.655281	-0.183010	-0.421923
10	6	0	0.325040	-0.275938	0.294111
11	6	0	0.094618	-1.666154	0.861862
12	7	0	0.015903	-1.958458	2.111171
13	8	0	0.081771	-0.830161	2.940367
14	15	0	-1.074643	0.464363	-0.731705
15	8	0	-1.029766	0.248326	-2.220775
16	6	0	-2.643604	-0.143262	-0.009633
17	6	0	-2.899643	-0.238547	1.366388
18	6	0	-4.143595	-0.680693	1.817215
19	6	0	-5.139779	-1.028778	0.902499
20	6	0	-4.888626	-0.940655	-0.467572
21	6	0	-3.645295	-0.501557	-0.923236
22	6	0	-0.956407	2.253117	-0.334044
23	6	0	-0.910746	2.767546	0.970254
24	6	0	-0.836220	4.143814	1.181356
25	6	0	-0.807895	5.018626	0.092508
26	6	0	-0.855103	4.513775	-1.207438
27	6	0	-0.929653	3.136547	-1.421290
28	6	0	0.005219	-2.886098	-0.022456
29	8	0	0.203305	-4.028217	0.321000
30	8	0	-0.360275	-2.512523	-1.261377
31	6	0	-0.515624	-3.565708	-2.222807
32	1	0	-0.824513	-3.068270	-3.141666
33	1	0	2.600301	-0.001638	2.382343
34	1	0	5.011516	0.238124	2.909259
35	1	0	6.705796	0.309854	1.106814
36	1	0	6.032076	0.143598	-1.281228
37	1	0	3.708363	-0.108326	-2.894109
38	1	0	1.210941	-0.309763	-2.589537
39	1	0	0.036893	-1.229702	3.824076
40	1	0	0.381435	0.387303	1.161751
41	1	0	-0.963501	2.727882	-2.426376
42	1	0	-0.831930	5.191605	-2.056635
43	1	0	-0.748384	6.090937	0.259210
44	1	0	-0.798835	4.533214	2.195195
45	1	0	-0.933059	2.103016	1.830098
46	1	0	-2.131328	0.006188	2.093706
47	1	0	-4.333409	-0.758004	2.884485
48	1	0	-6.107581	-1.372409	1.258216
49	1	0	-5.659512	-1.216149	-1.182371
50	1	0	-3.431801	-0.436236	-1.985634
51	1	0	0.431114	-4.094560	-2.362381
52	1	0	-1.276062	-4.276682	-1.889157

6a

HF=-210.1658908 NIMAG = 0

Zero-point correction= 0.082628 (Hartree/Particle)

Thermal correction to Energy= 0.086630

Thermal correction to Enthalpy= 0.087574

Thermal correction to Gibbs Free Energy= 0.056211

Sum of electronic and zero-point Energies= -210.083263

Sum of electronic and thermal Energies= -210.079261

Sum of electronic and thermal Enthalpies= -210.078317

Sum of electronic and thermal Free Energies= -210.109680

B3LYP (PCM)/6-31G* HF=-210.171054	M06-2X/6-31G* HF=-210.071803	B3LYP/6-311+G** HF=-210.230492	M06-2X/6-311+G** HF=-210.134909
	M06-2X(PCM)/6-31G* (HF=-210.07740)	B3LYP(PCM)/6-311+G** (HF=-210.235878)	M06-2X(PCM)/6-311+G** (HF=-210.140789)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.122355	0.000000
2	6	0	-1.125371	0.331556	0.000000
3	6	0	-0.712761	-0.983414	0.000000
4	6	0	0.712659	-0.983517	0.000000
5	6	0	1.125490	0.331398	0.000000
6	1	0	2.113917	0.767882	0.000000
7	1	0	1.360787	-1.849584	0.000000
8	1	0	-1.361033	-1.849372	0.000000
9	1	0	-2.113802	0.768052	0.000000
10	1	0	0.000029	2.130390	0.000000

6b

HF=-288.8065511 NIMAG = 0

Zero-point correction= 0.13837 (Hartree/Particle)

Thermal correction to Energy= 0.145727

Thermal correction to Enthalpy= 0.146671

Thermal correction to Gibbs Free Energy= 0.107153

Sum of electronic and zero-point Energies= -288.668181

Sum of electronic and thermal Energies= -288.660824

Sum of electronic and thermal Enthalpies= -288.659880

Sum of electronic and thermal Free Energies= -288.699398

B3LYP (PCM)/6-31G* HF=-288.811203	M06-2X/6-31G* HF=-288.6684876	B3LYP/6-311+G** HF=-288.8890488	M06-2X/6-311+G** HF=-288.7504714
	M06-2X(PCM)/6-31G* HF=-288,6736875	B3LYP(PCM)/6-311+G** HF=-288.8940755	M06-2X(PCM)/6-311+G** HF=-288.7560681

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000036	-0.808084	0.000196
2	6	0	1.137426	-0.023315	-0.000057
3	6	0	0.713149	1.288879	-0.000114
4	6	0	-0.713226	1.288832	0.000014
5	6	0	-1.137431	-0.023363	0.000077
6	1	0	0.000096	-1.817349	-0.000611
7	6	0	2.509780	-0.617541	0.000006
8	1	0	-1.362620	2.154745	0.000158
9	1	0	1.362491	2.154833	0.000031
10	6	0	-2.509748	-0.617569	-0.000060
11	1	0	2.695840	-1.241720	0.885388
12	1	0	2.695190	-1.243367	-0.884357
13	1	0	3.258767	0.179577	-0.000991
14	1	0	-2.695599	-1.242173	-0.885197
15	1	0	-2.695298	-1.242982	0.884549
16	1	0	-3.258818	0.179485	0.000458

7a

HF=-1525.2421976 NIMAG = 0

Zero-point correction= 0.360308 (Hartree/Particle)

Thermal correction to Energy= 0.384371

Thermal correction to Enthalpy= 0.385315

Thermal correction to Gibbs Free Energy= 0.303806

Sum of electronic and zero-point Energies= -1524.881890

Sum of electronic and thermal Energies= -1524.857826

Sum of electronic and thermal Enthalpies= -1524.856882
Sum of electronic and thermal Free Energies= -1524.938392

B3LYP (PCM)/6-31G* (HF=-1525.266150)	M06-2X/6-31G* HF=-1524.733457	B3LYP/6-311+G** HF=-1525.589926	M06-2X/6-311+G** HF=-1525.0902735
	M06-2X(PCM)/6-31G* (HF=-1524.758654)	B3LYP(PCM)/6-311+G** (HF=-1525.616832)	M06-2X(PCM)/6-311+G** (HF=-1525.118115)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.204963	-1.153883	1.521108
2	6	0	2.017942	-1.118530	0.130249
3	6	0	2.886586	-1.844861	-0.697537
4	6	0	3.933840	-2.581606	-0.143666
5	6	0	4.120532	-2.603579	1.239672
6	6	0	3.253555	-1.892325	2.071755
7	15	0	0.687881	-0.188624	-0.716867
8	8	0	0.402416	-0.710273	-2.095095
9	6	0	-0.810510	-0.375607	0.431403
10	6	0	-0.986920	0.721132	1.499008
11	6	0	-1.860546	1.895160	0.963956
12	8	0	-2.299868	1.750124	-0.427144
13	7	0	-2.738451	0.500074	-0.844202
14	6	0	-2.040810	-0.498083	-0.431670
15	6	0	-3.022260	1.929415	1.913026
16	6	0	-2.905942	0.931113	2.799099
17	7	0	-1.703305	0.218504	2.697279
18	6	0	-2.485139	-1.830171	-0.968913
19	6	0	1.187668	1.572176	-0.731001
20	6	0	2.046993	2.149556	0.215717
21	6	0	2.380822	3.502056	0.128719
22	6	0	1.865543	4.283920	-0.906837
23	6	0	1.021407	3.711081	-1.861044
24	6	0	0.683625	2.360924	-1.777270
25	1	0	-1.794116	-0.791712	2.758324
26	1	0	-3.598312	0.660699	3.589959
27	1	0	-0.625151	-1.336213	0.918907
28	1	0	-0.015122	1.107223	1.818583
29	1	0	-1.291652	2.825768	0.906262
30	1	0	2.475764	1.544828	1.009680
31	1	0	3.049983	3.940996	0.863842
32	1	0	2.128654	5.336152	-0.975095
33	1	0	0.627010	4.315037	-2.673413
34	1	0	0.038312	1.907249	-2.522388
35	1	0	2.719444	-1.837409	-1.770456
36	1	0	4.600676	-3.142986	-0.792415
37	1	0	4.935722	-3.178878	1.670261
38	1	0	3.389963	-1.914894	3.149577
39	1	0	1.534427	-0.616446	2.186859
40	1	0	-3.825858	2.650026	1.848278
41	8	0	-1.730691	-2.826507	-0.441051
42	8	0	-3.389248	-2.012920	-1.748038
43	6	0	-2.022181	-4.138526	-0.948360
44	1	0	-1.334917	-4.810498	-0.433623
45	1	0	-3.060264	-4.408886	-0.737617
46	1	0	-1.856371	-4.170309	-2.027928

7'a

HF=-1336.6920381 NIMAG = 0
Zero-point correction= 0.345338 (Hartree/Particle)
Thermal correction to Energy= 0.366292

Thermal correction to Enthalpy= 0.367237
Thermal correction to Gibbs Free Energy= 0.293822
Sum of electronic and zero-point Energies= -1336.346700
Sum of electronic and thermal Energies= -1336.325746
Sum of electronic and thermal Enthalpies= -1336.324802
Sum of electronic and thermal Free Energies= -1336.398216

B3LYP (PCM)/6-31G* (HF=-1336.712767)	M06-2X/6-31G* HF=-1336.2482831	B3LYP/6-311+G** HF=-1336.9831448	M06-2X/6-311+G** HF=-1336.5469831
	M06-2X(PCM)/6-31G* (HF=-1336.270581)	B3LYP(PCM)/6-311+G** (HF=-1337.006570)	M06-2X(PCM)/6-311+G** (HF=-1336.5717959

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.433616	-3.369098	-0.278186
2	7	0	1.561463	-2.733468	-1.060792
3	6	0	2.882505	-2.630423	-1.525491
4	1	0	3.445098	-3.546711	-1.674820
5	6	0	1.052966	-1.354395	-0.846737
6	6	0	2.182305	-0.417725	-1.386949
7	6	0	3.267342	-1.376708	-1.792384
8	8	0	2.620358	0.585672	-0.442760
9	7	0	2.916020	0.123412	0.865246
10	6	0	2.022039	-0.640466	1.378706
11	6	0	0.768884	-1.071394	0.644670
12	6	0	2.234998	-1.099167	2.792938
13	15	0	-0.624146	0.130286	1.038866
14	6	0	-0.331750	1.691719	0.142193
15	6	0	-0.565880	1.853071	-1.232065
16	6	0	-0.292768	3.072386	-1.850729
17	6	0	0.211409	4.138577	-1.101840
18	6	0	0.434687	3.987170	0.267356
19	6	0	0.163258	2.768828	0.889944
20	8	0	-0.714462	0.329448	2.527798
21	6	0	-2.130940	-0.595293	0.282813
22	6	0	-3.233342	0.249444	0.067240
23	6	0	-4.443049	-0.264623	-0.396670
24	6	0	-4.570754	-1.631118	-0.653735
25	6	0	-3.485823	-2.481376	-0.438813
26	6	0	-2.276064	-1.967817	0.030762
27	1	0	0.402420	-1.989855	1.123423
28	1	0	1.382929	-0.786866	3.407387
29	1	0	3.156890	-0.669415	3.191500
30	1	0	2.302172	-2.194507	2.843284
31	1	0	0.140604	-1.235769	-1.438517
32	1	0	1.817795	0.204661	-2.209219
33	1	0	-0.976984	1.035559	-1.818404
34	1	0	-0.478719	3.192626	-2.914648
35	1	0	0.423917	5.088184	-1.585745
36	1	0	0.820328	4.817628	0.852176
37	1	0	0.323245	2.642411	1.956120
38	1	0	-3.144508	1.313906	0.263501
39	1	0	-5.285613	0.402265	-0.557585
40	1	0	-5.512722	-2.031645	-1.018415
41	1	0	-3.578504	-3.545837	-0.635711
42	1	0	-1.449108	-2.651922	0.193876
43	1	0	4.209654	-1.064614	-2.221730

C2

HF=-1525.224096 NIMAG = 0
Zero-point correction= 0.354928 (Hartree/Particle)

Thermal correction to Energy= 0.381112
Thermal correction to Enthalpy= 0.382056
Thermal correction to Gibbs Free Energy= 0.294548
Sum of electronic and zero-point Energies= -1524.869168
Sum of electronic and thermal Energies= -1524.842984
Sum of electronic and thermal Enthalpies= -1524.842040
Sum of electronic and thermal Free Energies= -1524.929548

B3LYP (PCM)/6-31G* (HF=-1525.240002)	M06-2X/6-31G* HF=-1524.706883	B3LYP/6-311+G** HF=-1525.576623	M06-2X/6-311+G** HF=-1525.066746
	M06-2X(PCM)/6-31G* (HF=-1524.724033)	B3LYP(PCM)/6-311+G** (HF=-1525.594444)	M06-2X(PCM)/6-311+G** (HF=-1525.085689)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.732007	-1.081976	1.314597
2	6	0	-2.292528	-1.012700	-0.015700
3	6	0	-2.993227	-1.709636	-1.009267
4	6	0	-4.118639	-2.465079	-0.675867
5	6	0	-4.550589	-2.529881	0.649526
6	6	0	-3.855968	-1.838098	1.645077
7	15	0	-0.832361	-0.040958	-0.542559
8	8	0	-0.501609	-0.342676	-1.986124
9	6	0	0.420148	-0.534946	0.702957
10	6	0	1.648577	-0.029112	0.942553
11	6	0	2.241985	1.111815	0.191661
12	8	0	1.767389	1.562269	-0.833957
13	7	0	2.507535	-0.604633	1.986061
14	8	0	1.972775	-1.474531	2.650887
15	6	0	-1.234355	1.714745	-0.253538
16	6	0	-1.485979	2.505064	-1.381982
17	6	0	-1.849620	3.843221	-1.229987
18	6	0	-1.960283	4.398966	0.045728
19	6	0	-1.703373	3.615777	1.173349
20	6	0	-1.342554	2.276721	1.025895
21	8	0	3.339183	1.607211	0.788657
22	6	0	3.953554	2.716757	0.113532
23	7	0	1.855648	-1.853265	-1.696386
24	6	0	1.406876	-2.907722	-0.933937
25	6	0	2.455329	-3.347891	-0.141342
26	6	0	3.557055	-2.497922	-0.401180
27	6	0	3.145120	-1.570791	-1.354235
28	1	0	0.404747	-3.290450	-1.062588
29	1	0	3.679262	-0.756469	-1.822022
30	1	0	4.805641	2.995698	0.733358
31	1	0	0.143689	-1.365953	1.350945
32	1	0	2.426658	-4.183353	0.544603
33	1	0	1.208481	-1.227342	-2.179818
34	1	0	4.542121	-2.554017	0.041609
35	1	0	-1.376713	2.066732	-2.368976
36	1	0	-2.040133	4.453148	-2.108857
37	1	0	-2.241999	5.442066	0.162541
38	1	0	-1.780659	4.047800	2.167432
39	1	0	-1.130978	1.682228	1.910736
40	1	0	-2.640992	-1.656927	-2.034878
41	1	0	-4.655656	-3.004677	-1.451279
42	1	0	-5.425465	-3.119982	0.909003
43	1	0	-4.187693	-1.889701	2.678464
44	1	0	-2.200637	-0.551263	2.100667
45	1	0	4.284416	2.421623	-0.886041
46	1	0	3.250001	3.548431	0.023004

7c

HF=-1525.2457994 NIMAG = 0

Zero-point correction= 0.360215 (Hartree/Particle)

Thermal correction to Energy= 0.384009

Thermal correction to Enthalpy= 0.384953

Thermal correction to Gibbs Free Energy= 0.304858

Sum of electronic and zero-point Energies= -1524.885584

Sum of electronic and thermal Energies= -1524.861791

Sum of electronic and thermal Enthalpies= -1524.860847

Sum of electronic and thermal Free Energies= -1524.940941

B3LYP (PCM)/6-31G* (HF=-1525.265086)	M06-2X/6-31G* HF=-1524.7386701	B3LYP/6-311+G** HF=-1525.5928991	M06-2X/6-311+G** HF=-1525.0948986
	M06-2X(PCM)/6-31G* (HF=-1524.759360)	B3LYP(PCM)/6-311+G** (HF=-1525.614760)	M06-2X(PCM)/6-311+G** (HF=-1525.118049)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.542668	-2.667800	-1.381867
2	6	0	0.157372	-2.379885	0.004968
3	6	0	1.129284	-3.229969	0.880052
4	6	0	2.043756	-3.856639	-0.125510
5	6	0	1.693583	-3.437970	-1.356532
6	6	0	0.329566	-0.884905	0.409835
7	6	0	1.800153	-0.580919	0.601708
8	7	0	2.523178	-1.316073	1.373724
9	8	0	1.841275	-2.416647	1.892998
10	15	0	-0.754246	0.184517	-0.668991
11	8	0	-0.642397	-0.093645	-2.145019
12	6	0	2.520521	0.526530	-0.106338
13	6	0	-2.436309	-0.248916	-0.066094
14	6	0	-3.303307	-0.846100	-0.991861
15	6	0	-4.597580	-1.206687	-0.612525
16	6	0	-5.034858	-0.973792	0.691855
17	6	0	-4.177833	-0.374875	1.618811
18	6	0	-2.885288	-0.012085	1.241918
19	6	0	-0.485465	1.926843	-0.197971
20	6	0	-0.216128	2.346906	1.112659
21	6	0	-0.057485	3.704450	1.395376
22	6	0	-0.168691	4.648878	0.372977
23	6	0	-0.429591	4.233959	-0.934700
24	6	0	-0.584250	2.878168	-1.221909
25	1	0	-0.099862	-0.822828	1.421734
26	1	0	-0.885240	-2.669693	0.170860
27	1	0	0.603423	-3.931200	1.533546
28	1	0	2.854283	-4.525185	0.128323
29	1	0	-0.110421	1.624784	1.918287
30	1	0	0.156732	4.022131	2.412170
31	1	0	-0.046125	5.705636	0.594834
32	1	0	-0.505633	4.966354	-1.733757
33	1	0	-0.761869	2.541850	-2.238753
34	1	0	-2.238454	0.470759	1.969525
35	1	0	-4.517806	-0.186171	2.633502
36	1	0	-6.042424	-1.254321	0.987066
37	1	0	-5.263161	-1.668400	-1.336835
38	1	0	-2.950565	-1.017069	-2.004287
39	1	0	0.425907	-1.913583	-2.055942
40	1	0	2.173672	-3.683084	-2.298456
41	8	0	3.575876	0.988776	0.577733
42	8	0	2.178154	0.932743	-1.198435
43	6	0	4.340813	2.003104	-0.096283
44	1	0	5.144669	2.262038	0.592764

45	1	0	4.746856	1.616464	-1.034653
46	1	0	3.715938	2.874498	-0.308888

7'c

HF=-1336.6993544 NIMAG = 0

Zero-point correction= 0.345466 (Hartree/Particle)

Thermal correction to Energy= 0.366167

Thermal correction to Enthalpy= 0.367111

Thermal correction to Gibbs Free Energy= 0.294570

Sum of electronic and zero-point Energies= -1336.353888

Sum of electronic and thermal Energies= -1336.333187

Sum of electronic and thermal Enthalpies= -1336.332243

Sum of electronic and thermal Free Energies= -1336.404784

B3LYP (PCM)/6-31G* (HF=-1336.7152010)	M06-2X/6-31G* HF=-1336.2562508	B3LYP/6-311+G** HF=-1336.9902454	M06-2X/6-311+G** HF=-1336.5546772
	M06-2X(PCM)/6-31G* (HF=-1336.273322)	B3LYP(PCM)/6-311+G** (HF=-1337.008465)	M06-2X(PCM)/6-311+G** (HF=-1336.573958)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.766554	2.794008	1.008956
2	6	0	-0.888024	1.761346	0.069211
3	6	0	-1.310530	2.059835	-1.235069
4	6	0	-1.598614	3.375623	-1.594685
5	6	0	-1.472640	4.401453	-0.654141
6	6	0	-1.059459	4.109694	0.646341
7	15	0	-0.476215	0.068993	0.634199
8	6	0	-1.898906	-0.985426	0.180869
9	6	0	-2.148263	-1.443686	-1.121906
10	6	0	-3.274333	-2.222966	-1.388395
11	6	0	-4.158464	-2.549901	-0.357932
12	6	0	-3.912410	-2.102382	0.941399
13	6	0	-2.786299	-1.324978	1.212482
14	6	0	0.965030	-0.441881	-0.413451
15	6	0	1.488006	-1.860713	-0.229210
16	7	0	2.515802	-2.243207	-0.898909
17	8	0	3.029447	-1.230630	-1.755964
18	6	0	3.364270	-0.002413	-1.046205
19	6	0	2.148953	0.553331	-0.236220
20	6	0	4.429354	-0.163096	0.000327
21	6	0	3.923169	0.164705	1.200148
22	7	0	2.628652	0.678570	1.151407
23	6	0	0.888927	-2.866971	0.713543
24	8	0	-0.162108	0.033500	2.111695
25	1	0	0.669496	-0.351508	-1.469613
26	1	0	1.844754	1.537459	-0.607401
27	1	0	3.638520	0.656280	-1.875942
28	1	0	1.506077	-3.768360	0.712073
29	1	0	0.832254	-2.458745	1.728581
30	1	0	-0.131105	-3.134486	0.415483
31	1	0	5.430744	-0.514330	-0.206980
32	1	0	-1.461784	-1.213659	-1.932440
33	1	0	-3.456941	-2.579482	-2.398331
34	1	0	-5.033972	-3.158496	-0.567289
35	1	0	-4.594425	-2.363226	1.745991
36	1	0	-2.576086	-0.987279	2.223006
37	1	0	-1.430190	1.269889	-1.971680
38	1	0	-1.925387	3.600101	-2.606352
39	1	0	-1.699869	5.426019	-0.936174
40	1	0	-0.964325	4.905442	1.380012

41	1	0	-0.445512	2.552237	2.017488
42	1	0	1.969619	0.422170	1.883683
43	1	0	4.422189	0.121073	2.163186

***E*-8a**

HF=-1336.72690

Zero-point correction= 0.343685 (Hartree/Particle)

Thermal correction to Energy= 0.365992

Thermal correction to Enthalpy= 0.366936

Thermal correction to Gibbs Free Energy= 0.289269

Sum of electronic and zero-point Energies= -1336.383217

Sum of electronic and thermal Energies= -1336.360910

Sum of electronic and thermal Enthalpies= -1336.359966

Sum of electronic and thermal Free Energies= -1336.437633

B3LYP (PCM)/6-31G* (HF=-1336.740982)	M06-2X/6-31G* HF=-1336.279048	B3LYP/6-311+G** HF=-1337.029055	M06-2X/6-311+G** HF=-1336.586437
	M06-2X(PCM)/6-31G* (HF=-1336.294841)	B3LYP(PCM)/6-311+G** HF=-1337.044383)	M06-2X(PCM)/6-311+G** (HF=-1336.603519)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.518448	-2.241509	-1.387938
2	6	0	0.660540	-1.825081	-0.056287
3	6	0	1.432543	-2.589845	0.827665
4	6	0	2.058722	-3.755271	0.383168
5	6	0	1.918094	-4.162140	-0.944032
6	6	0	1.146794	-3.404632	-1.829468
7	15	0	-0.125597	-0.313607	0.610456
8	6	0	-1.925281	-0.478513	0.353552
9	6	0	-2.694002	-0.797566	1.482331
10	6	0	-4.071261	-0.984477	1.362619
11	6	0	-4.689216	-0.849953	0.118339
12	6	0	-3.930114	-0.520451	-1.006941
13	6	0	-2.552886	-0.333191	-0.892880
14	6	0	0.495430	1.079756	-0.474584
15	6	0	1.957260	1.328978	-0.191546
16	7	0	2.487945	1.296312	1.081599
17	6	0	3.821280	1.609019	1.035239
18	6	0	4.153755	1.870142	-0.279051
19	6	0	2.975920	1.692908	-1.055245
20	6	0	-0.353187	2.338077	-0.351709
21	6	0	-0.364913	3.125067	0.929711
22	7	0	-0.988757	2.645693	-1.423599
23	8	0	-1.724397	3.841534	-1.283207
24	8	0	0.216706	-0.101454	2.071192
25	1	0	-1.281355	3.712265	1.008936
26	1	0	-0.273643	2.458069	1.791472
27	1	0	0.485948	3.817339	0.952017
28	1	0	0.406501	0.744084	-1.513680
29	1	0	1.960744	0.948730	1.878569
30	1	0	4.422285	1.615086	1.933337
31	1	0	5.131642	2.157088	-0.641786
32	1	0	2.873857	1.828190	-2.124164
33	1	0	-2.203922	-0.885652	2.447234
34	1	0	-4.661176	-1.230882	2.241263
35	1	0	-5.762463	-0.993679	0.025452
36	1	0	-4.411962	-0.400674	-1.973499
37	1	0	-1.981890	-0.043851	-1.769665
38	1	0	1.534489	-2.260668	1.857154
39	1	0	2.657436	-4.343364	1.073403

40	1	0	2.407397	-5.068594	-1.290330
41	1	0	1.034565	-3.720511	-2.863054
42	1	0	-0.085843	-1.667258	-2.085391
43	1	0	-2.148998	3.915810	-2.151645

***Z*-8a**

HF=-1336.7280541

Zero-point correction= 0.344262 (Hartree/Particle)

Thermal correction to Energy= 0.366240

Thermal correction to Enthalpy= 0.367184

Thermal correction to Gibbs Free Energy= 0.291549

Sum of electronic and zero-point Energies= -1336.383792

Sum of electronic and thermal Energies= -1336.361814

Sum of electronic and thermal Enthalpies= -1336.360870

Sum of electronic and thermal Free Energies= -1336.436505

B3LYP (PCM)/6-31G* (HF=-1336.741565)	M06-2X/6-31G* HF=-1336.280638	B3LYP/6-311+G** HF=-1337.029358	M06-2X/6-311+G** HF=-1336.587511
	M06-2X(PCM)/6-31G* (HF=-1336.295737)	B3LYP(PCM)/6-311+G** (HF=-1337.044003)	M06-2X(PCM)/6-311+G** (HF=-1336.603790)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.485737	-3.047210	1.299482
2	6	0	0.086042	-2.434657	0.327150
3	8	0	-0.540265	-2.267636	2.487297
4	6	0	0.192684	-3.202843	-0.962553
5	6	0	0.683709	-1.036712	0.430602
6	15	0	-0.196354	0.202772	-0.663995
7	6	0	2.162516	-1.023255	0.124998
8	8	0	0.195395	0.065170	-2.120410
9	7	0	2.664322	-0.924201	-1.156170
10	6	0	4.032954	-0.991804	-1.122900
11	6	0	4.421012	-1.161586	0.190987
12	6	0	3.238918	-1.181447	0.980846
13	6	0	-1.996629	0.013866	-0.430053
14	6	0	-2.797900	0.259926	-1.555582
15	6	0	-4.187059	0.188786	-1.456241
16	6	0	-4.784789	-0.132562	-0.236106
17	6	0	-3.990989	-0.392015	0.882813
18	6	0	-2.600327	-0.320649	0.791293
19	6	0	0.270311	1.835144	0.015255
20	6	0	0.974528	2.707047	-0.824778
21	6	0	1.359794	3.966153	-0.361964
22	6	0	1.043953	4.359239	0.939082
23	6	0	0.337831	3.494409	1.779607
24	6	0	-0.050016	2.237006	1.320054
25	1	0	-0.321107	-4.161989	-0.867258
26	1	0	-0.242370	-2.635046	-1.792893
27	1	0	1.244555	-3.382450	-1.211683
28	1	0	0.559624	-0.699675	1.462568
29	1	0	-0.963896	-2.886129	3.102133
30	1	0	2.072968	-0.685211	-1.948428
31	1	0	4.615703	-0.906806	-2.029016
32	1	0	5.438309	-1.262133	0.544754
33	1	0	3.173053	-1.310712	2.053262
34	1	0	-2.321422	0.493184	-2.502992
35	1	0	-4.801644	0.379662	-2.331816
36	1	0	-5.867385	-0.189692	-0.158989
37	1	0	-4.454475	-0.659318	1.828734
38	1	0	-1.997852	-0.564618	1.661249

39	1	0	1.211250	2.388306	-1.835182
40	1	0	1.906802	4.638418	-1.017366
41	1	0	1.344935	5.339294	1.299591
42	1	0	0.087733	3.800989	2.791625
43	1	0	-0.609863	1.577658	1.978289

***E*-8b**

HF=-1376.0387356 NIMAG = 0

Zero-point correction= 0.373007 (Hartree/Particle)

Thermal correction to Energy= 0.396379

Thermal correction to Enthalpy= 0.397323

Thermal correction to Gibbs Free Energy= 0.318001

Sum of electronic and zero-point Energies= -1375.665728

Sum of electronic and thermal Energies= -1375.642357

Sum of electronic and thermal Enthalpies= -1375.641412

Sum of electronic and thermal Free Energies= -1375.720734

B3LYP (PCM)/6-31G* (HF=-1376.0.52581)	M06-2X(PCM)/6-31G* (HF=-1375.587382)	B3LYP(PCM)/6-311+G** (HF=-1376.365612)	M06-2X(PCM)/6-311+G** (HF=-1375.906484)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.535777	2.268629	1.168428
2	6	0	-1.626603	1.691599	0.298978
3	7	0	-2.129984	1.835844	-0.978422
4	6	0	-3.343098	2.471788	-0.929186
5	6	0	-3.619807	2.761668	0.391728
6	6	0	-0.285405	1.060541	0.581201
7	6	0	0.867538	2.060054	0.562974
8	7	0	1.557460	2.058491	1.647173
9	8	0	2.598780	3.011206	1.611509
10	15	0	-0.030540	-0.394890	-0.568468
11	8	0	-0.231594	-0.024776	-2.023137
12	6	0	-1.242673	-1.649298	-0.014323
13	6	0	-1.272916	-2.161687	1.290763
14	6	0	-2.218936	-3.121885	1.645262
15	6	0	-3.138547	-3.580692	0.698415
16	6	0	-3.109728	-3.078284	-0.602950
17	6	0	-2.165199	-2.114750	-0.960024
18	6	0	1.627100	-1.095687	-0.262102
19	6	0	2.298800	-1.624996	-1.374071
20	6	0	3.546208	-2.229386	-1.218057
21	6	0	4.132215	-2.306408	0.046583
22	6	0	3.472755	-1.771410	1.155288
23	6	0	2.224657	-1.166950	1.005083
24	6	0	1.115608	2.978655	-0.609994
25	6	0	2.284634	2.530016	-1.508956
26	1	0	0.201245	3.057916	-1.203479
27	1	0	1.335282	3.973670	-0.207721
28	1	0	-0.315270	0.650927	1.597328
29	1	0	-1.687941	1.403259	-1.785988
30	1	0	-3.908482	2.661258	-1.830393
31	1	0	-4.500248	3.271874	0.758674
32	1	0	-2.421283	2.335116	2.242577
33	1	0	1.839929	-1.546868	-2.355138
34	1	0	4.061213	-2.636149	-2.084111
35	1	0	5.104877	-2.775804	0.167951
36	1	0	3.933985	-1.817071	2.138139
37	1	0	1.741336	-0.724724	1.870345
38	1	0	-2.131365	-1.715757	-1.969154

39	1	0	-3.823134	-3.434540	-1.341130
40	1	0	-3.875069	-4.329762	0.976681
41	1	0	-2.238178	-3.513251	2.658759
42	1	0	-0.556286	-1.822486	2.034312
43	1	0	2.979692	2.923571	2.498838
44	1	0	2.458351	3.279976	-2.288814
45	1	0	3.204101	2.421391	-0.927347
46	1	0	2.060584	1.579902	-2.001791

Z-8b

HF=-1376.0408284 NIMAG = 0

Zero-point correction= 0.372976 (Hartree/Particle)

Thermal correction to Energy= 0.396329

Thermal correction to Enthalpy= 0.397273

Thermal correction to Gibbs Free Energy= 0.318146

Sum of electronic and zero-point Energies= -1375.667853

Sum of electronic and thermal Energies= -1375.644500

Sum of electronic and thermal Enthalpies= -1375.643556

Sum of electronic and thermal Free Energies= -1375.722682

B3LYP (PCM)/6-31G* (HF=-1376.054155)	M06-2X(PCM)/6-31G* (HF=-1375.588143)	B3LYP(PCM)/6-311+G** (HF=-1373.366775)	M06-2X(PCM)/6-311+G** (HF=-1375.906685)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.632316	2.408351	1.242673
2	6	0	0.782541	1.901235	-0.056322
3	6	0	1.622810	2.559462	-0.963183
4	6	0	2.309190	3.710508	-0.573231
5	6	0	2.160152	4.208402	0.721669
6	6	0	1.320668	3.556984	1.629329
7	15	0	-0.078803	0.398946	-0.644450
8	6	0	-1.867867	0.663501	-0.393480
9	6	0	-2.609674	1.004178	-1.534816
10	6	0	-3.973528	1.275539	-1.429147
11	6	0	-4.605743	1.204263	-0.186469
12	6	0	-3.874244	0.851936	0.949571
13	6	0	-2.508930	0.580966	0.851521
14	6	0	0.499058	-0.957540	0.510431
15	6	0	1.928846	-1.321689	0.188368
16	7	0	2.412359	-1.411667	-1.100614
17	6	0	3.725975	-1.802479	-1.075231
18	6	0	4.090257	-1.993509	0.242492
19	6	0	2.954812	-1.688607	1.042210
20	6	0	-0.431989	-2.166126	0.513366
21	6	0	-0.542520	-3.017200	-0.732391
22	7	0	-1.112837	-2.538555	1.534421
23	8	0	-0.937891	-1.689400	2.660752
24	8	0	0.238046	0.099621	-2.094972
25	6	0	-1.547449	-4.168011	-0.652135
26	1	0	-0.784095	-2.356671	-1.576348
27	1	0	0.459800	-3.407402	-0.954909
28	1	0	0.491656	-0.537888	1.519187
29	1	0	-1.491450	-2.132875	3.321723
30	1	0	1.881084	-1.073722	-1.899418
31	1	0	4.292380	-1.906432	-1.989695
32	1	0	5.061253	-2.317274	0.592541
33	1	0	2.882956	-1.743050	2.120673
34	1	0	-2.109824	1.041494	-2.497980
35	1	0	-4.542368	1.538270	-2.316951

36	1	0	-5.668885	1.414476	-0.104065
37	1	0	-4.369011	0.779590	1.914470
38	1	0	-1.963496	0.268800	1.737052
39	1	0	1.729755	2.159828	-1.966911
40	1	0	2.961119	4.216147	-1.280380
41	1	0	2.695942	5.103774	1.025473
42	1	0	1.201709	3.944750	2.637400
43	1	0	-0.025371	1.916724	1.954966
44	1	0	-1.556342	-4.720338	-1.597962
45	1	0	-1.291217	-4.863991	0.151899
46	1	0	-2.559531	-3.799582	-0.458267

***E*-8c**

HF=-1525.2701448 NIMAG = 0

Zero-point correction= 0.358529 (Hartree/Particle)

Thermal correction to Energy= 0.383801

Thermal correction to Enthalpy= 0.384746

Thermal correction to Gibbs Free Energy= 0.300402

Sum of electronic and zero-point Energies= -1524.911616

Sum of electronic and thermal Energies= -1524.886343

Sum of electronic and thermal Enthalpies= -1524.885399

Sum of electronic and thermal Free Energies= -1524.969743

B3LYP (PCM)/6-31G* (HF=-1525.289298)	M06-2X/6-31G* HF=-1524.757314	B3LYP/6-311+G** HF=-1525.6290259	M06-2X/6-311+G** HF=-1525.1232561
	M06-2X(PCM)/6-31G* (HF=-1524.778418	B3LYP(PCM)/6-311+G** (HF=-1525.649778)	M06-2X(PCM)/6-311+G** (HF=-1525.145994)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.124515	-2.979356	1.272339
2	6	0	-0.853488	-1.937561	0.402157
3	7	0	-1.086931	-2.393490	-0.878783
4	6	0	-1.470593	-3.707562	-0.835493
5	6	0	-1.514433	-4.098951	0.488307
6	6	0	-0.469028	-0.508014	0.683878
7	6	0	-1.673473	0.400868	0.841510
8	7	0	-1.682398	1.189618	1.849954
9	8	0	-2.847323	1.970263	1.897840
10	15	0	0.779782	0.093253	-0.599633
11	8	0	0.372722	-0.276988	-2.006508
12	6	0	2.343146	-0.718426	-0.105915
13	6	0	2.809505	-0.801776	1.215052
14	6	0	4.018143	-1.439435	1.495122
15	6	0	4.768191	-2.002033	0.459852
16	6	0	4.306844	-1.929007	-0.855335
17	6	0	3.098418	-1.291769	-1.138709
18	6	0	0.981194	1.893417	-0.376006
19	6	0	0.064998	2.727017	-1.039399
20	6	0	0.174333	4.112192	-0.925289
21	6	0	1.196076	4.676836	-0.158590
22	6	0	2.113271	3.852970	0.495294
23	6	0	2.008856	2.465706	0.386958
24	6	0	-2.792059	0.352616	-0.177483
25	8	0	-2.722793	0.856585	-1.277647
26	8	0	-3.845211	-0.324781	0.291027
27	6	0	-4.960199	-0.437180	-0.613742
28	1	0	0.049517	-0.465296	1.647532
29	1	0	-0.813807	-1.849482	-1.696249
30	1	0	-1.670844	-4.257985	-1.743700
31	1	0	-1.797552	-5.077440	0.852464

32	1	0	-1.066924	-2.929126	2.351956
33	1	0	-0.729559	2.287148	-1.633711
34	1	0	-0.538506	4.750930	-1.439621
35	1	0	1.280881	5.757310	-0.075658
36	1	0	2.916020	4.288301	1.084437
37	1	0	2.740151	1.836400	0.884058
38	1	0	2.721460	-1.240428	-2.155647
39	1	0	4.885334	-2.372149	-1.661350
40	1	0	5.708013	-2.501091	0.680413
41	1	0	4.370805	-1.501572	2.520992
42	1	0	2.237032	-0.371656	2.032902
43	1	0	-5.707359	-1.022788	-0.078752
44	1	0	-5.348622	0.553739	-0.861951
45	1	0	-4.653093	-0.946160	-1.530609
46	1	0	-2.704656	2.505719	2.694052

Z-8c

HF=-1525.2755861 NIMAG = 0

Zero-point correction= 0.359089 (Hartree/Particle)

Thermal correction to Energy= 0.384134

Thermal correction to Enthalpy= 0.385078

Thermal correction to Gibbs Free Energy= 0.300679

Sum of electronic and zero-point Energies= -1524.916497

Sum of electronic and thermal Energies= -1524.891452

Sum of electronic and thermal Enthalpies= -1524.890508

Sum of electronic and thermal Free Energies= -1524.974907

B3LYP (PCM)/6-31G* (HF=-1525.2939052)	M06-2X/6-31G* HF=-1524.7643431	B3LYP/6-311+G** HF=-1525.6324157	M06-2X/6-311+G** HF=-1525.1281454
	M06-2X(PCM)/6-31G* (HF=-1524.7843637)	B3LYP(PCM)/6-311+G** (HF=-1525.6521387)	M06-2X(PCM)/6-311+G** (HF=-1525.1496188)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.853895	-0.217430	1.203001
2	6	0	2.425942	-0.313743	-0.129831
3	6	0	3.341901	-0.690681	-1.121635
4	6	0	4.669105	-0.961109	-0.785933
5	6	0	5.090354	-0.858061	0.540460
6	6	0	4.181369	-0.487577	1.534366
7	15	0	0.717951	0.043685	-0.688797
8	6	0	0.438306	1.841068	-0.496196
9	6	0	0.063701	2.536222	-1.654641
10	6	0	-0.141336	3.915728	-1.607834
11	6	0	0.024436	4.607429	-0.407221
12	6	0	0.392795	3.918000	0.750693
13	6	0	0.600778	2.539889	0.708883
14	6	0	-0.367139	-0.851352	0.574620
15	6	0	-0.723855	-2.245792	0.117155
16	7	0	-0.968394	-2.580827	-1.193281
17	6	0	-1.306960	-3.902541	-1.276937
18	6	0	-1.304839	-4.429713	0.001198
19	6	0	-0.934809	-3.381846	0.884990
20	6	0	-1.585914	-0.075660	1.033372
21	6	0	-2.725774	0.105387	0.073196
22	7	0	-1.743234	0.456980	2.192593
23	8	0	-0.609764	0.318795	3.007150
24	8	0	0.511119	-0.393068	-2.117610
25	1	0	0.261096	-0.961676	1.460820
26	1	0	-0.902680	0.738997	3.831594
27	1	0	-0.778995	-1.934828	-1.955169

28	1	0	-1.512378	-4.363434	-2.232532
29	1	0	-1.542358	-5.450614	0.268505
30	1	0	-0.841111	-3.439105	1.961890
31	1	0	-0.063837	1.982393	-2.579238
32	1	0	-0.430701	4.448886	-2.509435
33	1	0	-0.134151	5.682103	-0.371302
34	1	0	0.517674	4.454397	1.687591
35	1	0	0.871317	2.015502	1.619872
36	1	0	2.996967	-0.778180	-2.147231
37	1	0	5.372099	-1.256480	-1.560117
38	1	0	6.123468	-1.070952	0.802088
39	1	0	4.504928	-0.414051	2.569159
40	1	0	2.158628	0.058804	1.991454
41	8	0	-3.894381	0.373975	0.672704
42	8	0	-2.573727	0.026672	-1.129086
43	6	0	-4.997070	0.602931	-0.221430
44	1	0	-5.854140	0.799783	0.422652
45	1	0	-4.794290	1.460847	-0.867982
46	1	0	-5.174700	-0.278627	-0.842766

9a

HF=-1603.877772 NIMAG = 0

Zero-point correction= 0.415917 (Hartree/Particle)

Thermal correction to Energy= 0.442989

Thermal correction to Enthalpy= 0.443933

Thermal correction to Gibbs Free Energy= 0.357117

Sum of electronic and zero-point Energies= -1603.461855

Sum of electronic and thermal Energies= -1603.434784

Sum of electronic and thermal Enthalpies= -1603.433839

Sum of electronic and thermal Free Energies= -1603.520655

B3LYP (PCM)/6-31G* HF=-1603.8951186	M06-2X/6-31G* HF=-1603.3313001	B3LYP/6-311+G** HF=-1604.2462336	M06-2X/6-311+G** HF=-1603.7099068
	M06-2X(PCM)/6-31G* HF=-1603.3499956	B3LYP(PCM)/6-311+G** HF=-1604.2656542	M06-2X(PCM)/6-311+G** HF=-1603,7305972

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.495039	-0.938009	-0.008368
2	6	0	-2.282214	-1.130764	0.667303
3	6	0	-2.065934	-2.343522	1.344680
4	6	0	-3.027991	-3.351096	1.317284
5	6	0	-4.224706	-3.157159	0.622727
6	6	0	-4.458616	-1.948365	-0.032508
7	15	0	-1.002576	0.166327	0.840911
8	8	0	-0.737227	0.521813	2.279801
9	6	0	-1.520452	1.630974	-0.122869
10	6	0	-1.544441	2.833816	0.597576
11	6	0	-1.926548	4.021728	-0.027646
12	6	0	-2.291454	4.018738	-1.373518
13	6	0	-2.272883	2.824142	-2.097807
14	6	0	-1.887510	1.637015	-1.477734
15	6	0	0.607213	-0.583191	0.187441
16	6	0	0.869555	-1.062641	-1.260556
17	6	0	1.319249	0.149762	-2.139865
18	8	0	1.407778	1.423912	-1.416143
19	7	0	2.066003	1.373411	-0.177527
20	6	0	1.678338	0.405915	0.571802
21	6	0	2.648781	-0.275126	-2.675572
22	6	0	3.056180	-1.402065	-2.064509
23	7	0	2.065307	-1.959334	-1.239371

24	6	0	-0.269579	-1.851503	-1.913761
25	6	0	2.390533	0.189911	1.872852
26	8	0	2.545113	-0.929113	2.329019
27	6	0	4.358893	-2.125544	-2.201923
28	8	0	2.852210	1.310605	2.429201
29	6	0	3.561700	1.133093	3.667552
30	1	0	3.857517	2.135694	3.975822
31	1	0	2.385225	-2.235638	-0.313120
32	1	0	0.696336	-1.444930	0.858944
33	1	0	0.571129	0.392306	-2.899758
34	1	0	-1.875271	0.720670	-2.059012
35	1	0	-2.555290	2.817621	-3.147110
36	1	0	-2.588879	4.943734	-1.860310
37	1	0	-1.937037	4.948863	0.538760
38	1	0	-1.259152	2.820989	1.644627
39	1	0	-3.696635	0.002922	-0.509130
40	1	0	-5.394772	-1.785742	-0.559784
41	1	0	-4.975671	-3.942330	0.602568
42	1	0	-2.847618	-4.284113	1.844074
43	1	0	-1.153410	-2.493008	1.915613
44	1	0	3.210201	0.293506	-3.405290
45	1	0	-1.177581	-1.254325	-2.036512
46	1	0	0.057591	-2.190971	-2.902006
47	1	0	-0.522092	-2.734468	-1.319488
48	1	0	5.032801	-1.592552	-2.877270
49	1	0	4.858155	-2.219070	-1.228010
50	1	0	4.203429	-3.141718	-2.583611
51	1	0	2.908852	0.675232	4.414886
52	1	0	4.440203	0.499487	3.519218

9'a

HF=-1415.324843 NIMAG = 0

Zero-point correction= 0.400989 (Hartree/Particle)

Thermal correction to Energy= 0.424823

Thermal correction to Enthalpy= 0.425767

Thermal correction to Gibbs Free Energy= 0.347711

Sum of electronic and zero-point Energies= -1414.923854

Sum of electronic and thermal Energies= -1414.900020

Sum of electronic and thermal Enthalpies= -1414.899076

Sum of electronic and thermal Free Energies= -1414.977132

B3LYP (PCM)/6-31G* HF=-1415.3405936	M06-2X/6-31G* HF=-1414.843162	B3LYP/6-311+G** HF=-1415.636082	M06-2X/6-311+G** HF=-1415.1630924
	M06-2X(PCM)/6-31G* HF=-1414.860120	B3LYP(PCM)/6-311+G** HF=-1415.653770	M06-2X(PCM)/6-311+G** HF=-1415.1630924

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.796932	-2.644856	0.941959
2	6	0	-1.894670	-1.420105	0.260403
3	6	0	-2.747640	-1.324862	-0.847317
4	6	0	-3.463962	-2.440838	-1.284269
5	6	0	-3.339747	-3.659965	-0.617549
6	6	0	-2.508673	-3.759107	0.501104
7	15	0	-0.962028	-0.006755	0.961487
8	8	0	-1.199302	0.110058	2.445197
9	6	0	0.884755	-0.390065	0.744681
10	6	0	1.597886	-0.739888	-0.595610
11	6	0	2.111786	0.577896	-1.271436
12	8	0	1.718484	1.777941	-0.566377
13	7	0	2.053670	1.773440	0.819212

14	6	0	1.637988	0.731174	1.441804
15	6	0	3.596092	0.389939	-1.346336
16	6	0	3.957261	-0.732351	-0.702917
17	7	0	2.851132	-1.489276	-0.278151
18	6	0	1.909259	0.650578	2.916664
19	6	0	-1.475719	1.505259	0.076767
20	6	0	-1.300027	1.748284	-1.293672
21	6	0	-1.772313	2.928755	-1.864256
22	6	0	-2.415642	3.881950	-1.070927
23	6	0	-2.586455	3.651475	0.293947
24	6	0	-2.120745	2.467383	0.867354
25	1	0	2.918592	-1.864293	0.664086
26	6	0	5.329554	-1.275373	-0.455220
27	1	0	0.925606	-1.284182	1.383066
28	1	0	0.962866	0.528992	3.453982
29	1	0	2.420156	1.555649	3.253695
30	1	0	2.540229	-0.219426	3.146315
31	6	0	0.797735	-1.600031	-1.578090
32	1	0	1.634985	0.727343	-2.246559
33	1	0	-0.788697	1.026544	-1.921779
34	1	0	-1.629088	3.109314	-2.926058
35	1	0	-2.778010	4.803987	-1.517769
36	1	0	-3.080595	4.393155	0.915509
37	1	0	-2.244761	2.275145	1.928329
38	1	0	-2.863606	-0.379065	-1.366672
39	1	0	-4.123255	-2.353951	-2.143727
40	1	0	-3.897297	-4.527567	-0.960042
41	1	0	-2.423029	-4.701429	1.035399
42	1	0	-1.181657	-2.718401	1.834709
43	1	0	4.264567	1.095464	-1.822297
44	1	0	-0.096236	-1.089230	-1.947883
45	1	0	1.439057	-1.835898	-2.433708
46	1	0	0.485232	-2.543350	-1.120546
47	1	0	6.092809	-0.601286	-0.851793
48	1	0	5.514982	-1.399463	0.620733
49	1	0	5.451747	-2.261366	-0.919765

C3

HF=-1603.863808 NIMAG = 0

Zero-point correction= 0.410629 (Hartree/Particle)

Thermal correction to Energy= 0.440167

Thermal correction to Enthalpy= 0.441111

Thermal correction to Gibbs Free Energy= 0.346711

Sum of electronic and zero-point Energies= -1603.453179

Sum of electronic and thermal Energies= -1603.423641

Sum of electronic and thermal Enthalpies= -1603.422697

Sum of electronic and thermal Free Energies= -1603.517097

B3LYP (PCM)/6-31G* HF=-1603.876279	M06-2X/6-31G* HF=-1603.3047315	B3LYP/6-311+G** HF=-1604.2346812	M06-2X/6-311+G** HF=-1603.684531
	M06-2X(PCM)/6-31G* HF=-1603.31821	B3LYP(PCM)/6-311+G** HF=-1604.248587	M06-2X(PCM)/6-311+G** HF=-1603.699348

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.770020	-2.909116	0.297294
2	6	0	1.680224	-2.818276	-0.555819
3	7	0	1.949902	-1.801012	-1.459476
4	6	0	3.153502	-1.215785	-1.164210
5	6	0	3.689977	-1.899523	-0.073714
6	6	0	0.489931	-3.713872	-0.708401

7	6	0	3.718490	-0.110390	-1.997388
8	6	0	0.263870	-0.391741	0.832396
9	6	0	1.409168	0.240729	1.169667
10	7	0	2.249969	-0.261879	2.262095
11	8	0	1.793083	-1.237446	2.834537
12	15	0	-0.943896	-0.021828	-0.489305
13	6	0	-1.474689	1.717626	-0.342258
14	6	0	-1.530173	2.474293	-1.518896
15	6	0	-1.984563	3.792515	-1.480044
16	6	0	-2.379103	4.362267	-0.268286
17	6	0	-2.320104	3.611811	0.908547
18	6	0	-1.872966	2.291454	0.872607
19	6	0	-2.391865	-1.024183	0.015683
20	6	0	-3.143971	-1.619995	-1.006997
21	6	0	-4.277923	-2.372540	-0.699296
22	6	0	-4.669169	-2.537127	0.630594
23	6	0	-3.923033	-1.950145	1.654861
24	6	0	-2.788942	-1.197126	1.349857
25	8	0	-0.510658	-0.384815	-1.892066
26	6	0	1.914172	1.473625	0.508604
27	8	0	2.857219	2.098913	1.233188
28	6	0	3.374736	3.307205	0.652925
29	8	0	1.499060	1.886669	-0.559187
30	1	0	4.102388	3.683335	1.372068
31	1	0	0.047514	-1.270375	1.439154
32	1	0	2.885254	-3.632262	1.093594
33	1	0	1.210920	-1.349849	-2.002021
34	1	0	4.653606	-1.698520	0.375681
35	1	0	-1.203960	2.023462	-2.450630
36	1	0	-2.024318	4.376208	-2.395766
37	1	0	-2.731293	5.390034	-0.239032
38	1	0	-2.623947	4.053737	1.853659
39	1	0	-1.832702	1.717611	1.794728
40	1	0	-2.823202	-1.496761	-2.037102
41	1	0	-4.853273	-2.833183	-1.497788
42	1	0	-5.550946	-3.125383	0.870082
43	1	0	-4.220069	-2.082718	2.691610
44	1	0	-2.213460	-0.755103	2.159413
45	1	0	4.617238	0.296308	-1.523571
46	1	0	4.002408	-0.466725	-2.996904
47	1	0	2.999741	0.706797	-2.128489
48	1	0	-0.392986	-3.169612	-1.057159
49	1	0	0.683795	-4.515222	-1.435501
50	1	0	0.245068	-4.190386	0.245922
51	1	0	3.854749	3.097038	-0.306508
52	1	0	2.571653	4.032416	0.497662

9c

HF=-1603.8823844 NIMAG = 0

Zero-point correction= 0.415519 (Hartree/Particle)

Thermal correction to Energy= 0.442467

Thermal correction to Enthalpy= 0.443412

Thermal correction to Gibbs Free Energy= 0.357419

Sum of electronic and zero-point Energies= -1603.466865

Sum of electronic and thermal Energies= -1603.439917

Sum of electronic and thermal Enthalpies= -1603.438973

Sum of electronic and thermal Free Energies= -1603.524965

B3LYP (PCM)/6-31G* HF=-1603.8974796	M06-2X/6-31G* HF=-1603.3395055	B3LYP/6-311+G** HF=-1604.2494464	M06-2X/6-311+G** HF=-1603.7169826
	M06-2X(PCM)/6-31G* HF=-1603.3557737	B3LYP(PCM)/6-311+G** HF=-1604.2664764	M06-2X(PCM)/6-311+G** HF=-1603.7351871

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.617687	2.343980	1.449443
2	6	0	1.363079	1.549232	0.323585
3	6	0	1.535173	2.091029	-0.958350
4	6	0	1.960219	3.411463	-1.110654
5	6	0	2.221156	4.196094	0.014805
6	6	0	2.049153	3.661248	1.293561
7	15	0	0.862290	-0.182312	0.639877
8	6	0	2.307059	-1.180982	0.100696
9	6	0	3.003723	-1.863812	1.107449
10	6	0	4.134204	-2.619405	0.792779
11	6	0	4.577427	-2.699657	-0.528084
12	6	0	3.889736	-2.019848	-1.536251
13	6	0	2.761527	-1.261779	-1.223720
14	6	0	-0.502158	-0.620176	-0.559049
15	6	0	-1.261450	-1.938845	-0.162170
16	6	0	-2.431041	-2.089599	-1.200001
17	8	0	-2.364229	-1.094646	-2.296831
18	7	0	-2.400065	0.225793	-1.831848
19	6	0	-1.519484	0.446009	-0.919832
20	6	0	-3.658277	-1.971625	-0.362175
21	6	0	-3.316973	-1.729932	0.922769
22	7	0	-1.945368	-1.798847	1.132124
23	6	0	-0.369820	-3.185386	-0.153620
24	6	0	-4.211617	-1.469020	2.093237
25	6	0	-1.696462	1.735688	-0.174215
26	8	0	-1.641188	1.789009	1.038066
27	8	0	0.525334	-0.452875	2.083108
28	8	0	-1.965165	2.774202	-0.973992
29	6	0	-2.231727	4.015271	-0.295203
30	1	0	-2.448943	4.734007	-1.085254
31	1	0	-0.013996	-0.854663	-1.515991
32	1	0	-2.340371	-3.013453	-1.779904
33	1	0	-4.664419	-2.050856	-0.751263
34	1	0	1.328621	1.498720	-1.845883
35	1	0	2.084684	3.826220	-2.107143
36	1	0	2.555660	5.223114	-0.105547
37	1	0	2.245569	4.271778	2.170771
38	1	0	1.457747	1.922558	2.436958
39	1	0	2.244291	-0.736105	-2.022227
40	1	0	4.231136	-2.080084	-2.566092
41	1	0	5.456043	-3.290130	-0.773602
42	1	0	4.666647	-3.146904	1.579594
43	1	0	2.642747	-1.800436	2.129670
44	1	0	-1.492235	-1.205001	1.823618
45	1	0	-1.001936	-4.063862	0.013011
46	1	0	0.156159	-3.310665	-1.107433
47	1	0	0.366025	-3.149926	0.652772
48	1	0	-5.262790	-1.485092	1.794837
49	1	0	-4.055259	-2.216737	2.880035
50	1	0	-3.990761	-0.485952	2.529058
51	1	0	-3.088356	3.908246	0.374966
52	1	0	-1.357419	4.326092	0.282176

9’c

HF= -1415.3331593 NIMAG = 0

Zero-point correction= 0.400901 (Hartree/Particle)

Thermal correction to Energy= 0.424730

Thermal correction to Enthalpy= 0.425674

Thermal correction to Gibbs Free Energy= 0.347217

Sum of electronic and zero-point Energies= -1414.932258

Sum of electronic and thermal Energies= -1414.908429
Sum of electronic and thermal Enthalpies= -1414.907485
Sum of electronic and thermal Free Energies= -1414.985942

B3LYP (PCM)/6-31G* HF=-1415.3458845	M06-2X/6-31G* HF=-1414.8529721	B3LYP/6-311+G** HF=-1415.6443549	M06-2X/6-311+G** HF=-1415.172567
	M06-2X(PCM)/6-31G* HF=-1414.8667005	B3LYP(PCM)/6-311+G** HF=-1415.6589747	M06-2X(PCM)/6-311+G** HF=-1415.1881427

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.610749	2.545068	1.146205
2	6	0	-1.457679	1.595668	0.126659
3	6	0	-1.958756	1.870781	-1.153928
4	6	0	-2.589387	3.086506	-1.413888
5	6	0	-2.732343	4.033007	-0.395806
6	6	0	-2.246158	3.759928	0.883428
7	15	0	-0.645345	0.017817	0.584157
8	6	0	-1.931221	-1.241264	0.243203
9	6	0	-2.277248	-1.678254	-1.044245
10	6	0	-3.304080	-2.606404	-1.217688
11	6	0	-3.994722	-3.101901	-0.109181
12	6	0	-3.652749	-2.672852	1.174398
13	6	0	-2.623753	-1.747417	1.351961
14	6	0	0.763461	-0.287944	-0.593623
15	6	0	1.340066	-1.707571	-0.538949
16	7	0	2.291739	-2.030167	-1.338845
17	8	0	2.701382	-0.950513	-2.165076
18	6	0	3.104837	0.203641	-1.375455
19	6	0	1.953501	0.730835	-0.441574
20	6	0	4.230990	-0.052338	-0.424151
21	6	0	3.828562	0.171064	0.842568
22	7	0	2.536618	0.696050	0.914080
23	6	0	4.600905	-0.006353	2.112431
24	6	0	0.912694	-2.783438	0.424333
25	8	0	-0.194489	0.021685	2.026791
26	1	0	0.389716	-0.151708	-1.619135
27	6	0	1.608945	2.178068	-0.815329
28	1	0	3.329437	0.929300	-2.164623
29	1	0	1.599674	-3.627179	0.326924
30	1	0	0.934768	-2.411510	1.454647
31	1	0	-0.104704	-3.132739	0.225466
32	1	0	5.214355	-0.383769	-0.730566
33	1	0	-1.739619	-1.316578	-1.916838
34	1	0	-3.560667	-2.946389	-2.217236
35	1	0	-4.793809	-3.825262	-0.246839
36	1	0	-4.183499	-3.062172	2.038940
37	1	0	-2.337827	-1.419670	2.347107
38	1	0	-1.863892	1.141813	-1.954206
39	1	0	-2.970770	3.294959	-2.409774
40	1	0	-3.224803	4.979719	-0.600886
41	1	0	-2.359831	4.492301	1.678038
42	1	0	-1.223081	2.320587	2.135417
43	1	0	1.917561	0.404440	1.668139
44	1	0	2.536436	2.760557	-0.820988
45	1	0	1.158253	2.238265	-1.813490
46	1	0	0.932677	2.642646	-0.096458
47	1	0	5.596297	-0.410248	1.911408
48	1	0	4.706679	0.948147	2.642368
49	1	0	4.082502	-0.696311	2.791643

10

HF=-1603.8846409 NIMAG = 0

Zero-point correction= 0.415378 (Hartree/Particle)

Thermal correction to Energy= 0.442342

Thermal correction to Enthalpy= 0.443286

Thermal correction to Gibbs Free Energy= 0.356861

Sum of electronic and zero-point Energies= -1603.469263

Sum of electronic and thermal Energies= -1603.442299

Sum of electronic and thermal Enthalpies= -1603.441355

Sum of electronic and thermal Free Energies= -1603.527780

B3LYP (PCM)/6-31G* HF=-1603.9053901	M06-2X/6-31G* HF=-1603.3406178	B3LYP/6-311+G** HF=-1604.2465245	M06-2X/6-311+G** HF=-1603.7132945
	M06-2X(PCM)/6-31G* HF=-1603.3626828	B3LYP(PCM)/6-311+G** HF=-1604.2698378	M06-2X(PCM)/6-311+G** HF=-1603.7378783

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.370072	-1.298761	-1.107201
2	6	0	1.516688	-1.667010	0.033971
3	6	0	2.470621	-1.817135	1.270155
4	6	0	3.872283	-1.864054	0.638034
5	6	0	3.602392	-1.412730	-0.787666
6	8	0	2.339863	-0.745453	2.232902
7	7	0	2.318261	0.553393	1.668921
8	6	0	1.419597	0.680252	0.757208
9	6	0	0.541028	-0.492973	0.388527
10	15	0	-0.929053	-0.237417	-0.751757
11	8	0	-0.734922	-0.408814	-2.227211
12	6	0	0.811740	-2.988025	-0.297387
13	6	0	1.438600	1.990322	0.017787
14	8	0	1.226422	2.071587	-1.171597
15	6	0	4.709966	-1.137900	-1.759207
16	6	0	-1.634624	1.393156	-0.294292
17	6	0	-2.090320	2.190185	-1.352923
18	6	0	-2.672342	3.431763	-1.096691
19	6	0	-2.796847	3.890870	0.216499
20	6	0	-2.337317	3.105272	1.275576
21	6	0	-1.759902	1.860004	1.022293
22	6	0	-2.157692	-1.460967	-0.122603
23	6	0	-2.786271	-2.252833	-1.093629
24	6	0	-3.755441	-3.186972	-0.724927
25	6	0	-4.107283	-3.338986	0.616902
26	6	0	-3.490536	-2.550301	1.590938
27	6	0	-2.523317	-1.614667	1.222963
28	8	0	1.736308	3.025341	0.816802
29	6	0	1.804627	4.300559	0.153790
30	1	0	2.056648	5.017839	0.934877
31	1	0	0.088691	-0.799185	1.343854
32	1	0	2.236062	-2.699944	1.868871
33	1	0	4.576045	-1.216030	1.171489
34	1	0	-1.402187	1.267844	1.860519
35	1	0	-2.425413	3.460810	2.298640
36	1	0	-3.248826	4.859176	0.415067
37	1	0	-3.023121	4.043761	-1.923386
38	1	0	-1.965524	1.830360	-2.369490
39	1	0	-2.066137	-1.003747	1.997012
40	1	0	-3.763645	-2.661599	2.636924
41	1	0	-4.861066	-4.067097	0.904660
42	1	0	-4.234786	-3.796319	-1.486539
43	1	0	-2.499181	-2.126005	-2.133115
44	1	0	1.558198	-3.785269	-0.392873

45	1	0	0.100446	-3.273361	0.484188
46	1	0	0.284973	-2.906746	-1.250849
47	1	0	5.363819	-0.340502	-1.383309
48	1	0	5.338915	-2.027871	-1.892920
49	1	0	4.297844	-0.839738	-2.725422
50	1	0	4.296679	-2.877072	0.649032
51	1	0	2.573867	4.288469	-0.622586
52	1	0	0.839888	4.542777	-0.299399

Z1c

HF=-1678.854747

Zero-point correction= 0.404964 (Hartree/Particle)

Thermal correction to Energy= 0.432190

Thermal correction to Enthalpy= 0.433134

Thermal correction to Gibbs Free Energy= 0.344959

Sum of electronic and zero-point Energies= -1678.449783

Sum of electronic and thermal Energies= -1678.422556

Sum of electronic and thermal Enthalpies= -1678.421612

Sum of electronic and thermal Free Energies= -1678.509788

B3LYP (PCM)/6-31G* HF=-1678.889582	M06-2X/6-31G* HF=-1678.278195	B3LYP/6-311+G** HF=-1679.242247	M06-2X/6-311+G** HF=-1678.674958
	M06-2X(PCM)/6-31G* HF=-1.678.3153896	B3LYP(PCM)/6-311+G** HF=-1679.27999	M06-2X(PCM)/6-311+G** HF=-1678.71457

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.499069	-1.348160	1.276815
2	6	0	2.328974	-1.110707	-0.095931
3	6	0	3.027505	-1.884835	-1.032467
4	6	0	3.897872	-2.886165	-0.600743
5	6	0	4.069326	-3.119081	0.764820
6	6	0	3.368711	-2.353097	1.699752
7	15	0	1.258639	0.207170	-0.751628
8	6	0	2.078109	1.803055	-0.364706
9	6	0	2.197537	2.300249	0.943806
10	6	0	2.842160	3.516491	1.170520
11	6	0	3.370739	4.243033	0.100481
12	6	0	3.251473	3.754149	-1.201671
13	6	0	2.606707	2.538533	-1.434953
14	6	0	-0.308586	0.250570	0.266876
15	6	0	-0.711395	-0.954238	1.058573
16	6	0	-1.191524	-2.181982	0.471556
17	8	0	-1.571626	-3.212857	0.987473
18	6	0	-1.440537	0.867997	-0.610782
19	6	0	-2.791741	1.039852	0.046791
20	6	0	-3.775299	0.593468	-0.841016
21	7	0	-3.102872	0.099871	-1.999642
22	6	0	-1.799889	0.162646	-1.874355
23	6	0	-3.165839	1.503462	1.301230
24	6	0	-4.531436	1.541315	1.608784
25	6	0	-5.499734	1.121245	0.688526
26	6	0	-5.134550	0.625304	-0.567098
27	7	0	-0.676892	-0.891152	2.404658
28	8	0	-0.238575	0.191488	2.922682
29	8	0	1.015691	0.085224	-2.243827
30	8	0	-1.181314	-2.062542	-0.937461
31	6	0	-1.573222	-3.246742	-1.634703
32	1	0	-0.945888	-4.090954	-1.338517
33	1	0	-2.415608	1.775468	2.038005

34	1	0	-4.845218	1.889767	2.587994
35	1	0	-6.550664	1.160758	0.958077
36	1	0	-5.877935	0.271987	-1.275517
37	1	0	-3.577062	-0.313858	-2.795281
38	1	0	-1.082925	-0.128874	-2.632810
39	1	0	-1.071890	1.854561	-0.951970
40	1	0	-0.119045	0.982125	1.069098
41	1	0	2.874197	-1.698888	-2.091367
42	1	0	4.437518	-3.485381	-1.329481
43	1	0	4.744110	-3.901799	1.101872
44	1	0	3.489583	-2.543867	2.762374
45	1	0	1.944515	-0.776281	2.015560
46	1	0	2.500967	2.148944	-2.443225
47	1	0	3.659796	4.319000	-2.035775
48	1	0	3.872803	5.189799	0.282376
49	1	0	2.930013	3.897108	2.184573
50	1	0	1.781750	1.750795	1.785576
51	1	0	-1.433124	-3.032664	-2.697402
52	1	0	-2.617115	-3.505006	-1.426412

TS1a

HF=-1490.2909134 NIMAG = 1 (-408.570)
Zero-point correction= 0.388415 (Hartree/Particle)
Thermal correction to Energy= 0.412564
Thermal correction to Enthalpy= 0.413508
Thermal correction to Gibbs Free Energy= 0.333284
Sum of electronic and zero-point Energies= -1489.902498
Sum of electronic and thermal Energies= -1489.878350
Sum of electronic and thermal Enthalpies= -1489.877406
Sum of electronic and thermal Free Energies= -1489.957629

B3LYP (PCM)/6-31G* HF=-1490.306494	M06-2X/6-31G* HF=-1489.771464	B3LYP/6-311+G** HF=-1490.619597	M06-2X/6-311+G** HF=-1490.107969
	M06-2X(PCM)/6-31G* HF=-1489.788143	B3LYP(PCM)/6-311+G** HF=-1490.637186	M06-2X(PCM)/6-311+G** HF=-1490.126489

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.607902	1.353908	0.263450
2	6	0	4.651650	0.098900	-0.344850
3	6	0	3.633922	-0.797294	-0.025417
4	6	0	2.568689	-0.462420	0.841205
5	6	0	2.556487	0.795420	1.453225
6	6	0	3.582341	1.693208	1.160674
7	6	0	1.672616	-1.619444	0.907308
8	6	0	2.323799	-2.638709	0.136877
9	7	0	3.478209	-2.136846	-0.384596
10	6	0	-0.130877	-1.259849	-0.257631
11	15	0	-0.918686	0.127260	0.643750
12	6	0	-0.330210	1.645587	-0.196942
13	6	0	-0.721702	-2.528955	-0.433859
14	6	0	-1.935939	-3.068816	0.274442
15	7	0	-0.051291	-3.445437	-1.185691
16	8	0	1.082901	-3.034679	-1.629745
17	6	0	-2.715485	0.096266	0.275089
18	8	0	-0.670525	0.141186	2.131419
19	1	0	1.075042	-1.841179	1.780571
20	1	0	0.520734	-0.984952	-1.083792
21	1	0	2.178948	-3.703627	0.202528
22	1	0	-2.007133	-4.139580	0.063552

23	1	0	-1.866714	-2.932129	1.360964
24	1	0	-2.862665	-2.586656	-0.052568
25	1	0	4.029951	-2.618615	-1.079378
26	1	0	1.754542	1.052972	2.136700
27	1	0	3.587014	2.672659	1.630086
28	1	0	5.457287	-0.172059	-1.021648
29	1	0	5.390290	2.075854	0.045820
30	6	0	-0.259637	2.809473	0.582918
31	6	0	0.123825	4.020676	0.008571
32	6	0	0.439921	4.081802	-1.350313
33	6	0	0.371559	2.928402	-2.133255
34	6	0	-0.012599	1.714977	-1.560572
35	1	0	-0.495148	2.751609	1.641747
36	1	0	0.178286	4.916308	0.621748
37	1	0	0.741222	5.025276	-1.797693
38	1	0	0.622387	2.970103	-3.189744
39	1	0	-0.054951	0.827027	-2.185089
40	6	0	-3.592697	0.101710	1.366764
41	6	0	-4.972999	0.110933	1.156573
42	6	0	-5.483009	0.113146	-0.142350
43	6	0	-4.611382	0.111196	-1.235222
44	6	0	-3.232754	0.107437	-1.028490
45	1	0	-3.179578	0.098283	2.370936
46	1	0	-5.648825	0.115168	2.007646
47	1	0	-6.557460	0.118268	-0.305628
48	1	0	-5.006057	0.115099	-2.247675
49	1	0	-2.564834	0.109877	-1.885866

TS2a

HF=-1490.2955522 NIMAG = 1 (-399.050)
Zero-point correction= 0.387911 (Hartree/Particle)
Thermal correction to Energy= 0.412317
Thermal correction to Enthalpy= 0.413261
Thermal correction to Gibbs Free Energy= 0.331514
Sum of electronic and zero-point Energies= -1489.907641
Sum of electronic and thermal Energies= -1489.883236
Sum of electronic and thermal Enthalpies= -1489.882291
Sum of electronic and thermal Free Energies= -1489.964038

B3LYP (PCM)/6-31G* HF=-1490.310607	M06-2X/6-31G* HF=-1489.774168	B3LYP/6-311+G** HF=-1490.624187	M06-2X/6-311+G** HF=-1490.110314
	M06-2X(PCM)/6-31G* HF=-1489.790371	B3LYP(PCM)/6-311+G** HF=-1490.641119	M06-2X(PCM)/6-311+G** HF=-1490.131876

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.206761	2.008793	1.067563
2	6	0	1.629527	1.677157	-0.167687
3	6	0	1.528580	2.657232	-1.164481
4	6	0	1.992722	3.952511	-0.926894
5	6	0	2.560845	4.276672	0.305746
6	6	0	2.668314	3.303319	1.302847
7	15	0	0.996723	0.002581	-0.569539
8	6	0	2.410015	-1.142617	-0.344794
9	6	0	3.087072	-1.548378	-1.503742
10	6	0	4.193628	-2.392991	-1.410269
11	6	0	4.629557	-2.840246	-0.161657
12	6	0	3.952975	-2.448068	0.995543
13	6	0	2.846205	-1.603602	0.906285
14	6	0	-0.151110	-0.368698	0.798727

15	6	0	-0.760678	-1.615871	1.003858
16	6	0	-0.805742	-2.745871	0.014491
17	7	0	-1.540407	-1.765609	2.114302
18	8	0	-1.572593	-0.739585	2.884626
19	8	0	0.435825	-0.050230	-1.965945
20	6	0	-2.469728	0.956022	1.770254
21	7	0	-3.724491	0.452751	1.580704
22	6	0	-3.905091	0.109261	0.238200
23	6	0	-2.758827	0.525657	-0.474174
24	6	0	-1.804337	1.038939	0.507455
25	1	0	0.045741	0.167348	1.725757
26	1	0	-1.095211	1.829654	0.296251
27	1	0	-2.213844	1.465148	2.685422
28	6	0	-5.003807	-0.479989	-0.385684
29	1	0	-4.276700	0.076497	2.338558
30	1	0	-1.394430	-3.563518	0.440360
31	1	0	-1.269907	-2.431671	-0.927463
32	1	0	0.196790	-3.119175	-0.225193
33	1	0	2.728570	-1.208838	-2.470960
34	1	0	4.711444	-2.706059	-2.312897
35	1	0	5.490170	-3.499984	-0.089825
36	1	0	4.281493	-2.805821	1.967593
37	1	0	2.313499	-1.326855	1.811854
38	1	0	1.086643	2.389277	-2.119598
39	1	0	1.910958	4.706820	-1.704895
40	1	0	2.922455	5.284702	0.490613
41	1	0	3.114306	3.552172	2.262031
42	1	0	2.309258	1.258371	1.847321
43	6	0	-4.942797	-0.630815	-1.770123
44	1	0	-5.873381	-0.802548	0.180012
45	1	0	-5.782048	-1.083138	-2.291605
46	6	0	-3.817618	-0.212154	-2.500759
47	6	0	-2.717160	0.358703	-1.864038
48	1	0	-3.800562	-0.349341	-3.578174
49	1	0	-1.823504	0.626982	-2.416559

TS3a

HF=-1490.2801921 NIMAG= 1 (-274.200)
Zero-point correction= 0.387416 (Hartree/Particle)
Thermal correction to Energy= 0.411879
Thermal correction to Enthalpy= 0.412823
Thermal correction to Gibbs Free Energy= 0.330755
Sum of electronic and zero-point Energies= -1489.892776
Sum of electronic and thermal Energies= -1489.868313
Sum of electronic and thermal Enthalpies= -1489.867369
Sum of electronic and thermal Free Energies= -1489.949437

B3LYP (PCM)/6-31G* HF=-1490.304603	M06-2X/6-31G* HF=-1489.759023	B3LYP/6-311+G** HF=-1490.610810	M06-2X/6-311+G** HF=-1490.097386
	M06-2X(PCM)/6-31G* HF=-1489.7862214	B3LYP(PCM)/6-311+G** HF=-1490.638480	M06-2X(PCM)/6-311+G** HF=-1490.127850

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.709501	1.997361	1.295901
2	6	0	1.575204	1.771445	-0.083199
3	6	0	1.746104	2.839247	-0.975247
4	6	0	2.043979	4.116195	-0.495356
5	6	0	2.172444	4.334522	0.877052
6	6	0	2.005306	3.274054	1.771994

7	15	0	1.180328	0.122482	-0.787282
8	6	0	2.487387	-1.005838	-0.198334
9	6	0	3.564823	-1.247975	-1.062695
10	6	0	4.616921	-2.069045	-0.656946
11	6	0	4.597427	-2.652957	0.611173
12	6	0	3.522007	-2.421627	1.471593
13	6	0	2.465190	-1.602250	1.072792
14	6	0	-0.349400	-0.399848	0.092961
15	6	0	-0.694131	-1.789005	0.148931
16	6	0	-0.635817	-2.723333	-1.019904
17	7	0	-1.128369	-2.315508	1.331604
18	8	0	-1.147554	-1.547269	2.341724
19	6	0	-1.624239	0.728547	-0.603729
20	6	0	-2.931083	0.519947	0.072564
21	6	0	-3.802672	-0.072980	-0.858673
22	7	0	-3.109916	-0.152775	-2.080272
23	6	0	-1.879615	0.367959	-1.975094
24	6	0	-3.380742	0.739524	1.373408
25	6	0	-4.690998	0.384431	1.697147
26	6	0	-5.540906	-0.204946	0.747969
27	6	0	-5.108349	-0.450110	-0.554186
28	8	0	1.066691	0.190988	-2.292683
29	1	0	-2.719979	1.156863	2.125924
30	1	0	-5.054732	0.550518	2.706503
31	1	0	-6.551621	-0.481980	1.033036
32	1	0	-5.759006	-0.912961	-1.290514
33	1	0	-3.483395	-0.570256	-2.922895
34	1	0	-1.178262	0.400546	-2.797697
35	1	0	-1.092315	1.664031	-0.434040
36	1	0	-0.374422	-0.032731	1.130327
37	1	0	-1.197381	-2.341181	-1.886702
38	1	0	-1.056172	-3.689654	-0.723567
39	1	0	0.390278	-2.889382	-1.378137
40	1	0	3.562611	-0.803087	-2.053643
41	1	0	5.447346	-2.257137	-1.332235
42	1	0	5.415912	-3.294877	0.926422
43	1	0	3.497586	-2.888448	2.452361
44	1	0	1.621668	-1.458484	1.742250
45	1	0	1.647378	2.652618	-2.040705
46	1	0	2.177637	4.938668	-1.193131
47	1	0	2.404902	5.328180	1.250917
48	1	0	2.108288	3.441080	2.840780
49	1	0	1.593625	1.178764	2.001590

TS3'a

HF=-1490.274342 NIMAG=1 (**-200.280)**

Zero-point correction= 0.387759 (Hartree/Particle)

Thermal correction to Energy= 0.412122

Thermal correction to Enthalpy= 0.413066

Thermal correction to Gibbs Free Energy= 0.332122

Sum of electronic and zero-point Energies= -1489.886583

Sum of electronic and thermal Energies= -1489.862220

Sum of electronic and thermal Enthalpies= -1489.861276

Sum of electronic and thermal Free Energies= -1489.942220

B3LYP (PCM)/6-31G* HF=-1490.300580	M06-2X/6-31G* HF=-1489.752487	B3LYP/6-311+G** HF=-1490.606524	M06-2X/6-311+G** HF=-1490.092695
	M06-2X(PCM)/6-31G* HF=-1489.783495	B3LYP(PCM)/6-311+G** HF=-1490.636995	M06-2X(PCM)/6-311+G** HF=- 1490.127797

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.772589	-0.493188	0.273528
2	6	0	-3.546744	-1.144936	0.175105
3	6	0	-2.513392	-0.737795	-0.689996
4	6	0	-2.738746	0.348971	-1.536549
5	6	0	-3.965729	1.012141	-1.460936
6	6	0	-4.964655	0.606112	-0.562580
7	7	0	-3.108636	-2.311581	0.825775
8	6	0	-1.884085	-2.660236	0.424346
9	6	0	-1.359473	-1.683949	-0.524194
10	6	0	0.157227	-1.212244	0.203897
11	6	0	1.068618	-2.355619	0.175520
12	6	0	1.803743	-2.821810	-1.048002
13	15	0	0.722940	0.344396	-0.642099
14	6	0	0.018020	1.721939	0.348682
15	6	0	-0.473588	2.829375	-0.355929
16	6	0	-0.976314	3.935844	0.329397
17	6	0	-0.992040	3.946588	1.724936
18	6	0	-0.499215	2.849374	2.434796
19	6	0	0.006306	1.743656	1.751057
20	6	0	2.529881	0.468808	-0.383970
21	6	0	3.171789	0.118998	0.813113
22	6	0	4.549067	0.293118	0.942553
23	6	0	5.293458	0.817462	-0.117195
24	6	0	4.659624	1.163062	-1.311296
25	6	0	3.281262	0.989194	-1.446693
26	8	0	0.345938	0.448856	-2.098955
27	7	0	0.954174	-3.124809	1.275592
28	8	0	1.655002	-4.170350	1.388746
29	1	0	-0.968334	-2.075995	-1.467449
30	1	0	-0.105043	-0.988398	1.240677
31	1	0	-1.337117	-3.466469	0.894743
32	1	0	2.497865	-2.072371	-1.444276
33	1	0	2.365059	-3.716893	-0.762345
34	1	0	1.123088	-3.088598	-1.873317
35	1	0	-3.623256	-2.789537	1.554864
36	1	0	-1.959912	0.663476	-2.222636
37	1	0	-4.151979	1.861163	-2.112305
38	1	0	-5.547840	-0.829363	0.956261
39	1	0	-5.905997	1.146512	-0.523755
40	1	0	-0.459508	2.810591	-1.441525
41	1	0	-1.355530	4.789191	-0.226638
42	1	0	-1.384281	4.807812	2.259310
43	1	0	-0.505894	2.854776	3.521493
44	1	0	0.396593	0.904859	2.321350
45	1	0	2.778495	1.240539	-2.375738
46	1	0	5.237251	1.562201	-2.140750
47	1	0	6.367312	0.948593	-0.013028
48	1	0	5.042378	0.009375	1.868087
49	1	0	2.611725	-0.319925	1.633022

TS4a

HF=-1490.2840148 NImag = 1 (-319.310)
Zero-point correction= 0.387655 (Hartree/Particle)
Thermal correction to Energy= 0.411894
Thermal correction to Enthalpy= 0.412838
Thermal correction to Gibbs Free Energy= 0.332394
Sum of electronic and zero-point Energies= -1489.896360
Sum of electronic and thermal Energies= -1489.872121
Sum of electronic and thermal Enthalpies= -1489.871177
Sum of electronic and thermal Free Energies= -1489.951621

	M06-2X/6-31G*	B3LYP/6-311+G**	M06-2X/6-311+G**

B3LYP (PCM)/6-31G* HF=-1490.305174	HF=-1489.765852	HF=-1490.613654	HF=-1490.103632
	M06-2X(PCM)/6-31G* HF=-1489.788860	B3LYP(PCM)/6-311+G** HF=-1490.637673	M06-2X(PCM)/6-311+G** HF=-1490.129374

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.280423	-0.905898	-1.480225
2	6	0	2.568614	-0.488413	-0.347184
3	6	0	3.219817	-0.428626	0.893963
4	6	0	4.562998	-0.789555	0.998209
5	6	0	5.264927	-1.213001	-0.132946
6	6	0	4.623688	-1.268280	-1.371445
7	15	0	0.795968	-0.088354	-0.584346
8	6	0	-0.104113	-1.542528	0.072935
9	6	0	-0.890912	-2.275793	-0.823917
10	6	0	-1.570099	-3.416389	-0.392832
11	6	0	-1.465200	-3.833552	0.934543
12	6	0	-0.678659	-3.108737	1.833604
13	6	0	0.000841	-1.969472	1.404995
14	6	0	0.427212	1.294387	0.568342
15	6	0	1.256774	2.459163	0.627382
16	6	0	2.245288	2.889162	-0.421367
17	7	0	1.002498	3.370755	1.603997
18	8	0	0.036488	3.081829	2.392081
19	6	0	-1.361117	1.934461	0.178677
20	6	0	-2.492030	0.994735	0.255470
21	6	0	-3.048199	0.879125	-1.036387
22	7	0	-2.326489	1.738966	-1.871974
23	6	0	-1.348272	2.348424	-1.179820
24	6	0	-3.075321	0.284759	1.309208
25	6	0	-4.169666	-0.534829	1.039536
26	6	0	-4.692181	-0.648270	-0.260787
27	6	0	-4.141128	0.064680	-1.323848
28	8	0	0.457949	0.185579	-2.028297
29	1	0	-2.679726	0.368931	2.317041
30	1	0	-4.630421	-1.095787	1.847426
31	1	0	-5.545579	-1.295909	-0.439969
32	1	0	-4.552127	-0.007919	-2.326898
33	1	0	-2.390698	1.746081	-2.880936
34	1	0	-0.651670	3.010236	-1.672691
35	1	0	-1.194930	2.631550	1.024592
36	1	0	0.121685	0.986088	1.572086
37	1	0	1.796578	2.932336	-1.424616
38	1	0	2.608256	3.887502	-0.159386
39	1	0	3.106514	2.215053	-0.497656
40	1	0	-0.963986	-1.940123	-1.853807
41	1	0	-2.180051	-3.979363	-1.094299
42	1	0	-1.992550	-4.722895	1.269535
43	1	0	-0.592389	-3.432358	2.867415
44	1	0	0.616732	-1.422096	2.113713
45	1	0	2.694240	-0.074972	1.776610
46	1	0	5.063231	-0.732901	1.961147
47	1	0	6.311873	-1.492120	-0.048824
48	1	0	5.169989	-1.588023	-2.254802
49	1	0	2.775834	-0.928604	-2.441553

TS4'a

HF=-1490.2759862 NIMAG = 1 (-445.530)

Zero-point correction= 0.387549 (Hartree/Particle)

Thermal correction to Energy= 0.412120

Thermal correction to Enthalpy= 0.413064
Thermal correction to Gibbs Free Energy= 0.331205
Sum of electronic and zero-point Energies= -1489.888437
Sum of electronic and thermal Energies= -1489.863866
Sum of electronic and thermal Enthalpies= -1489.862922
Sum of electronic and thermal Free Energies= -1489.944781

B3LYP (PCM)/6-31G* HF=-1490.2992994	M06-2X/6-31G* HF=-1489.7544071	B3LYP/6-311+G** HF=-1490.6098399	M06-2X/6-311+G** HF=-1490.0951489
	M06-2X(PCM)/6-31G* HF=-1489.7817878	B3LYP(PCM)/6-311+G** HF=-1490.6356986	M06-2X(PCM)/6-311+G** HF=-1490.125978

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.644905	0.805426	1.805054
2	6	0	2.607804	0.801519	0.410749
3	6	0	3.748244	0.386305	-0.301191
4	6	0	4.922645	-0.039852	0.312689
5	6	0	4.940370	-0.024138	1.707096
6	6	0	3.821424	0.399484	2.440528
7	6	0	1.541595	1.104361	-0.588156
8	6	0	2.234372	1.013998	-1.859001
9	7	0	3.467426	0.536625	-1.669339
10	6	0	0.301144	-0.214619	-0.724368
11	6	0	0.880136	-1.541923	-0.848699
12	7	0	1.408042	-1.718853	-2.073625
13	8	0	1.949866	-2.812086	-2.394362
14	15	0	-0.944939	0.139875	0.598547
15	8	0	-0.417434	0.347369	1.993909
16	6	0	-1.775581	1.662407	-0.012283
17	6	0	-2.456596	1.731960	-1.237272
18	6	0	-3.061672	2.922093	-1.639309
19	6	0	-2.995390	4.052743	-0.820212
20	6	0	-2.327210	3.988960	0.403100
21	6	0	-1.720397	2.797884	0.807490
22	6	0	-2.198754	-1.186894	0.495307
23	6	0	-2.914032	-1.464956	1.669497
24	6	0	-3.920044	-2.431241	1.665402
25	6	0	-4.216921	-3.127029	0.491975
26	6	0	-3.500613	-2.861984	-0.677043
27	6	0	-2.493402	-1.896503	-0.678533
28	6	0	1.123526	-2.511171	0.275059
29	1	0	-0.135097	0.097550	-1.677269
30	1	0	0.910834	1.979442	-0.432879
31	1	0	1.849177	1.188766	-2.852010
32	1	0	4.063168	0.198676	-2.414571
33	1	0	0.202002	-2.780447	0.804392
34	1	0	1.552870	-3.413956	-0.170570
35	1	0	1.824671	-2.120905	1.024186
36	1	0	-2.663242	-0.932277	2.582022
37	1	0	-4.466709	-2.645079	2.579873
38	1	0	-4.998343	-3.882343	0.490161
39	1	0	-3.716688	-3.415020	-1.587004
40	1	0	-1.916782	-1.729063	-1.583193
41	1	0	-1.205797	2.729688	1.761488
42	1	0	-2.280192	4.864488	1.045217
43	1	0	-3.469470	4.978828	-1.134404
44	1	0	-3.589852	2.966472	-2.588009
45	1	0	-2.532395	0.854164	-1.874298
46	1	0	5.783423	-0.367613	-0.262738
47	1	0	5.835419	-0.347458	2.230786
48	1	0	3.865328	0.397043	3.525762

49	1	0	1.760714	1.073267	2.371952

TS5a

HF=-1336.646382 NIMAG = 1 (-354.470)
Zero-point correction= 0.341185 (Hartree/Particle)
Thermal correction to Energy= 0.362641
Thermal correction to Enthalpy= 0.363585
Thermal correction to Gibbs Free Energy= 0.288969
Sum of electronic and zero-point Energies= -1336.305197
Sum of electronic and thermal Energies= -1336.283741
Sum of electronic and thermal Enthalpies= -1336.282797
Sum of electronic and thermal Free Energies= -1336.357413

B3LYP (PCM)/6-31G* (HF=-1336.663800)	M06-2X/6-31G* HF=-1336.185390	B3LYP/6-311+G** HF=-1336.941070	M06-2X/6-311+G** HF=-1336.486259
	M06-2X(PCM)/6-31G* (HF=-1336.203680)	B3LYP(PCM)/6-311+G** (HF=-1336.961439)	M06-2X(PCM)/6-311+G** (HF=-1336.507212)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.909762	-2.655495	-0.890001
2	6	0	-1.322296	-1.441567	-0.318152
3	6	0	-2.494614	-1.409820	0.449441
4	6	0	-3.226502	-2.578455	0.663904
5	6	0	-2.795619	-3.786630	0.113378
6	6	0	-1.637973	-3.823398	-0.667128
7	15	0	-0.329524	0.046436	-0.700396
8	6	0	-1.363123	1.506074	-0.333650
9	6	0	-1.492335	2.065903	0.946342
10	6	0	-2.311553	3.178805	1.141524
11	6	0	-3.000326	3.739908	0.064234
12	6	0	-2.866105	3.192307	-1.213467
13	6	0	-2.049182	2.080185	-1.414987
14	6	0	1.102515	0.208922	0.444532
15	6	0	1.104403	-0.131320	1.818850
16	6	0	0.277826	-1.176611	2.519854
17	7	0	2.112495	0.385765	2.602169
18	8	0	2.925784	1.152725	2.009303
19	8	0	0.085588	0.010674	-2.159874
20	6	0	2.626564	-0.770737	-0.482235
21	6	0	3.846867	-0.389957	0.182979
22	6	0	4.572623	0.431319	-0.684118
23	6	0	3.828896	0.546066	-1.857752
24	7	0	2.730411	-0.237092	-1.782485
25	1	0	2.190485	-1.759958	-0.390970
26	1	0	4.014710	1.154730	-2.733323
27	1	0	4.166060	-0.755826	1.145487
28	1	0	1.602730	1.168762	0.282728
29	1	0	1.882392	-0.145215	-2.352958
30	1	0	5.514117	0.920986	-0.479354
31	1	0	0.637332	-1.240898	3.551432
32	1	0	-0.793212	-0.947451	2.543392
33	1	0	0.376054	-2.169902	2.061647
34	1	0	-2.842792	-0.473274	0.874605
35	1	0	-4.135796	-2.543183	1.257636
36	1	0	-3.366604	-4.695608	0.282324
37	1	0	-1.308883	-4.758520	-1.111929
38	1	0	-0.034982	-2.677127	-1.533468
39	1	0	-1.922874	1.658554	-2.407586
40	1	0	-3.392810	3.634900	-2.054540

41	1	0	-3.634598	4.608657	0.219236
42	1	0	-2.403069	3.612166	2.133624
43	1	0	-0.938549	1.650756	1.783438

TS6a

HF=-1336.653010 NIMAG = 1 (-361.900)

Zero-point correction= 0.341287 (Hartree/Particle)

Thermal correction to Energy= 0.362783

Thermal correction to Enthalpy= 0.363727

Thermal correction to Gibbs Free Energy= 0.289286

Sum of electronic and zero-point Energies= -1336.311723

Sum of electronic and thermal Energies= -1336.290227

Sum of electronic and thermal Enthalpies= -1336.289283

Sum of electronic and thermal Free Energies= -1336.363724

B3LYP (PCM)/6-31G* (HF=-1336.6709027)	M06-2X/6-31G* HF=-1336.196822	B3LYP/6-311+G** HF=-1336.9481952	M06-2X/6-311+G** HF=-1336.4983951
	M06-2X(PCM)/6-31G* (HF=-1336.2158789)	B3LYP(PCM)/6-311+G** (HF=-1336.969100)2	M06-2X(PCM)/6-311+G** (HF=-1336.5202416)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.650600	-0.493633	-1.482811
2	6	0	2.316836	-1.001081	-0.205934
3	6	0	3.499990	-0.843677	0.599047
4	6	0	4.399102	-0.070224	-0.130048
5	6	0	3.813898	0.183196	-1.375075
6	1	0	1.702949	-1.895823	-0.174563
7	1	0	4.182924	0.788888	-2.192722
8	6	0	0.998001	0.308081	0.472100
9	6	0	1.565509	1.609440	0.506887
10	7	0	2.462273	1.888837	1.506336
11	8	0	2.696966	0.931894	2.304214
12	15	0	-0.424779	-0.068556	-0.612396
13	6	0	-1.747397	1.134163	-0.243102
14	6	0	-2.628301	1.459892	-1.284179
15	6	0	-3.686593	2.339342	-1.055090
16	6	0	-3.869902	2.899133	0.210793
17	6	0	-2.989653	2.584843	1.248646
18	6	0	-1.929996	1.705523	1.024902
19	6	0	-1.043632	-1.695043	-0.039671
20	6	0	-1.429182	-1.934998	1.287967
21	6	0	-1.886069	-3.195948	1.668139
22	6	0	-1.964937	-4.225110	0.725734
23	6	0	-1.587737	-3.991313	-0.597272
24	6	0	-1.127996	-2.729948	-0.980959
25	8	0	-0.066865	-0.110352	-2.085590
26	6	0	1.332107	2.713070	-0.490723
27	1	0	0.973229	-0.144160	1.466481
28	1	0	3.646638	-1.274632	1.576565
29	1	0	1.898922	-0.299196	-2.148475
30	1	0	5.358211	0.302691	0.200466
31	1	0	0.327206	3.146741	-0.400885
32	1	0	2.060310	3.507946	-0.303676
33	1	0	1.435509	2.372521	-1.527079
34	1	0	-2.466878	1.033661	-2.269886
35	1	0	-4.364006	2.591842	-1.866292
36	1	0	-4.693037	3.586334	0.387227
37	1	0	-3.121881	3.030670	2.230585
38	1	0	-1.233958	1.490356	1.830924

39	1	0	-0.831547	-2.532801	-2.006991
40	1	0	-1.651199	-4.789689	-1.331692
41	1	0	-2.322128	-5.207038	1.024294
42	1	0	-2.182034	-3.375563	2.698028
43	1	0	-1.382760	-1.139232	2.026987

TS7a

HF=-1336.6317945 NIMAG = 1 (-324.680)
Zero-point correction= 0.340905 (Hartree/Particle)
Thermal correction to Energy= 0.362552
Thermal correction to Enthalpy= 0.363496
Thermal correction to Gibbs Free Energy= 0.288963
Sum of electronic and zero-point Energies= -1336.290890
Sum of electronic and thermal Energies= -1336.269242
Sum of electronic and thermal Enthalpies= -1336.268298
Sum of electronic and thermal Free Energies= -1336.342832

B3LYP (PCM)/6-31G* (HF=-1336.6540194)	M06-2X/6-31G* HF=-1336.17076	B3LYP/6-311+G** HF=-1336.9266953	M06-2X/6-311+G** HF=-1336.4720791
	M06-2X(PCM)/6-31G* (HF=-1336.194143)	B3LYP(PCM)/6-311+G** (HF=-1336.952278)	M06-2X(PCM)/6-311+G** (HF=-1336.498444)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.553888	-1.294207	-1.855381
2	6	0	-2.344531	-1.602920	-0.481537
3	7	0	-3.255725	-0.785882	0.213030
4	6	0	-3.956643	-0.017671	-0.648125
5	6	0	-3.538713	-0.307944	-1.949736
6	6	0	-0.476538	-1.325655	0.175683
7	6	0	-0.577301	-1.473509	1.585569
8	7	0	-0.929568	-2.707968	2.074831
9	8	0	-1.113560	-3.619315	1.209342
10	15	0	0.350402	0.025100	-0.775491
11	8	0	-0.025396	0.027028	-2.232215
12	6	0	0.028485	1.654392	-0.001494
13	6	0	0.888201	2.251027	0.931321
14	6	0	0.601242	3.516017	1.446138
15	6	0	-0.542591	4.198832	1.029202
16	6	0	-1.393430	3.619577	0.085076
17	6	0	-1.106340	2.357438	-0.434621
18	6	0	2.130163	-0.342693	-0.534696
19	6	0	2.682698	-0.886200	0.634661
20	6	0	4.056533	-1.118705	0.718008
21	6	0	4.885794	-0.815671	-0.363525
22	6	0	4.339601	-0.287040	-1.534967
23	6	0	2.967502	-0.053889	-1.623738
24	6	0	-0.586406	-0.379843	2.619846
25	1	0	-2.209589	-2.624448	-0.089781
26	1	0	-4.686360	0.698834	-0.295140
27	1	0	-3.903913	0.167655	-2.849286
28	1	0	-2.004031	-1.738672	-2.671168
29	1	0	-3.364477	-0.799366	1.217095
30	1	0	-0.179056	-2.275038	-0.280980
31	1	0	-1.367193	0.371975	2.434238
32	1	0	-0.778097	-0.842587	3.593042
33	1	0	0.357889	0.172374	2.681770
34	1	0	2.529391	0.335900	-2.537546
35	1	0	4.981214	-0.062521	-2.382784

36	1	0	5.954669	-1.000619	-0.296639
37	1	0	4.475897	-1.546124	1.624740
38	1	0	2.043233	-1.153485	1.470423
39	1	0	1.789134	1.735534	1.250093
40	1	0	1.275634	3.970357	2.166978
41	1	0	-0.763684	5.184804	1.429374
42	1	0	-2.274303	4.157090	-0.256309
43	1	0	-1.746731	1.919064	-1.193893

TS7'a

HF=-1336.6407325 NImag =1 (-181.160)
Zero-point correction= 0.340798 (Hartree/Particle)
Thermal correction to Energy= 0.362504
Thermal correction to Enthalpy= 0.363448
Thermal correction to Gibbs Free Energy= 0.287989
Sum of electronic and zero-point Energies= -1336.299935
Sum of electronic and thermal Energies= -1336.278229
Sum of electronic and thermal Enthalpies= -1336.277285
Sum of electronic and thermal Free Energies= -1336.352744

B3LYP (PCM)/6-31G* (HF=-1336.664411)	M06-2X/6-31G* HF=-1336.2050379	B3LYP/6-311+G** HF=-1336.9670486	M06-2X/6-311+G** HF=-1336.5137667
	M06-2X(PCM)/6-31G* (HF=-1336.205038)	B3LYP(PCM)/6-311+G** (HF=-1336.967049)	M06-2X(PCM)/6-311+G** (HF=-1336.5137667)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.690024	2.094771	1.324915
2	6	0	-0.734025	1.810379	-0.049982
3	6	0	-1.220198	2.776116	-0.944677
4	6	0	-1.669361	4.007743	-0.469007
5	6	0	-1.633466	4.284241	0.899313
6	6	0	-1.140888	3.330398	1.792145
7	15	0	-0.197066	0.220365	-0.771519
8	6	0	-1.612462	-0.923298	-0.627163
9	6	0	-1.918285	-1.712856	-1.744392
10	6	0	-3.003944	-2.589100	-1.705777
11	6	0	-3.791692	-2.674773	-0.557031
12	6	0	-3.498478	-1.879006	0.553721
13	6	0	-2.414732	-1.002989	0.520360
14	6	0	1.201587	-0.301550	0.354248
15	6	0	0.923511	-1.200620	1.444497
16	6	0	0.418206	-2.610155	1.315017
17	7	0	1.382681	-0.743499	2.646142
18	8	0	1.209730	-1.522549	3.625586
19	8	0	0.192498	0.366045	-2.236181
20	6	0	2.541362	-0.909039	-0.702645
21	6	0	3.792648	-0.830456	0.035287
22	6	0	4.612600	0.099114	-0.567980
23	6	0	3.923423	0.587065	-1.702774
24	7	0	2.760908	-0.056023	-1.825974
25	1	0	2.140055	-1.885881	-0.972375
26	1	0	5.584471	0.435047	-0.233143
27	1	0	3.977844	-1.359725	0.960372
28	1	0	4.204767	1.377218	-2.387156
29	1	0	1.949888	0.206953	-2.406397
30	1	0	1.628249	0.618517	0.764853
31	1	0	-1.229148	2.558895	-2.008661
32	1	0	-2.042974	4.752376	-1.166755

33	1	0	-1.982826	5.244673	1.269025
34	1	0	-1.100351	3.547491	2.855923
35	1	0	-0.286724	1.370294	2.027394
36	1	0	-2.197036	-0.384346	1.385492
37	1	0	-4.115851	-1.938584	1.445679
38	1	0	-4.638148	-3.355726	-0.527800
39	1	0	-3.236804	-3.199074	-2.574399
40	1	0	-1.311078	-1.620454	-2.639455
41	1	0	0.196168	-2.886203	0.280278
42	1	0	1.164808	-3.305279	1.722950
43	1	0	-0.486968	-2.768885	1.912100

TS8a

HF = -1336.6453437 NIMAG =1 (-359,040)
Zero-point correction= 0.340490 (Hartree/Particle)
Thermal correction to Energy= 0.362224
Thermal correction to Enthalpy= 0.363168
Thermal correction to Gibbs Free Energy= 0.288126
Sum of electronic and zero-point Energies= -1336.304853
Sum of electronic and thermal Energies= -1336.283120
Sum of electronic and thermal Enthalpies= -1336.282176
Sum of electronic and thermal Free Energies= -1336.357218

B3LYP (PCM)/6-31G* (HF=-1336.663724)	M06-2X/6-31G* HF=-1336.1834755	B3LYP/6-311+G** HF=-1336.9398606	M06-2X/6-311+G** HF=-1336.4846432
	M06-2X(PCM)/6-31G* (HF=-1336.203234)	B3LYP(PCM)/6-311+G** (HF=-1336.961540)	M06-2X(PCM)/6-311+G** (HF=-1336.507513)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.444013	2.795264	-0.874714
2	6	0	0.207927	1.723451	-0.002736
3	6	0	0.400755	1.903507	1.374724
4	6	0	0.830688	3.134425	1.869536
5	6	0	1.067062	4.197366	0.994227
6	6	0	0.872064	4.026947	-0.377296
7	15	0	-0.400205	0.164730	-0.751812
8	6	0	-2.136304	0.007005	-0.190706
9	6	0	-2.500635	-0.276608	1.133933
10	6	0	-3.846876	-0.337893	1.491392
11	6	0	-4.837548	-0.115313	0.531472
12	6	0	-4.480472	0.162705	-0.788725
13	6	0	-3.133953	0.222481	-1.151433
14	6	0	0.540353	-1.172969	0.097338
15	6	0	0.041702	-2.505874	0.148615
16	6	0	-0.896052	-3.102209	-0.864761
17	7	0	0.495965	-3.378671	1.092069
18	8	0	1.484991	-2.999328	1.810342
19	8	0	-0.279719	0.173275	-2.252389
20	6	0	2.253909	-1.215293	-0.964165
21	7	0	3.118206	-1.775378	0.014065
22	6	0	4.008401	-0.844522	0.392650
23	6	0	3.871961	0.302311	-0.410798
24	6	0	2.814639	0.064559	-1.277964
25	1	0	4.677025	-1.024312	1.224541
26	1	0	1.849938	-1.864386	-1.731310
27	1	0	2.758381	-2.490426	0.673421
28	1	0	4.490334	1.187612	-0.353337
29	1	0	2.438426	0.707133	-2.060503

30	1	0	1.014054	-0.875037	1.034522
31	1	0	-1.836080	-2.548048	-0.958996
32	1	0	-0.442065	-3.126374	-1.866326
33	1	0	-1.121756	-4.129870	-0.566418
34	1	0	0.292083	2.648527	-1.940214
35	1	0	1.053310	4.852319	-1.060642
36	1	0	1.400663	5.156099	1.382308
37	1	0	0.980701	3.263919	2.937969
38	1	0	0.218405	1.089286	2.071137
39	1	0	-1.741623	-0.469530	1.886865
40	1	0	-4.122566	-0.565195	2.517494
41	1	0	-5.886067	-0.164475	0.812921
42	1	0	-5.249250	0.328499	-1.538619
43	1	0	-2.841995	0.424034	-2.177726

TS8'a

HF=-1336.639117 NIMAG =1 (-233.310)

Zero-point correction= 0.340684 (Hartree/Particle)

Thermal correction to Energy= 0.362439

Thermal correction to Enthalpy= 0.363383

Thermal correction to Gibbs Free Energy= 0.287602

Sum of electronic and zero-point Energies= -1336.298432

Sum of electronic and thermal Energies= -1336.276677

Sum of electronic and thermal Enthalpies= -1336.275733

Sum of electronic and thermal Free Energies= -1336.351515

B3LYP (PCM)/6-31G* (HF=-1336.662884)	M06-2X/6-31G* HF=-1336.1764031	B3LYP/6-311+G** HF=-1336.936084	M06-2X/6-311+G** HF=-1336.4802341
	M06-2X(PCM)/6-31G* (HF=-1336.204097)	B3LYP(PCM)/6-311+G** (HF=-1336.964541)	M06-2X(PCM)/6-311+G** (HF=-1336.512598)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.935130	0.144726	1.024409
2	6	0	-2.196498	-1.094616	0.827700
3	7	0	-3.030055	-1.849859	-0.064079
4	6	0	-4.049276	-1.094607	-0.480088
5	6	0	-4.039779	0.146240	0.196913
6	1	0	-1.870762	-1.609992	1.729796
7	1	0	-4.716182	-1.439814	-1.260350
8	6	0	-0.658353	-1.047458	-0.077821
9	6	0	-0.122147	-2.397999	-0.153794
10	7	0	-0.777312	-3.183536	-1.041452
11	8	0	-0.396355	-4.379266	-1.190036
12	15	0	0.341225	0.275146	0.753122
13	8	0	0.175465	0.311178	2.249842
14	6	0	-0.222804	1.840592	-0.022446
15	6	0	-0.543969	2.898551	0.839139
16	6	0	-0.950798	4.129621	0.321942
17	6	0	-1.039275	4.312541	-1.058839
18	6	0	-0.715625	3.264002	-1.923919
19	6	0	-0.306013	2.034492	-1.409111
20	6	0	2.076430	0.070578	0.220709
21	6	0	2.450944	-0.351842	-1.063389
22	6	0	3.800137	-0.434037	-1.405993
23	6	0	4.782493	-0.094326	-0.472350
24	6	0	4.414622	0.320374	0.808454
25	6	0	3.065765	0.401951	1.156639
26	6	0	0.842370	-2.990960	0.836289
27	1	0	-2.588813	-2.606858	-0.619726

28	1	0	-4.773822	0.931348	0.074863
29	1	0	-2.636843	0.906861	1.729854
30	1	0	-1.026598	-0.699653	-1.046227
31	1	0	0.634873	-4.062563	0.917080
32	1	0	1.886351	-2.889968	0.511980
33	1	0	0.760992	-2.516682	1.821680
34	1	0	-0.470612	2.741337	1.911539
35	1	0	-1.197441	4.944741	0.997064
36	1	0	-1.356062	5.270614	-1.462297
37	1	0	-0.779164	3.405194	-2.999483
38	1	0	-0.045767	1.233088	-2.095990
39	1	0	1.698637	-0.649672	-1.788235
40	1	0	4.084264	-0.772148	-2.398681
41	1	0	5.833110	-0.161638	-0.741872
42	1	0	5.177052	0.574229	1.539892
43	1	0	2.768545	0.705933	2.155908

TS9a

HF=-1415.284201 NIMAG = 1 (-348.140)
Zero-point correction= 0.397277 (Hartree/Particle)
Thermal correction to Energy= 0.421958
Thermal correction to Enthalpy= 0.422902
Thermal correction to Gibbs Free Energy= 0.341688
Sum of electronic and zero-point Energies= -1414.886924
Sum of electronic and thermal Energies= -1414.862243
Sum of electronic and thermal Enthalpies= -1414.861299
Sum of electronic and thermal Free Energies= -1414.942513

B3LYP (PCM)/6-31G* HF=-1415.2988756	M06-2X/6-31G* HF=-1414.784793	B3LYP/6-311+G** HF=-1415.598355	M06-2X/6-311+G** HF=-1415.1065485
	M06-2X(PCM)/6-31G* HF=-1414.800475	B3LYP(PCM)/6-311+G** HF=-1415.6156359	M06-2X(PCM)/6-311+G** HF=-1415.124692

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.916330	0.739499	0.268835
2	6	0	-3.046399	1.826821	0.303245
3	6	0	-1.991660	1.598291	-0.673371
4	7	0	-2.411557	0.422906	-1.354913
5	6	0	-3.476360	-0.134497	-0.735899
6	6	0	-0.456678	0.987281	0.442360
7	6	0	0.076961	2.112727	1.138488
8	7	0	-0.677896	2.623231	2.154230
9	8	0	-1.729253	1.961441	2.448208
10	6	0	-1.444413	2.721302	-1.528280
11	6	0	-4.004543	-1.476429	-1.126182
12	15	0	0.525132	-0.163409	-0.612531
13	8	0	0.181127	-0.132377	-2.091679
14	6	0	0.165746	-1.809620	0.111572
15	6	0	-0.009649	-2.035084	1.485760
16	6	0	-0.254454	-3.324521	1.959666
17	6	0	-0.334101	-4.396347	1.067865
18	6	0	-0.169546	-4.177862	-0.301393
19	6	0	0.080453	-2.890334	-0.778918
20	6	0	2.321512	0.087305	-0.384650
21	6	0	2.983106	-0.162528	0.826341
22	6	0	4.360555	0.028837	0.923026
23	6	0	5.086860	0.464891	-0.188689

24	6	0	4.434433	0.703558	-1.398828
25	6	0	3.055222	0.513712	-1.499497
26	6	0	1.282188	2.942162	0.775492
27	1	0	-3.171123	2.737039	0.865904
28	1	0	-1.109574	0.422481	1.111226
29	1	0	-1.759205	-0.042144	-1.988992
30	1	0	-4.781052	0.576382	0.897857
31	1	0	1.205450	3.896442	1.305807
32	1	0	2.225936	2.469360	1.071691
33	1	0	1.353114	3.146977	-0.298901
34	1	0	2.429122	-0.507040	1.694790
35	1	0	4.867761	-0.164940	1.864171
36	1	0	6.160778	0.612084	-0.110954
37	1	0	4.998424	1.034400	-2.266749
38	1	0	2.537247	0.681628	-2.438638
39	1	0	0.203044	-2.708518	-1.842724
40	1	0	-0.236008	-5.009222	-0.998178
41	1	0	-0.528805	-5.398754	1.439701
42	1	0	-0.391192	-3.489450	3.024853
43	1	0	0.030469	-1.209315	2.191059
44	1	0	-4.177575	-1.538228	-2.207281
45	1	0	-3.293594	-2.270053	-0.861651
46	1	0	-4.947921	-1.681143	-0.613943
47	1	0	-1.062071	3.519322	-0.885899
48	1	0	-0.639737	2.361948	-2.175242
49	1	0	-2.236703	3.141420	-2.159068

TS10a

HF=-1415.287754 NIMAG =1 (-353.700)
Zero-point correction= 0.397102 (Hartree/Particle)
Thermal correction to Energy= 0.421680
Thermal correction to Enthalpy= 0.422625
Thermal correction to Gibbs Free Energy= 0.342611
Sum of electronic and zero-point Energies= -1414.890651
Sum of electronic and thermal Energies= -1414.866074
Sum of electronic and thermal Enthalpies= -1414.865129
Sum of electronic and thermal Free Energies= -1414.945143

B3LYP (PCM)/6-31G* HF=-1415.302624	M06-2X/6-31G* HF=-1414.794249	B3LYP/6-311+G** HF=-1415.602854	M06-2X/6-311+G** HF=-1415.116883
	M06-2X(PCM)/6-31G* HF=-1414.810171	B3LYP(PCM)/6-311+G** HF=-1415.620368	M06-2X(PCM)/6-311+G** HF=-1415.135320

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.033308	1.779163	1.166339
2	6	0	1.714034	1.396302	-0.144577
3	6	0	2.318119	2.060226	-1.221592
4	6	0	3.224863	3.095282	-0.990507
5	6	0	3.536726	3.473523	0.316600
6	6	0	2.940021	2.814777	1.394068
7	15	0	0.581485	0.011671	-0.543110
8	8	0	0.122629	0.057810	-1.989878
9	6	0	-0.795931	0.073480	0.663794
10	6	0	-1.485516	-1.134770	0.994411
11	6	0	-1.496412	-2.421113	0.209818
12	7	0	-2.265598	-1.134971	2.116406
13	8	0	-2.310396	-0.029053	2.741342
14	6	0	1.587356	-1.481891	-0.212403

15	6	0	1.993033	-2.242670	-1.316109
16	6	0	2.798953	-3.367778	-1.132476
17	6	0	3.200229	-3.738650	0.151501
18	6	0	2.795553	-2.983419	1.255829
19	6	0	1.994403	-1.857012	1.076114
20	6	0	-2.070245	1.409642	-0.097328
21	6	0	-3.197162	1.375451	0.812750
22	6	0	-4.141546	0.508993	0.289417
23	6	0	-3.665786	0.048893	-0.953266
24	7	0	-2.521787	0.701780	-1.250944
25	1	0	-0.614204	0.665251	1.564275
26	6	0	-1.325218	2.709569	-0.329571
27	1	0	-3.280499	1.977785	1.703676
28	1	0	-1.822708	0.388117	-1.930224
29	6	0	-4.262962	-0.967866	-1.869129
30	1	0	-5.073110	0.201375	0.745052
31	1	0	-2.351176	-3.018485	0.541980
32	1	0	-1.577649	-2.256393	-0.871623
33	1	0	-0.591333	-3.020776	0.367020
34	1	0	1.663475	-1.949189	-2.308181
35	1	0	3.108974	-3.955997	-1.992054
36	1	0	3.824668	-4.616524	0.294465
37	1	0	3.100923	-3.274287	2.257191
38	1	0	1.673154	-1.286581	1.943198
39	1	0	2.059757	1.765835	-2.234740
40	1	0	3.685815	3.607167	-1.831001
41	1	0	4.241385	4.280928	0.496706
42	1	0	3.177604	3.109002	2.412751
43	1	0	1.575120	1.279803	2.015885
44	1	0	-3.720067	-1.920221	-1.803521
45	1	0	-5.305737	-1.159018	-1.603164
46	1	0	-4.223232	-0.636280	-2.912699
47	1	0	-0.560917	2.609645	-1.101412
48	1	0	-2.028124	3.486415	-0.652144
49	1	0	-0.845493	3.048851	0.593174

TS11a

HF=-1415.2619514 NIMAG =1 (-280.160)
Zero-point correction= 0.396282 (Hartree/Particle)
Thermal correction to Energy= 0.421412
Thermal correction to Enthalpy= 0.422356
Thermal correction to Gibbs Free Energy= 0.339965
Sum of electronic and zero-point Energies= -1414.865669
Sum of electronic and thermal Energies= -1414.840539
Sum of electronic and thermal Enthalpies= -1414.839595
Sum of electronic and thermal Free Energies= -1414.921986

B3LYP (PCM)/6-31G* HF=-1415.282459	M06-2X/6-31G* HF=-1414.761662	B3LYP/6-311+G** HF=-1415.576976	M06-2X/6-311+G** HF=-1415.084456
	M06-2X(PCM)/6-31G* HF=-1414.783492	B3LYP(PCM)/6-311+G** HF=-1415.60085	M06-2X(PCM)/6-311+G** HF=-1415.109471

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.409645	-0.091341	2.808848
2	6	0	-3.091555	0.441306	1.922878
3	6	0	-2.120932	1.427533	1.840665
4	1	0	-1.558892	1.849749	2.660231
5	6	0	-3.572467	0.202757	0.622733

6	7	0	-2.925458	1.035239	-0.217144
7	6	0	-1.947301	1.822850	0.462538
8	6	0	-0.169651	1.290340	-0.199664
9	6	0	-0.119953	1.402700	-1.621481
10	7	0	0.420687	2.540775	-2.199545
11	8	0	0.856550	3.442801	-1.441758
12	15	0	0.478029	-0.156014	0.758140
13	8	0	0.048331	-0.178649	2.203062
14	6	0	0.068623	-1.749395	-0.058225
15	6	0	-1.031794	-2.462162	0.441067
16	6	0	-1.375231	-3.702551	-0.099044
17	6	0	-0.613885	-4.250136	-1.133730
18	6	0	0.498577	-3.559308	-1.618053
19	6	0	0.841937	-2.318044	-1.080223
20	6	0	2.295567	0.044948	0.612367
21	6	0	3.037093	-0.316353	1.748670
22	6	0	4.427725	-0.214257	1.742154
23	6	0	5.089578	0.256136	0.606085
24	6	0	4.357182	0.630717	-0.521552
25	6	0	2.964850	0.528820	-0.522257
26	6	0	-0.641930	0.414991	-2.631419
27	6	0	-4.551194	-0.816292	0.140941
28	1	0	-3.066406	1.075784	-1.216445
29	6	0	-1.955864	3.298696	0.089227
30	1	0	0.363169	2.161493	0.206653
31	1	0	-0.017824	-0.479669	-2.741910
32	1	0	-1.646487	0.040024	-2.387607
33	1	0	-0.679236	0.913461	-3.605609
34	1	0	2.510786	-0.660396	2.633666
35	1	0	4.993783	-0.495602	2.626253
36	1	0	6.173269	0.340026	0.602880
37	1	0	4.866446	1.015385	-1.400891
38	1	0	2.406726	0.851331	-1.394751
39	1	0	1.723438	-1.801460	-1.448126
40	1	0	1.106958	-3.991055	-2.408213
41	1	0	-0.876413	-5.219103	-1.550104
42	1	0	-2.224880	-4.250561	0.300610
43	1	0	-1.592353	-2.050312	1.274638
44	1	0	-2.938227	3.732450	0.309225
45	1	0	-1.196342	3.845852	0.651406
46	1	0	-1.738191	3.431808	-0.974031
47	1	0	-5.145276	-1.199659	0.974313
48	1	0	-5.236450	-0.398284	-0.605835
49	1	0	-4.030289	-1.664813	-0.322994

TS11'a

HF=-1415.2670651 NIMAG =1 (-184.210)

Zero-point correction= 0.396697 (Hartree/Particle)

Thermal correction to Energy= 0.421564

Thermal correction to Enthalpy= 0.422508

Thermal correction to Gibbs Free Energy= 0.341080

Sum of electronic and zero-point Energies= -1414.870368

Sum of electronic and thermal Energies= -1414.845501

Sum of electronic and thermal Enthalpies= -1414.844557

Sum of electronic and thermal Free Energies= -1414.925985

B3LYP (PCM)/6-31G* HF=-1415.2900963	M06-2X/6-31G* HF=-1414.7683814	B3LYP/6-311+G** HF=-1415.5844372	M06-2X/6-311+G** HF=-1415.0936155
	M06-2X(PCM)/6-31G* HF=-1414.793654	B3LYP(PCM)/6-311+G** HF=-1415.615398	M06-2X(PCM)/6-311+G** HF=-1415.1226881

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.951603	-0.705776	0.442286
2	6	0	2.330327	-0.119888	-0.671983
3	6	0	3.113438	0.293532	-1.761861
4	6	0	4.498818	0.138595	-1.730252
5	6	0	5.113463	-0.434486	-0.614971
6	6	0	4.339150	-0.859495	0.465881
7	15	0	0.529007	0.168518	-0.836147
8	6	0	0.159606	1.710294	0.085470
9	6	0	-0.871510	2.522230	-0.410649
10	6	0	-1.195831	3.719252	0.229902
11	6	0	-0.485119	4.120627	1.363289
12	6	0	0.557358	3.328221	1.848264
13	6	0	0.882125	2.130485	1.210696
14	6	0	-0.226811	-1.312648	0.005712
15	6	0	-0.230165	-1.456569	1.440390
16	6	0	-0.814360	-0.503027	2.448835
17	7	0	0.247009	-2.664771	1.874918
18	8	0	0.233188	-2.831126	3.127032
19	8	0	0.122808	0.302235	-2.283959
20	6	0	-1.866130	-1.710275	-0.724168
21	6	0	-2.095180	-1.168631	-2.057948
22	6	0	-3.102155	-0.223397	-2.015728
23	6	0	-3.551546	-0.135834	-0.681568
24	7	0	-2.868667	-1.029577	0.051479
25	6	0	-4.543192	0.804176	-0.080435
26	6	0	-1.902626	-3.234598	-0.593388
27	1	0	-3.475447	0.376027	-2.835096
28	1	0	-1.552233	-1.495431	-2.931758
29	1	0	-2.935310	-1.122784	1.056239
30	1	0	0.341467	-2.157371	-0.400570
31	1	0	-0.048600	-0.129882	3.140633
32	1	0	-1.300204	0.361208	1.990749
33	1	0	-1.524716	-1.042745	3.092826
34	1	0	2.623779	0.720029	-2.631988
35	1	0	5.097463	0.460063	-2.578438
36	1	0	6.193171	-0.557467	-0.591726
37	1	0	4.811648	-1.321308	1.328463
38	1	0	2.359291	-1.069584	1.275399
39	1	0	1.703811	1.528619	1.586506
40	1	0	1.123398	3.645633	2.719781
41	1	0	-0.733677	5.055229	1.859202
42	1	0	-1.990188	4.347293	-0.165619
43	1	0	-1.392769	2.218928	-1.313688
44	1	0	-2.918263	-3.610766	-0.755244
45	1	0	-1.244671	-3.684623	-1.343122
46	1	0	-1.545656	-3.542485	0.395925
47	1	0	-5.235864	1.170175	-0.842695
48	1	0	-5.123775	0.325095	0.715426
49	1	0	-4.031701	1.673212	0.354995

TS12a

HF=-1415.2858897 NIMAG =1 (-344.310)
Zero-point correction= 0.396494 (Hartree/Particle)
Thermal correction to Energy= 0.421376
Thermal correction to Enthalpy= 0.422320
Thermal correction to Gibbs Free Energy= 0.341043
Sum of electronic and zero-point Energies= -1414.889396
Sum of electronic and thermal Energies= -1414.864513
Sum of electronic and thermal Enthalpies= -1414.863569

Sum of electronic and thermal Free Energies= -1414.944847

B3LYP (PCM)/6-31G* HF=-1415.300836	M06-2X/6-31G* HF=-1414.7867724	B3LYP/6-311+G** HF=-1415.6002794	M06-2X/6-311+G** HF=-1415.1090876
	M06-2X(PCM)/6-31G* HF=-1414.8028692	B3LYP(PCM)/6-311+G** HF=-1415.617907	M06-2X(PCM)/6-311+G** HF=-1415.1277451

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.574873	-0.004920	1.623050
2	6	0	3.679067	-0.035869	0.427576
3	7	0	3.090000	-1.170239	0.012761
4	1	0	2.873060	-1.936229	0.680027
5	6	0	3.289623	1.018908	-0.431800
6	6	0	2.387610	0.500958	-1.342172
7	6	0	2.155390	-0.886291	-1.031271
8	6	0	0.445253	-1.015126	0.072601
9	6	0	0.114925	-2.397636	0.233442
10	7	0	0.750658	-3.158485	1.162701
11	8	0	1.717546	-2.617480	1.812241
12	15	0	-0.735258	0.130431	-0.753884
13	8	0	-0.731121	0.084233	-2.260784
14	6	0	-2.392368	-0.224442	-0.055716
15	6	0	-2.618441	-0.509504	1.299087
16	6	0	-3.916112	-0.721844	1.762892
17	6	0	-4.996694	-0.648251	0.880013
18	6	0	-4.777021	-0.367814	-0.469289
19	6	0	-3.479131	-0.157756	-0.937975
20	6	0	-0.324845	1.805084	-0.125120
21	6	0	-0.085105	2.092301	1.226282
22	6	0	0.180697	3.400071	1.631025
23	6	0	0.203174	4.433641	0.690945
24	6	0	-0.043466	4.156352	-0.654533
25	6	0	-0.307693	2.847546	-1.061473
26	6	0	-0.914261	-3.138914	-0.587671
27	1	0	3.643449	2.039172	-0.363237
28	1	0	1.903626	1.015127	-2.160444
29	1	0	0.913470	-0.599796	0.967205
30	1	0	-1.936314	-2.949926	-0.236612
31	1	0	-0.880487	-2.853356	-1.643954
32	1	0	-0.727992	-4.213256	-0.502926
33	1	0	-0.497897	2.616896	-2.105745
34	1	0	-0.030698	4.958301	-1.387931
35	1	0	0.408847	5.452382	1.008818
36	1	0	0.368388	3.613076	2.680053
37	1	0	-0.103480	1.301628	1.971630
38	1	0	-1.786043	-0.592336	1.992377
39	1	0	-4.083324	-0.950901	2.811831
40	1	0	-6.006935	-0.815285	1.244153
41	1	0	-5.614864	-0.317525	-1.159538
42	1	0	-3.293928	0.047652	-1.988066
43	6	0	1.971876	-1.923221	-2.113878
44	1	0	1.163161	-1.612865	-2.779905
45	1	0	2.895182	-2.030271	-2.694990
46	1	0	1.725924	-2.897315	-1.680096
47	1	0	4.701478	1.017836	1.987341
48	1	0	4.165232	-0.619724	2.432138
49	1	0	5.568896	-0.402338	1.380151

TS12'a

HF=-1415.279749 NIMAG =1 (-254.890)
Zero-point correction= 0.396761 (Hartree/Particle)
Thermal correction to Energy= 0.421567
Thermal correction to Enthalpy= 0.422511
Thermal correction to Gibbs Free Energy= 0.341104
Sum of electronic and zero-point Energies= -1414.882988
Sum of electronic and thermal Energies= -1414.858182
Sum of electronic and thermal Enthalpies= -1414.857238
Sum of electronic and thermal Free Energies= -1414.938645

B3LYP (PCM)/6-31G* HF=-1415.298709	M06-2X/6-31G* HF=-1414.779405	B3LYP/6-311+G** HF=-1415.596610	M06-2X/6-311+G** HF=-1415.104168
	M06-2X(PCM)/6-31G* HF=-1414.801104	B3LYP(PCM)/6-311+G** HF=-1415.619287	M06-2X(PCM)/6-311+G** HF=-1415.129596

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.470261	2.962370	1.002252
2	6	0	0.483766	1.895882	0.093118
3	6	0	0.351722	2.160596	-1.277675
4	6	0	0.190092	3.469946	-1.729237
5	6	0	0.167867	4.527685	-0.816227
6	6	0	0.311360	4.273067	0.548530
7	15	0	0.747202	0.213316	0.782166
8	6	0	2.331568	-0.338528	0.051517
9	6	0	2.461372	-0.830250	-1.255549
10	6	0	3.717533	-1.180483	-1.750186
11	6	0	4.851329	-1.042520	-0.945864
12	6	0	4.726708	-0.559687	0.357696
13	6	0	3.471694	-0.209144	0.856769
14	6	0	-0.588978	-0.831960	0.036136
15	6	0	-0.366586	-2.266615	-0.057791
16	6	0	0.593984	-3.068563	0.779129
17	7	0	-1.234809	-2.898426	-0.884048
18	8	0	-1.087380	-4.141328	-1.065417
19	8	0	0.773589	0.241414	2.288852
20	6	0	-2.157566	-0.512777	0.942518
21	7	0	-3.088755	-0.999223	-0.046574
22	6	0	-3.742283	0.016511	-0.624090
23	6	0	-3.405076	1.220049	0.049618
24	6	0	-2.476214	0.906487	1.017574
25	6	0	-4.639739	-0.183121	-1.801166
26	6	0	-2.099404	-1.301096	2.244212
27	1	0	-2.835634	-1.877217	-0.542954
28	1	0	-3.815486	2.194423	-0.181770
29	1	0	-2.036107	1.576609	1.743059
30	1	0	-0.894775	-0.392563	-0.916983
31	1	0	1.482080	-3.358914	0.201967
32	1	0	0.928952	-2.521567	1.664812
33	1	0	0.108818	-4.002706	1.083208
34	1	0	0.585802	2.748257	2.060989
35	1	0	0.301983	5.094214	1.260402
36	1	0	0.045322	5.547857	-1.170321
37	1	0	0.087075	3.665955	-2.793186
38	1	0	0.382978	1.350172	-2.001488
39	1	0	1.584526	-0.974965	-1.880287
40	1	0	3.808958	-1.571076	-2.759989
41	1	0	5.828276	-1.319590	-1.332929
42	1	0	5.605250	-0.461704	0.989708
43	1	0	3.362308	0.150530	1.875619

44	1	0	-1.319759	-0.884447	2.886396
45	1	0	-3.065034	-1.254618	2.758470
46	1	0	-1.865900	-2.349523	2.039044
47	1	0	-5.589588	-0.639637	-1.494700
48	1	0	-4.863554	0.770266	-2.286033
49	1	0	-4.179706	-0.853740	-2.536357

TS1c

HF=-1678.8369466 NIMAG = 1 (-353.020)

Zero-point correction= 0.403130 (Hartree/Particle)

Thermal correction to Energy= 0.430365

Thermal correction to Enthalpy= 0.431310

Thermal correction to Gibbs Free Energy= 0.343770

Sum of electronic and zero-point Energies= -1678.433817

Sum of electronic and thermal Energies= -1678.406581

Sum of electronic and thermal Enthalpies= -1678.405637

Sum of electronic and thermal Free Energies= -1678.493177

B3LYP (PCM)/6-31G* HF=-1678.859779	M06-2X/6-31G* HF=-1678.256366	B3LYP/6-311+G** HF=-1679.222433	M06-2X/6-311+G** HF=-1678.651154
	M06-2X(PCM)/6-31G* HF=-1678.280352	B3LYP(PCM)/6-311+G** HF=-1679.248062	M06-2X(PCM)/6-311+G** HF=-1678.677583

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.591362	1.819916	1.723700
2	6	0	-0.385733	1.900238	0.337660
3	6	0	-0.092428	3.148512	-0.237358
4	6	0	-0.014697	4.293701	0.556733
5	6	0	-0.216722	4.204455	1.934846
6	6	0	-0.501054	2.966723	2.515106
7	15	0	-0.448440	0.507029	-0.861837
8	6	0	-2.215834	0.184954	-1.221285
9	6	0	-3.225633	1.081760	-0.846716
10	6	0	-4.545407	0.864703	-1.246658
11	6	0	-4.868509	-0.249238	-2.023141
12	6	0	-3.866507	-1.142874	-2.407734
13	6	0	-2.546713	-0.924401	-2.015755
14	6	0	0.245732	-1.063329	-0.156186
15	6	0	-0.441723	-2.116957	0.488972
16	6	0	-1.766583	-2.096516	1.159225
17	8	0	-2.499394	-3.053274	1.275716
18	7	0	0.158609	-3.351079	0.591919
19	8	0	1.341572	-3.387426	0.146932
20	8	0	0.326064	0.853953	-2.104225
21	8	0	-2.080238	-0.866624	1.653804
22	6	0	-3.389992	-0.762671	2.237127
23	6	0	2.019827	-0.494948	0.952346
24	6	0	2.539864	-1.764369	1.347159
25	7	0	3.744099	-1.968899	0.771982
26	6	0	4.069406	-0.895560	-0.063367
27	6	0	3.049292	0.072564	0.070004
28	6	0	5.193718	-0.713036	-0.864236
29	6	0	5.300857	0.503702	-1.535663
30	6	0	4.315132	1.494069	-1.400422
31	6	0	3.187715	1.289046	-0.607657
32	1	0	0.942362	-1.460259	-0.894422
33	1	0	1.430905	0.103013	1.634448
34	1	0	2.178978	-2.421526	2.121408

35	1	0	4.205355	-2.868099	0.757039
36	1	0	2.427557	2.056158	-0.528677
37	1	0	4.428013	2.434036	-1.932390
38	1	0	6.163429	0.687652	-2.169823
39	1	0	5.958206	-1.479437	-0.955049
40	1	0	-2.983897	1.950462	-0.242348
41	1	0	-5.320267	1.567409	-0.951474
42	1	0	-5.896745	-0.419252	-2.330928
43	1	0	-4.111480	-2.010369	-3.013992
44	1	0	-1.774258	-1.619960	-2.330929
45	1	0	0.086333	3.204357	-1.307106
46	1	0	0.210033	5.253156	0.098633
47	1	0	-0.149851	5.094421	2.555013
48	1	0	-0.654173	2.891528	3.588579
49	1	0	-0.830449	0.866958	2.180588
50	1	0	-3.487181	-1.451644	3.079769
51	1	0	-3.479182	0.271867	2.570839
52	1	0	-4.155961	-0.991785	1.493051

TS2c

HF=-1678.850795 NImag= 1 (-315.870)
Zero-point correction= 0.403112 (Hartree/Particle)
Thermal correction to Energy= 0.430511
Thermal correction to Enthalpy= 0.431455
Thermal correction to Gibbs Free Energy= 0.342545
Sum of electronic and zero-point Energies= -1678.447683
Sum of electronic and thermal Energies= -1678.420284
Sum of electronic and thermal Enthalpies= -1678.419340
Sum of electronic and thermal Free Energies= -1678.508250

B3LYP (PCM)/6-31G* HF=-1678.923243	M06-2X/6-31G* HF=-1678.273038	B3LYP/6-311+G** HF=-1679.236721	M06-2X/6-311+G** HF=-1678.668172
	M06-2X(PCM)/6-31G* HF=-1678.295962	B3LYP(PCM)/6-311+G** HF=-1679.260828	M06-2X(PCM)/6-311+G** HF=-1678.693331

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.317559	-1.812499	1.075656
2	6	0	2.012630	-1.384730	-0.224340
3	6	0	2.493329	-2.112049	-1.322098
4	6	0	3.275258	-3.249794	-1.120760
5	6	0	3.581085	-3.668947	0.175275
6	6	0	3.099273	-2.951306	1.271993
7	15	0	1.060506	0.128465	-0.609857
8	6	0	2.226436	1.530344	-0.365862
9	6	0	2.911734	1.769527	0.835150
10	6	0	3.783350	2.852125	0.944762
11	6	0	3.980744	3.705211	-0.144570
12	6	0	3.306922	3.471056	-1.343705
13	6	0	2.433933	2.386841	-1.455752
14	6	0	-0.110913	0.387656	0.799516
15	6	0	-0.891727	-0.574995	1.477743
16	6	0	-1.382165	-1.856797	0.927653
17	8	0	-2.017770	-2.699843	1.525641
18	7	0	-1.373195	-0.269759	2.735662
19	8	0	-1.042149	0.866917	3.172500
20	8	0	-1.017411	-1.983180	-0.374501
21	6	0	-1.431876	-3.187577	-1.027343
22	6	0	-1.344954	1.859605	-0.025315

23	6	0	-2.431628	1.196492	-0.757308
24	6	0	-3.540869	1.148881	0.110852
25	7	0	-3.186674	1.842567	1.278741
26	6	0	-1.933191	2.316219	1.190110
27	6	0	-4.748913	0.543593	-0.226988
28	6	0	-4.833419	-0.016498	-1.500390
29	6	0	-3.744519	0.026652	-2.387843
30	6	0	-2.534762	0.618194	-2.026261
31	8	0	0.522193	0.155824	-2.013661
32	1	0	0.305943	1.087524	1.525431
33	1	0	-0.546615	2.410614	-0.507597
34	1	0	-1.508818	2.932612	1.965469
35	1	0	-3.745105	1.879914	2.121060
36	1	0	2.237341	-1.785138	-2.325444
37	1	0	3.641734	-3.810911	-1.976277
38	1	0	4.188337	-4.556561	0.331556
39	1	0	3.323987	-3.281836	2.282322
40	1	0	1.928586	-1.280560	1.938978
41	1	0	1.907240	2.187333	-2.384175
42	1	0	3.461364	4.130359	-2.193755
43	1	0	4.661231	4.548085	-0.057273
44	1	0	4.310224	3.028923	1.878553
45	1	0	2.778252	1.107859	1.687124
46	1	0	-5.585463	0.510237	0.464672
47	1	0	-5.758405	-0.495363	-1.808934
48	1	0	-3.845498	-0.419945	-3.372960
49	1	0	-1.674520	0.605261	-2.685004
50	1	0	-2.522556	-3.264826	-1.026675
51	1	0	-1.053025	-3.108250	-2.046405
52	1	0	-1.011537	-4.062927	-0.524526

TS3c

HF=-1678.8509011 NImag= 1 (-267.840)

Zero-point correction= 0.402906 (Hartree/Particle)

Thermal correction to Energy= 0.430340

Thermal correction to Enthalpy= 0.431284

Thermal correction to Gibbs Free Energy= 0.342189

Sum of electronic and zero-point Energies= -1678.447996

Sum of electronic and thermal Energies= -1678.420561

Sum of electronic and thermal Enthalpies= -1678.419617

Sum of electronic and thermal Free Energies= -1678.508712

B3LYP (PCM)/6-31G* HF=-1678.873117	M06-2X/6-31G* HF=-1678.272594	B3LYP/6-311+G** HF=-1679.237196	M06-2X/6-311+G** HF=-1678.668027
	M06-2X(PCM)/6-31G* HF=-1678.296034	B3LYP(PCM)/6-311+G** HF=-1679.2616940	M06-2X(PCM)/6-311+G** HF=-1678.693618

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.909059	-0.055076	-0.326098
2	6	0	-3.630290	0.175697	-0.826548
3	6	0	-2.855675	1.298206	-0.473688
4	6	0	-3.386995	2.236853	0.414426
5	6	0	-4.670355	2.030309	0.915193
6	6	0	-5.418364	0.896416	0.555346
7	7	0	-2.883713	-0.558777	-1.766655
8	6	0	-1.719265	0.043733	-2.030827
9	6	0	-1.566743	1.157723	-1.159535
10	6	0	-0.319724	0.274909	0.176453

11	6	0	-0.823845	-0.899998	0.789553
12	7	0	-1.435503	-0.840677	2.042418
13	8	0	-1.516870	0.285845	2.566655
14	15	0	1.275805	0.366082	-0.770126
15	8	0	1.163814	0.376623	-2.273235
16	6	0	1.993361	1.945284	-0.166968
17	6	0	1.974140	2.351025	1.177068
18	6	0	2.558336	3.560284	1.553917
19	6	0	3.164536	4.375287	0.594815
20	6	0	3.182849	3.980654	-0.743805
21	6	0	2.599396	2.771293	-1.124423
22	6	0	2.359672	-0.967473	-0.151476
23	6	0	3.018836	-1.739795	-1.116306
24	6	0	3.895625	-2.751320	-0.722779
25	6	0	4.114623	-2.999207	0.633256
26	6	0	3.454872	-2.234838	1.598778
27	6	0	2.580663	-1.220416	1.209855
28	6	0	-0.753203	-2.198235	0.127899
29	1	0	-2.809541	3.106409	0.713914
30	1	0	-5.098091	2.751927	1.604679
31	1	0	-6.412033	0.757410	0.970899
32	1	0	-5.485388	-0.931460	-0.607856
33	1	0	-3.144857	-1.462964	-2.137194
34	1	0	-0.986695	-0.358298	-2.714212
35	1	0	-0.927275	1.992109	-1.420378
36	1	0	-0.425837	1.097914	0.888723
37	1	0	2.827343	-1.542823	-2.166265
38	1	0	4.403425	-3.348300	-1.475648
39	1	0	4.796431	-3.788414	0.939394
40	1	0	3.617803	-2.429914	2.655195
41	1	0	2.067339	-0.641609	1.971916
42	1	0	2.597883	2.457014	-2.163821
43	1	0	3.649145	4.614922	-1.493075
44	1	0	3.617864	5.317446	0.891500
45	1	0	2.536499	3.867313	2.596036
46	1	0	1.498292	1.736209	1.936834
47	8	0	-1.118970	-3.244780	0.901719
48	8	0	-0.399067	-2.338293	-1.042130
49	6	0	-1.040072	-4.525738	0.269016
50	1	0	-1.330970	-5.246063	1.034896
51	1	0	-1.721550	-4.586377	-0.585849
52	1	0	-0.023536	-4.726124	-0.080945

TS3'c

HF=-1678.8440885 NImag = 1 (-260.750)
Zero-point correction= 0.402925 (Hartree/Particle)
Thermal correction to Energy= 0.430301
Thermal correction to Enthalpy= 0.431245
Thermal correction to Gibbs Free Energy= 0.342400
Sum of electronic and zero-point Energies= -1678.441163
Sum of electronic and thermal Energies= -1678.413787
Sum of electronic and thermal Enthalpies= -1678.412843
Sum of electronic and thermal Free Energies= -1678.501688

B3LYP (PCM)/6-31G* HF=-1678.868640	M06-2X/6-31G* HF=-1678.266006	B3LYP/6-311+G** HF=-1679.231515	M06-2X/6-311+G** HF=-1678.662409
	M06-2X(PCM)/6-31G* HF=-1678.292150	B3LYP(PCM)/6-311+G** HF=-1679.258585	M06-2X(PCM)/6-311+G** HF=-1678.6909250

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.929643	0.239434	-0.387644
2	6	0	-3.636143	0.412884	-0.867948
3	6	0	-2.782241	1.443823	-0.434831
4	6	0	-3.241156	2.340322	0.529387
5	6	0	-4.540715	2.192723	1.016794
6	6	0	-5.371421	1.154903	0.567776
7	7	0	-2.934340	-0.316582	-1.849307
8	6	0	-1.719960	0.197020	-2.053998
9	6	0	-1.482428	1.240126	-1.101220
10	6	0	-0.334887	0.386089	0.182524
11	6	0	-0.856017	-0.793461	0.807255
12	7	0	-1.419021	-0.526357	2.055775
13	8	0	-1.909028	-1.466260	2.700401
14	15	0	1.285256	0.405006	-0.749376
15	8	0	1.180637	0.499709	-2.250652
16	6	0	2.096482	1.910608	-0.074875
17	6	0	2.165266	2.214869	1.293891
18	6	0	2.812831	3.372143	1.725366
19	6	0	3.396840	4.236554	0.795780
20	6	0	3.329858	3.942247	-0.566656
21	6	0	2.682308	2.784449	-1.001407
22	6	0	2.296435	-1.010554	-0.193742
23	6	0	2.979404	-1.716809	-1.192642
24	6	0	3.813905	-2.781387	-0.851371
25	6	0	3.967624	-3.148861	0.486535
26	6	0	3.283763	-2.451384	1.485015
27	6	0	2.451546	-1.383619	1.148960
28	6	0	-0.825618	-2.051212	0.066719
29	1	0	-2.601866	3.137716	0.897456
30	1	0	-4.913717	2.887171	1.763621
31	1	0	-6.374201	1.057948	0.972941
32	1	0	-5.567218	-0.568861	-0.733528
33	1	0	-3.271635	-1.160449	-2.293975
34	1	0	-1.019952	-0.200914	-2.772038
35	1	0	-0.840469	2.069345	-1.379643
36	1	0	-0.366391	1.201961	0.906951
37	1	0	2.838105	-1.428020	-2.229309
38	1	0	4.339443	-3.326450	-1.631026
39	1	0	4.616117	-3.979734	0.752134
40	1	0	3.393345	-2.740827	2.526542
41	1	0	1.912849	-0.863336	1.934773
42	1	0	2.617384	2.545345	-2.058623
43	1	0	3.780578	4.613997	-1.292464
44	1	0	3.900814	5.137828	1.134758
45	1	0	2.860350	3.599619	2.786909
46	1	0	1.714040	1.556305	2.031634
47	8	0	-1.179106	-3.155055	0.751076
48	8	0	-0.496020	-2.096588	-1.123580
49	6	0	-1.107657	-4.379390	0.011113
50	1	0	-1.384624	-5.160284	0.720488
51	1	0	-1.803754	-4.370530	-0.833808
52	1	0	-0.096651	-4.545902	-0.371093

TS4c

HF=-1678.849018 NImag = 1 (-259.590)
Zero-point correction= 0.402995 (Hartree/Particle)
Thermal correction to Energy= 0.430471
Thermal correction to Enthalpy= 0.431415
Thermal correction to Gibbs Free Energy= 0.342225
Sum of electronic and zero-point Energies= -1678.446023
Sum of electronic and thermal Energies= -1678.418547
Sum of electronic and thermal Enthalpies= -1678.417603

Sum of electronic and thermal Free Energies= -1678.506793

B3LYP (PCM)/6-31G* HF=-1678.869781	M06-2X/6-31G* HF=-1678.268494	B3LYP/6-311+G** HF=-1679.234927	M06-2X/6-311+G** HF=-1678.663821
	M06-2X(PCM)/6-31G* HF=-1678.290503	B3LYP(PCM)/6-311+G** HF=-1679.257990	M06-2X(PCM)/6-311+G** HF=-1678.688009

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.070293	-1.261244	-1.711985
2	6	0	2.845479	-1.690723	-1.209296
3	6	0	2.531232	-1.669654	0.165332
4	6	0	3.491268	-1.224802	1.078918
5	6	0	4.724200	-0.794024	0.591636
6	6	0	5.007302	-0.806006	-0.784960
7	7	0	1.741085	-2.235313	-1.878806
8	6	0	0.755980	-2.506566	-1.012055
9	6	0	1.155777	-2.156864	0.305722
10	6	0	-0.257428	-0.758116	0.759965
11	6	0	-1.423623	-1.467814	1.141598
12	7	0	-1.483750	-2.075134	2.386873
13	8	0	-0.434006	-1.997942	3.070020
14	15	0	-0.208307	0.575833	-0.529836
15	8	0	0.221562	0.189255	-1.919504
16	6	0	0.962590	1.788917	0.197948
17	6	0	0.953397	2.177102	1.546375
18	6	0	1.862533	3.126582	2.012494
19	6	0	2.789497	3.697040	1.137103
20	6	0	2.805756	3.314701	-0.204921
21	6	0	1.896532	2.365434	-0.673433
22	6	0	-1.849913	1.384748	-0.510876
23	6	0	-2.427674	1.654464	-1.758149
24	6	0	-3.658267	2.307737	-1.833484
25	6	0	-4.320424	2.690753	-0.666020
26	6	0	-3.750979	2.418982	0.580261
27	6	0	-2.519253	1.769658	0.659436
28	6	0	-2.489753	-1.789158	0.188395
29	8	0	-3.637128	-2.199172	0.763635
30	6	0	-4.681181	-2.561984	-0.149087
31	1	0	-5.520256	-2.866268	0.477675
32	8	0	-2.347017	-1.709726	-1.028476
33	1	0	3.276233	-1.208966	2.143477
34	1	0	5.480735	-0.440828	1.286294
35	1	0	5.975676	-0.459678	-1.134341
36	1	0	4.290201	-1.280524	-2.775434
37	1	0	1.577241	-2.124933	-2.871168
38	1	0	-0.218542	-2.828326	-1.351964
39	1	0	0.835157	-2.685473	1.198122
40	1	0	0.316749	-0.498805	1.650891
41	1	0	1.904204	2.052632	-1.712873
42	1	0	3.527839	3.754232	-0.888025
43	1	0	3.497671	4.436222	1.502300
44	1	0	1.848229	3.418595	3.059108
45	1	0	0.242907	1.742817	2.244952
46	1	0	-2.096720	1.553943	1.636271
47	1	0	-4.266785	2.708994	1.491569
48	1	0	-5.280002	3.197783	-0.725254
49	1	0	-4.101845	2.512149	-2.804352
50	1	0	-1.907833	1.337423	-2.656478
51	1	0	-4.958814	-1.711291	-0.777585
52	1	0	-4.366132	-3.388361	-0.793007

TS4'c

HF=-1678.8423116 NImag = 1 (-252.750)
Zero-point correction= 0.403056 (Hartree/Particle)
Thermal correction to Energy= 0.430380
Thermal correction to Enthalpy= 0.431324
Thermal correction to Gibbs Free Energy= 0.342800
Sum of electronic and zero-point Energies= -1678.439256
Sum of electronic and thermal Energies= -1678.411932
Sum of electronic and thermal Enthalpies= -1678.410988
Sum of electronic and thermal Free Energies= -1678.499511

B3LYP (PCM)/6-31G* HF=-1678.865720	M06-2X/6-31G* HF=-1678.2610434	B3LYP/6-311+G** HF=-1679.2287441	M06-2X/6-311+G** HF=-1678.6565815
	M06-2X(PCM)/6-31G* HF=-1678.286017	B3LYP(PCM)/6-311+G** HF=-1679.254567	M06-2X(PCM)/6-311+G** HF=-1678.683804

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.942583	-0.852795	0.503512
2	6	0	-2.356931	-0.449374	-0.704771
3	6	0	-2.825519	-0.979782	-1.913972
4	6	0	-3.860581	-1.914376	-1.913436
5	6	0	-4.432863	-2.324090	-0.707559
6	6	0	-3.974211	-1.791793	0.499934
7	15	0	-1.027198	0.798541	-0.808918
8	6	0	-1.547040	2.177443	0.283530
9	6	0	-1.381626	2.179567	1.678047
10	6	0	-1.830269	3.264632	2.432887
11	6	0	-2.441988	4.352078	1.806096
12	6	0	-2.599682	4.359211	0.418676
13	6	0	-2.152610	3.278127	-0.341026
14	6	0	0.508600	0.192987	0.063933
15	6	0	0.472523	-0.966630	0.897063
16	6	0	0.042902	-2.249278	0.316228
17	8	0	0.014063	-2.440528	-0.899429
18	7	0	1.064432	-0.756245	2.145145
19	8	0	1.112190	-1.704554	2.944434
20	8	0	-0.822138	1.264096	-2.230936
21	8	0	-0.299547	-3.198432	1.203056
22	6	0	-0.707857	-4.449165	0.630830
23	6	0	1.861550	-0.051756	-1.335156
24	6	0	3.157747	-0.183585	-0.646834
25	6	0	3.895355	0.993647	-0.889021
26	7	0	3.124327	1.787633	-1.754155
27	6	0	1.974846	1.167865	-2.065271
28	6	0	3.707099	-1.162243	0.184204
29	6	0	4.968628	-0.938585	0.738387
30	6	0	5.680858	0.242931	0.480432
31	6	0	5.151049	1.237395	-0.342166
32	1	0	-1.605849	-4.317220	0.020619
33	1	0	3.166353	-2.077596	0.397936
34	1	0	5.406202	-1.691828	1.386666
35	1	0	6.659545	0.388110	0.928235
36	1	0	5.697338	2.154229	-0.545359
37	1	0	3.388189	2.706433	-2.084179
38	1	0	1.232077	1.605847	-2.716244
39	1	0	1.336481	-0.905021	-1.758513
40	1	0	0.944465	1.024821	0.620379
41	1	0	-2.256782	3.280491	-1.422002
42	1	0	-3.067838	5.208081	-0.072718

43	1	0	-2.789522	5.195013	2.397675
44	1	0	-1.695371	3.260751	3.511068
45	1	0	-0.887226	1.351444	2.178678
46	1	0	-2.600980	-0.439691	1.447457
47	1	0	-4.421926	-2.103071	1.439744
48	1	0	-5.240210	-3.051931	-0.707718
49	1	0	-4.218985	-2.323313	-2.854286
50	1	0	-2.372921	-0.651648	-2.844046
51	1	0	0.085608	-4.870786	0.007652
52	1	0	-0.912921	-5.100175	1.481512

TS5c

HF=-1525.2102973 NImag = 1(-233.700)
Zero-point correction= 0.355667 (Hartree/Particle)
Thermal correction to Energy= 0.380555
Thermal correction to Enthalpy= 0.381499
Thermal correction to Gibbs Free Energy= 0.298080
Sum of electronic and zero-point Energies= -1524.854630
Sum of electronic and thermal Energies= -1524.829743
Sum of electronic and thermal Enthalpies= -1524.828798
Sum of electronic and thermal Free Energies= -1524.912217

B3LYP (PCM)/6-31G* (HF=-1525.228908)	M06-2X/6-31G* HF=-1524.6875761	B3LYP/6-311+G** HF=-1525.5617342	M06-2X/6-311+G** HF=-1525.0466745
	M06-2X(PCM)/6-31G* (HF=-1524.706769)	B3LYP(PCM)/6-311+G** (HF=-1525.582822)	M06-2X(PCM)/6-311+G** (HF=-1525.068045)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.013619	2.006280	-1.841360
2	6	0	-0.942979	2.496723	-1.096581
3	6	0	-1.478806	3.521443	-0.268428
4	6	0	-2.858973	3.563829	-0.476151
5	6	0	-3.159384	2.594468	-1.441644
6	6	0	-0.360573	0.983333	0.330787
7	6	0	0.772469	1.470932	0.990249
8	7	0	0.651478	2.207660	2.177748
9	8	0	-0.514651	2.377306	2.580947
10	15	0	-0.404735	-0.550072	-0.714734
11	8	0	-0.775244	-0.363346	-2.171058
12	6	0	1.168776	-1.457813	-0.547572
13	6	0	1.885130	-1.719945	-1.722260
14	6	0	3.079292	-2.438509	-1.665104
15	6	0	3.564622	-2.894311	-0.438043
16	6	0	2.850782	-2.637517	0.735137
17	6	0	1.652750	-1.925554	0.682047
18	6	0	-1.658510	-1.557232	0.163727
19	6	0	-1.836474	-1.539384	1.555990
20	6	0	-2.794014	-2.361623	2.150886
21	6	0	-3.581858	-3.203643	1.363411
22	6	0	-3.414555	-3.220660	-0.022636
23	6	0	-2.457985	-2.400967	-0.621671
24	6	0	2.088929	1.492533	0.332217
25	1	0	0.054032	2.426673	-1.513959
26	1	0	-4.117184	2.282226	-1.835645
27	1	0	-0.906569	4.125541	0.420853
28	1	0	-1.255772	1.097817	0.941903
29	1	0	-1.893858	1.149519	-2.387088

30	1	0	-3.576702	4.199013	0.024008
31	1	0	1.102817	-1.739339	1.599838
32	1	0	3.223749	-2.994526	1.691131
33	1	0	4.495908	-3.453000	-0.394678
34	1	0	3.632345	-2.638048	-2.578882
35	1	0	1.500318	-1.352447	-2.667698
36	1	0	-2.329570	-2.399041	-1.700010
37	1	0	-4.031083	-3.869980	-0.638432
38	1	0	-4.328376	-3.841198	1.829419
39	1	0	-2.928246	-2.338393	3.228784
40	1	0	-1.243745	-0.878475	2.182999
41	8	0	3.122596	1.669500	1.174110
42	8	0	2.219641	1.385166	-0.881373
43	6	0	4.411977	1.751828	0.549014
44	1	0	5.117389	1.922649	1.362833
45	1	0	4.644512	0.819920	0.026293
46	1	0	4.443617	2.577985	-0.166632

TS6c

HF=-1525.2167974 NImag =1 (-280.760)

Zero-point correction= 0.356345 (Hartree/Particle)

Thermal correction to Energy= 0.380822

Thermal correction to Enthalpy= 0.381766

Thermal correction to Gibbs Free Energy= 0.300440

Sum of electronic and zero-point Energies= -1524.860452

Sum of electronic and thermal Energies= -1524.835976

Sum of electronic and thermal Enthalpies= -1524.835032

Sum of electronic and thermal Free Energies= -1524.916357

B3LYP (PCM)/6-31G* (HF=-1525.2368764)	M06-2X/6-31G* HF=-1524.7013003	B3LYP/6-311+G** HF=-1525.5677648	M06-2X/6-311+G** HF=-1525.060146
	M06-2X(PCM)/6-31G* (HF=-1524.7223225)	B3LYP(PCM)/6-311+G** (HF=-1525.5905319)	M06-2X(PCM)/6-311+G** (HF=-1525.0836616)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.296116	-1.034800	-1.072906
2	6	0	-2.423533	-0.560585	-0.083590
3	6	0	-2.833629	-0.573926	1.258526
4	6	0	-4.095566	-1.055612	1.603634
5	6	0	-4.960044	-1.526934	0.612020
6	6	0	-4.559526	-1.516200	-0.724568
7	15	0	-0.786433	0.059742	-0.634584
8	8	0	-0.607990	-0.214554	-2.110938
9	6	0	0.373588	-0.833361	0.492506
10	6	0	1.655288	-0.384856	0.863121
11	6	0	2.426837	0.573009	0.057261
12	7	0	2.267491	-0.899929	2.009706
13	8	0	1.616496	-1.780441	2.605303
14	6	0	-0.735072	1.832948	-0.211480
15	6	0	-0.833198	2.739701	-1.274709
16	6	0	-0.853305	4.111484	-1.022544
17	6	0	-0.771135	4.584238	0.288341
18	6	0	-0.664145	3.683307	1.350286
19	6	0	-0.646676	2.310647	1.103512
20	6	0	0.539139	-2.581415	-0.622160
21	7	0	1.360260	-2.089314	-1.648003
22	6	0	2.635795	-2.375320	-1.349017
23	6	0	2.673432	-3.244584	-0.240948
24	6	0	1.364810	-3.419227	0.185392
25	1	0	-0.510703	-2.742030	-0.833849

26	1	0	3.450987	-1.964128	-1.928840
27	1	0	-0.115024	-1.337294	1.327041
28	1	0	1.020958	-4.015456	1.017652
29	1	0	1.016363	-1.323994	-2.235778
30	1	0	3.568778	-3.666119	0.194056
31	1	0	-0.875513	2.359185	-2.290329
32	1	0	-0.925706	4.810796	-1.851126
33	1	0	-0.784390	5.653341	0.483229
34	1	0	-0.588602	4.048303	2.370913
35	1	0	-0.542468	1.622427	1.937545
36	1	0	-2.969429	-1.023256	-2.108320
37	1	0	-5.229713	-1.882757	-1.497506
38	1	0	-5.943268	-1.902062	0.883215
39	1	0	-4.403749	-1.064093	2.645546
40	1	0	-2.174347	-0.208491	2.041539
41	8	0	3.533149	1.035977	0.675632
42	8	0	2.095965	0.932935	-1.065721
43	6	0	4.302662	1.977549	-0.082689
44	1	0	5.138734	2.253045	0.561202
45	1	0	4.667635	1.526402	-1.010327
46	1	0	3.703108	2.857036	-0.333161

TS7c

HF=-1525.1960762 NImag =1 (-239.410)

Zero-point correction= 0.355978 (Hartree/Particle)

Thermal correction to Energy= 0.380849

Thermal correction to Enthalpy= 0.381793

Thermal correction to Gibbs Free Energy= 0.299241

Sum of electronic and zero-point Energies= -1524.840098

Sum of electronic and thermal Energies= -1524.815227

Sum of electronic and thermal Enthalpies= -1524.814283

Sum of electronic and thermal Free Energies= -1524.896835

B3LYP (PCM)/6-31G* (HF=-1525.216147)	M06-2X/6-31G* HF=-1524.672979	B3LYP/6-311+G** HF=-1525.5468523	M06-2X/6-311+G** HF=-1525.0320692
	M06-2X(PCM)/6-31G* (HF=-1524.693647)	B3LYP(PCM)/6-311+G** (HF=-1525.569735)	M06-2X(PCM)/6-311+G** (HF=-1525.068045)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.056144	2.207386	-1.691624
2	6	0	1.396066	1.578857	-0.626085
3	6	0	1.962791	1.615449	0.656587
4	6	0	3.176908	2.267937	0.865694
5	6	0	3.833797	2.887719	-0.200505
6	6	0	3.271836	2.858420	-1.477187
7	15	0	-0.193057	0.763343	-1.039008
8	6	0	-1.415349	1.278116	0.227830
9	6	0	-1.364602	1.007974	1.603386
10	6	0	-2.330451	1.545309	2.456651
11	6	0	-3.351262	2.352730	1.950143
12	6	0	-3.407324	2.621987	0.581990
13	6	0	-2.445140	2.089002	-0.276221
14	6	0	0.247515	-1.040694	-1.068147
15	6	0	1.174962	-1.805164	-0.347254
16	6	0	1.372772	-1.767867	1.104529
17	7	0	1.844575	-2.868319	-0.985491
18	8	0	1.444429	-3.142147	-2.128790
19	8	0	-0.664193	1.141188	-2.415907
20	6	0	-1.570420	-2.230302	-1.049100
21	6	0	-2.652016	-1.717804	-1.805158

22	6	0	-3.650083	-1.309919	-0.917975
23	6	0	-3.190164	-1.592318	0.373064
24	7	0	-1.978964	-2.180560	0.291589
25	1	0	-0.905446	-3.016738	-1.384038
26	1	0	-3.631562	-1.353875	1.330545
27	1	0	-4.594573	-0.843297	-1.159824
28	1	0	-2.675717	-1.666958	-2.885055
29	1	0	-1.323425	-2.254320	1.067541
30	1	0	0.347306	-1.267883	-2.133188
31	1	0	1.600680	2.186726	-2.676823
32	1	0	3.777499	3.344207	-2.307291
33	1	0	4.780040	3.395441	-0.033341
34	1	0	3.609203	2.296431	1.862341
35	1	0	1.459929	1.146883	1.496333
36	1	0	-0.601271	0.355188	2.008922
37	1	0	-2.283303	1.330372	3.521218
38	1	0	-4.098569	2.770534	2.619922
39	1	0	-4.199318	3.248601	0.180452
40	1	0	-2.477242	2.290739	-1.342010
41	8	0	2.603381	-2.121941	1.494239
42	8	0	0.479523	-1.488487	1.909826
43	6	0	2.806601	-2.240052	2.911122
44	1	0	3.836313	-2.578295	3.026039
45	1	0	2.663003	-1.274528	3.403687
46	1	0	2.112436	-2.966723	3.341607

TS7'c

HF=-1525.2031871 NImag =1 (-257.950)
Zero-point correction= 0.355766 (Hartree/Particle)
Thermal correction to Energy= 0.380569
Thermal correction to Enthalpy= 0.381513
Thermal correction to Gibbs Free Energy= 0.298390
Sum of electronic and zero-point Energies= -1524.847421
Sum of electronic and thermal Energies= -1524.822618
Sum of electronic and thermal Enthalpies= -1524.821674
Sum of electronic and thermal Free Energies= -1524.904797

B3LYP (PCM)/6-31G* (HF=-1525.223106)	M06-2X/6-31G* HF=-1524.679930	B3LYP/6-311+G** HF=-1525.555314	M06-2X/6-311+G** HF=-1525.039626
	M06-2X(PCM)/6-31G* (HF=-1524.700720)	B3LYP(PCM)/6-311+G** (HF=-1525.577883)	M06-2X(PCM)/6-311+G** (HF=-1525.062790)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.726729	-2.381389	-1.771124
2	6	0	0.587787	-2.620301	-0.989448
3	6	0	0.914389	-3.756991	-0.190208
4	6	0	2.236202	-4.106180	-0.441075
5	6	0	2.717537	-3.212836	-1.415778
6	6	0	0.330884	-1.076060	0.338998
7	6	0	-0.875108	-1.256882	1.057266
8	7	0	-0.664922	-1.782422	2.338523
9	8	0	-1.652686	-1.999685	3.053288
10	15	0	0.628773	0.432621	-0.722550
11	8	0	1.087653	0.173105	-2.144084
12	6	0	1.921285	1.302732	0.240769
13	6	0	1.967889	1.323401	1.643913
14	6	0	2.972857	2.035637	2.299399
15	6	0	3.937126	2.727567	1.563407
16	6	0	3.899692	2.703924	0.168002
17	6	0	2.896815	1.993999	-0.492590

18	6	0	-0.833756	1.522197	-0.707247
19	6	0	-1.426210	1.808865	-1.944147
20	6	0	-2.523021	2.667883	-2.010220
21	6	0	-3.034355	3.241445	-0.844514
22	6	0	-2.443384	2.961158	0.390021
23	6	0	-1.342450	2.108004	0.460556
24	6	0	-2.159667	-1.146098	0.339967
25	8	0	-2.225768	-1.230769	-0.885057
26	8	0	-3.236892	-0.962135	1.115777
27	6	0	-4.488677	-0.880740	0.416653
28	1	0	-0.383954	-2.402933	-1.423936
29	1	0	2.810270	-4.891669	0.030800
30	1	0	0.246461	-4.213297	0.527990
31	1	0	3.709785	-3.118940	-1.836873
32	1	0	1.783182	-1.514808	-2.316834
33	1	0	1.198730	-1.270761	0.968304
34	1	0	2.865849	1.959392	-1.577467
35	1	0	4.653157	3.235478	-0.407006
36	1	0	4.719379	3.279567	2.077554
37	1	0	3.004948	2.043994	3.385381
38	1	0	1.235618	0.775269	2.230781
39	1	0	-0.887714	1.904270	1.424998
40	1	0	-2.836398	3.408918	1.298509
41	1	0	-3.889345	3.910451	-0.896887
42	1	0	-2.979235	2.886493	-2.971841
43	1	0	-1.020546	1.353828	-2.841560
44	1	0	-4.668137	-1.789228	-0.164411
45	1	0	-5.244423	-0.767548	1.194452
46	1	0	-4.495339	-0.019570	-0.257227

TS8c

HF=-1525.2034653 NImag =1 (-260.230)
Zero-point correction= 0.355397 (Hartree/Particle)
Thermal correction to Energy= 0.380453
Thermal correction to Enthalpy= 0.381398
Thermal correction to Gibbs Free Energy= 0.297650
Sum of electronic and zero-point Energies= -1524.848068
Sum of electronic and thermal Energies= -1524.823012
Sum of electronic and thermal Enthalpies= -1524.822068
Sum of electronic and thermal Free Energies= -1524.905815

B3LYP (PCM)/6-31G* (HF=-1525.224464)	M06-2X/6-31G* HF=-1524.6803137	B3LYP/6-311+G** HF=-1525.5540358	M06-2X/6-311+G** HF=-1525.0388791
	M06-2X(PCM)/6-31G* (HF=-1524.702275)	B3LYP(PCM)/6-311+G** (HF=-1525.577786)	M06-2X(PCM)/6-311+G** (HF=-1525.063322)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.397625	-1.781614	-1.614685
2	6	0	1.212112	-2.335012	-1.064298
3	7	0	1.636887	-3.285887	-0.117328
4	6	0	2.976810	-3.213693	0.017541
5	6	0	3.487326	-2.307358	-0.920246
6	6	0	0.191654	-0.992815	0.278000
7	6	0	-0.992487	-1.627167	0.696356
8	7	0	-1.027872	-2.472103	1.794994
9	8	0	0.084323	-2.844715	2.244022
10	15	0	0.266143	0.583680	-0.709822
11	8	0	0.434870	0.463581	-2.197467
12	6	0	1.703350	1.437178	0.051352

13	6	0	2.544885	2.141071	-0.821788
14	6	0	3.640934	2.849228	-0.327570
15	6	0	3.907405	2.860091	1.042476
16	6	0	3.076202	2.159290	1.919135
17	6	0	1.979888	1.450880	1.426930
18	6	0	-1.205512	1.569707	-0.250777
19	6	0	-1.561887	1.871222	1.071032
20	6	0	-2.684014	2.657383	1.331942
21	6	0	-3.453429	3.150318	0.275379
22	6	0	-3.100738	2.853798	-1.042446
23	6	0	-1.981788	2.063688	-1.307320
24	6	0	-2.242128	-1.513587	-0.082857
25	1	0	3.488044	-3.780059	0.784417
26	1	0	0.282105	-2.468352	-1.599867
27	1	0	1.034120	-3.614538	0.635786
28	1	0	4.533124	-2.074062	-1.065046
29	1	0	2.400503	-1.066517	-2.423589
30	1	0	0.985212	-1.081493	1.019098
31	1	0	2.331632	2.118549	-1.886233
32	1	0	4.287531	3.390851	-1.012881
33	1	0	4.761266	3.411233	1.427545
34	1	0	3.282224	2.161421	2.986088
35	1	0	1.349282	0.907652	2.126057
36	1	0	-0.974595	1.494568	1.903421
37	1	0	-2.956924	2.884099	2.358978
38	1	0	-4.326400	3.764459	0.480643
39	1	0	-3.699355	3.233672	-1.866046
40	1	0	-1.702307	1.811728	-2.325028
41	8	0	-3.347327	-1.863856	0.599424
42	8	0	-2.253909	-1.156368	-1.250727
43	6	0	-4.569899	-1.792007	-0.150083
44	1	0	-5.351253	-2.107637	0.541854
45	1	0	-4.748913	-0.770090	-0.494975
46	1	0	-4.532054	-2.457499	-1.017011

TS8'c

HF=-1525.2045738 NImag =1 (-259,330)

Zero-point correction= 0.356033 (Hartree/Particle)

Thermal correction to Energy= 0.380690

Thermal correction to Enthalpy= 0.381635

Thermal correction to Gibbs Free Energy= 0.299424

Sum of electronic and zero-point Energies= -1524.848541

Sum of electronic and thermal Energies= -1524.823883

Sum of electronic and thermal Enthalpies= -1524.822939

Sum of electronic and thermal Free Energies= -1524.905150

B3LYP (PCM)/6-31G* (HF=-1525.228360)	M06-2X/6-31G* HF=-1524.688982	B3LYP/6-311+G** HF=-1525.556419	M06-2X/6-311+G** HF=-1525.048549
	M06-2X(PCM)/6-31G* (HF=-1524.714342)	B3LYP(PCM)/6-311+G** (HF=-1525.583284)	M06-2X(PCM)/6-311+G** (HF=-1525.076807)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.764339	2.659187	-1.363048
2	6	0	0.645610	1.782222	-0.276632
3	6	0	0.425908	2.294241	1.010045
4	6	0	0.334055	3.672490	1.205241
5	6	0	0.462729	4.543997	0.121556
6	6	0	0.675177	4.036383	-1.161561
7	15	0	0.850529	0.007683	-0.636057
8	6	0	2.510600	-0.461594	-0.004506

9	6	0	3.426737	-0.974210	-0.933401
10	6	0	4.707855	-1.350230	-0.524541
11	6	0	5.082620	-1.215719	0.812659
12	6	0	4.175206	-0.703063	1.743913
13	6	0	2.895553	-0.326729	1.338338
14	6	0	-0.291218	-0.966442	0.473260
15	6	0	-1.584544	-0.479332	0.867017
16	6	0	-2.372698	0.358151	-0.044748
17	6	0	-0.346762	-2.568634	-0.539854
18	6	0	-1.035014	-3.543924	0.268003
19	6	0	-2.360749	-3.537599	-0.100675
20	6	0	-2.477703	-2.655556	-1.207134
21	7	0	-1.270648	-2.213835	-1.553057
22	7	0	-1.925150	-0.929782	2.145915
23	8	0	-2.987813	-0.551557	2.657510
24	8	0	0.748270	-0.340328	-2.102707
25	1	0	0.686318	-2.691678	-0.848863
26	1	0	-3.363766	-2.350909	-1.747940
27	1	0	-1.061571	-1.416196	-2.158680
28	1	0	-3.179735	-4.076308	0.355408
29	1	0	-0.589215	-4.080601	1.094476
30	1	0	0.237534	-1.344623	1.349104
31	1	0	3.120844	-1.070537	-1.970845
32	1	0	5.412062	-1.746744	-1.251120
33	1	0	6.079728	-1.507958	1.131116
34	1	0	4.465046	-0.595318	2.785586
35	1	0	2.204322	0.077944	2.073133
36	1	0	0.296537	1.627214	1.857157
37	1	0	0.154867	4.063901	2.202826
38	1	0	0.390654	5.617202	0.277190
39	1	0	0.764361	4.712114	-2.007891
40	1	0	0.908248	2.250296	-2.358216
41	8	0	-3.477890	0.908201	0.491593
42	8	0	-2.044478	0.563183	-1.214809
43	6	0	-4.228354	1.752024	-0.391345
44	1	0	-5.069516	2.111344	0.202743
45	1	0	-3.618642	2.589292	-0.742149
46	1	0	-4.586209	1.191673	-1.260412

TS9c

HF=-1603.8483606 NImag =1 (-279.020)

Zero-point correction= 0.411683 (Hartree/Particle)

Thermal correction to Energy= 0.439675

Thermal correction to Enthalpy= 0.440620

Thermal correction to Gibbs Free Energy= 0.351373

Sum of electronic and zero-point Energies= -1603.436677

Sum of electronic and thermal Energies= -1603.408685

Sum of electronic and thermal Enthalpies= -1603.407741

Sum of electronic and thermal Free Energies= -1603.496988

B3LYP (PCM)/6-31G* HF=-1603.865549	M06-2X/6-31G* HF=-1603.288247	B3LYP/6-311+G** HF=-1604.218691	M06-2X/6-311+G** HF=-1603.667945
	M06-2X(PCM)/6-31G* HF=-1603.306104	B3LYP(PCM)/6-311+G** HF=-1604.238242	M06-2X(PCM)/6-311+G** HF=-1603.687945

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.173515	-1.527502	-1.349106
2	6	0	1.167692	-2.324378	-0.760393
3	6	0	1.848059	-3.039296	0.286208
4	6	0	3.154446	-2.576499	0.359274

5	6	0	3.327067	-1.615158	-0.657288
6	6	0	0.120891	-2.928306	-1.662628
7	6	0	4.512156	-0.758655	-0.961418
8	6	0	0.061905	-0.920947	0.398017
9	6	0	-1.102459	-1.550258	0.884915
10	7	0	-1.031122	-2.357091	2.015646
11	8	0	0.100481	-2.423975	2.550338
12	15	0	0.085815	0.615354	-0.633861
13	8	0	0.423649	0.440724	-2.101090
14	6	0	-1.450905	1.567722	-0.389139
15	6	0	-2.120154	2.011928	-1.535901
16	6	0	-3.269535	2.792493	-1.412925
17	6	0	-3.757715	3.127461	-0.148729
18	6	0	-3.092424	2.684414	0.996978
19	6	0	-1.938296	1.910623	0.879122
20	6	0	1.386861	1.622626	0.190823
21	6	0	1.590909	1.663735	1.578622
22	6	0	2.576040	2.489053	2.122237
23	6	0	3.368447	3.280179	1.287658
24	6	0	3.173837	3.244050	-0.094501
25	6	0	2.187854	2.420122	-0.640657
26	6	0	-2.378892	-1.531845	0.151502
27	8	0	-2.496323	-1.111556	-0.991592
28	8	0	-3.417956	-2.015058	0.863789
29	6	0	-4.675133	-2.016814	0.175349
30	1	0	-5.390035	-2.444041	0.879633
31	1	0	1.390448	-3.798954	0.902546
32	1	0	0.827181	-0.902119	1.172387
33	1	0	1.909410	-0.796074	-2.015305
34	1	0	3.916860	-2.871638	1.067694
35	1	0	-1.430745	1.572161	1.777909
36	1	0	-3.470390	2.942243	1.982541
37	1	0	-4.655253	3.733151	-0.054572
38	1	0	-3.787576	3.132910	-2.305454
39	1	0	-1.737988	1.730378	-2.511567
40	1	0	2.031889	2.382503	-1.714885
41	1	0	3.787632	3.858287	-0.748162
42	1	0	4.135314	3.921466	1.713820
43	1	0	2.726712	2.509962	3.198104
44	1	0	0.992144	1.049546	2.245761
45	1	0	5.396443	-1.132061	-0.438760
46	1	0	4.727090	-0.741724	-2.036127
47	1	0	4.340155	0.277687	-0.643073
48	1	0	-0.651117	-3.412783	-1.059471
49	1	0	-0.352669	-2.168132	-2.286512
50	1	0	0.575966	-3.691216	-2.306398
51	1	0	-4.967090	-0.999407	-0.099983
52	1	0	-4.621060	-2.624894	-0.732315

TS10c

HF=-1603.8553437 NImag =1 (-269.170)

Zero-point correction= 0.412071 (Hartree/Particle)

Thermal correction to Energy= 0.439701

Thermal correction to Enthalpy= 0.440645

Thermal correction to Gibbs Free Energy= 0.353505

Sum of electronic and zero-point Energies= -1603.443273

Sum of electronic and thermal Energies= -1603.415643

Sum of electronic and thermal Enthalpies= -1603.414699

Sum of electronic and thermal Free Energies= -1603.501839

B3LYP (PCM)/6-31G* HF=-1603.871034	M06-2X/6-31G* HF=-1603.301033	B3LYP/6-311+G** HF=-1604.225366	M06-2X/6-311+G** HF=-1603.680300
	M06-2X(PCM)/6-31G* HF=-1603.317434	B3LYP(PCM)/6-311+G** HF=-1604.243272	M06-2X(PCM)/6-311+G** HF=-1603.698785

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.412245	-0.999509	-1.094512
2	6	0	-2.510835	-0.660354	-0.075179
3	6	0	-2.909374	-0.792368	1.263315
4	6	0	-4.186918	-1.258657	1.575177
5	6	0	-5.078323	-1.595262	0.554285
6	6	0	-4.689329	-1.465125	-0.780102
7	15	0	-0.873268	-0.009328	-0.592350
8	8	0	-0.596005	-0.365174	-2.038737
9	6	0	0.299601	-0.722295	0.641746
10	6	0	1.432233	-0.028218	1.117715
11	6	0	2.104615	1.039682	0.366777
12	8	0	1.900080	1.274365	-0.820279
13	7	0	1.998729	-0.382496	2.343089
14	8	0	1.472085	-1.368413	2.899025
15	6	0	-0.997659	1.794909	-0.324810
16	6	0	-0.958680	2.611810	-1.461308
17	6	0	-1.108291	3.992925	-1.333811
18	6	0	-1.290751	4.564457	-0.073281
19	6	0	-1.325697	3.752714	1.062987
20	6	0	-1.183722	2.370730	0.939148
21	8	0	2.970003	1.761353	1.109653
22	6	0	3.626074	2.830937	0.418155
23	1	0	4.240026	3.327150	1.170823
24	6	0	0.893711	-2.543166	-0.306148
25	7	0	1.600323	-1.940863	-1.374918
26	6	0	2.901686	-1.829662	-1.059962
27	6	0	3.124738	-2.526059	0.153750
28	6	0	1.906265	-3.008214	0.593479
29	6	0	-0.369457	-3.316851	-0.600663
30	6	0	3.862469	-1.070082	-1.911127
31	1	0	-0.176204	-1.274219	1.451962
32	1	0	1.716623	-3.603344	1.474738
33	1	0	1.088111	-1.338034	-2.028882
34	1	0	4.089314	-2.637241	0.630721
35	1	0	-0.796767	2.154472	-2.431956
36	1	0	-1.075159	4.622822	-2.218765
37	1	0	-1.404177	5.640892	0.025443
38	1	0	-1.462711	4.194699	2.046144
39	1	0	-1.206995	1.752022	1.831771
40	1	0	-3.095735	-0.905745	-2.129097
41	1	0	-5.379510	-1.728268	-1.577236
42	1	0	-6.072350	-1.959739	0.799331
43	1	0	-4.483764	-1.361959	2.615352
44	1	0	-2.229095	-0.538394	2.071791
45	1	0	4.875780	-1.143602	-1.508621
46	1	0	3.868596	-1.454283	-2.938127
47	1	0	3.568471	-0.013846	-1.950650
48	1	0	-1.003259	-2.793736	-1.317468
49	1	0	-0.116626	-4.296811	-1.023907
50	1	0	-0.939641	-3.485589	0.317680
51	1	0	4.255484	2.448403	-0.391086
52	1	0	2.895277	3.526667	-0.002975

TS11c

HF=-1603.8443519 NImag = 1 (-168.640)

Zero-point correction= 0.411124 (Hartree/Particle)

Thermal correction to Energy= 0.439329

Thermal correction to Enthalpy= 0.440273

Thermal correction to Gibbs Free Energy= 0.350353
Sum of electronic and zero-point Energies= -1603.433228
Sum of electronic and thermal Energies= -1603.405023
Sum of electronic and thermal Enthalpies= -1603.404079
Sum of electronic and thermal Free Energies= -1603.493999

B3LYP (PCM)/6-31G* HF=-1603.858474	M06-2X/6-31G* HF=-1603.280562	B3LYP/6-311+G** HF=-1604.215311	M06-2X/6-311+G** HF=-1603.660530
	M06-2X(PCM)/6-31G* HF=-1603.295160	B3LYP(PCM)/6-311+G** HF=-1604.231346	M06-2X(PCM)/6-311+G** HF=-1603.676886

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.445725	-2.906255	-0.733822
2	6	0	0.761827	-2.648028	0.610859
3	6	0	2.169076	-2.451660	0.629241
4	6	0	2.647365	-2.548014	-0.674713
5	6	0	1.544029	-2.791576	-1.512750
6	6	0	-0.019626	-3.334125	1.694393
7	6	0	1.471783	-2.825033	-3.000146
8	6	0	-0.193795	-0.531026	0.902078
9	6	0	-1.537217	-0.790026	1.166930
10	7	0	-2.027776	-0.800306	2.491415
11	8	0	-1.185656	-0.664624	3.390640
12	15	0	0.417600	0.509625	-0.487363
13	8	0	0.608503	-0.094598	-1.851637
14	6	0	1.988384	1.194622	0.165914
15	6	0	2.127964	1.730252	1.454762
16	6	0	3.350322	2.261015	1.867166
17	6	0	4.441724	2.265243	0.995467
18	6	0	4.308546	1.736493	-0.289470
19	6	0	3.087208	1.203412	-0.703359
20	6	0	-0.768200	1.909174	-0.557740
21	6	0	-1.099656	2.376265	-1.836901
22	6	0	-1.964569	3.461632	-1.985759
23	6	0	-2.503330	4.085809	-0.860029
24	6	0	-2.180630	3.621032	0.417452
25	6	0	-1.318093	2.536280	0.570390
26	6	0	-2.516983	-1.131801	0.120938
27	8	0	-2.218456	-1.677557	-0.939074
28	8	0	-3.782961	-0.822528	0.443006
29	6	0	-4.778468	-1.214441	-0.514550
30	1	0	-5.730543	-0.905061	-0.082809
31	1	0	3.667489	-2.425199	-1.012751
32	1	0	2.752393	-2.313792	1.530931
33	1	0	-0.508692	-2.781580	-1.075969
34	1	0	0.356194	-0.367086	1.830011
35	1	0	2.970291	0.782942	-1.697355
36	1	0	5.155836	1.738709	-0.970205
37	1	0	5.392768	2.680650	1.318168
38	1	0	3.449615	2.671421	2.868401
39	1	0	1.288762	1.740582	2.145348
40	1	0	-1.095796	2.173957	1.569896
41	1	0	-2.607218	4.097877	1.295644
42	1	0	-3.177992	4.930048	-0.975745
43	1	0	-2.219730	3.815803	-2.981057
44	1	0	-0.681787	1.873251	-2.703425
45	1	0	0.149652	-4.417666	1.653517
46	1	0	0.283235	-2.970547	2.679248
47	1	0	-1.096282	-3.162339	1.591842
48	1	0	1.135311	-1.844465	-3.356250
49	1	0	2.454235	-3.039574	-3.430155
50	1	0	0.763980	-3.583478	-3.352664

51	1	0	-4.608265	-0.714721	-1.471774
52	1	0	-4.760505	-2.296732	-0.670054

TS11'c

HF=-1603.839607 NImag= 1 (-235.680)
Zero-point correction= 0.411429 (Hartree/Particle)
Thermal correction to Energy= 0.439490
Thermal correction to Enthalpy= 0.440434
Thermal correction to Gibbs Free Energy= 0.350969
Sum of electronic and zero-point Energies= -1603.428178
Sum of electronic and thermal Energies= -1603.400116
Sum of electronic and thermal Enthalpies= -1603.399172
Sum of electronic and thermal Free Energies= -1603.488637

B3LYP (PCM)/6-31G* HF=-1603.855702	M06-2X/6-31G* HF=-1603.277013	B3LYP/6-311+G** HF=-1604.211837	M06-2X/6-311+G** HF=-1603.658150
	M06-2X(PCM)/6-31G* HF=-1604.230164	B3LYP(PCM)/6-311+G** HF=-1604.248587	M06-2X(PCM)/6-311+G** HF=-1603.677201

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.221189	2.512577	-0.604971
2	6	0	0.619754	1.920306	0.515670
3	6	0	0.827833	2.478313	1.785107
4	6	0	1.620652	3.617471	1.930626
5	6	0	2.210286	4.206432	0.811217
6	6	0	2.011790	3.651393	-0.455156
7	15	0	-0.497056	0.466304	0.446432
8	6	0	-2.087779	1.090734	-0.222931
9	6	0	-2.226579	1.646110	-1.503414
10	6	0	-3.462339	2.133946	-1.928860
11	6	0	-4.567745	2.078815	-1.076667
12	6	0	-4.434459	1.535152	0.202112
13	6	0	-3.199928	1.043344	0.627812
14	6	0	0.167227	-0.587794	-0.917981
15	6	0	1.552939	-0.752731	-1.127275
16	6	0	2.497165	-1.056032	-0.026661
17	8	0	2.251161	-1.836487	0.893960
18	6	0	-0.729898	-2.513172	-0.716289
19	7	0	-0.369168	-2.900745	0.596645
20	6	0	-1.434451	-2.888417	1.411779
21	6	0	-2.581949	-2.608965	0.633494
22	6	0	-2.156927	-2.378611	-0.663175
23	6	0	-0.034842	-3.206480	-1.863239
24	6	0	-1.312037	-3.023597	2.889907
25	7	0	1.910751	-0.760145	-2.483132
26	8	0	3.102740	-0.940070	-2.771176
27	8	0	-0.671968	-0.139826	1.813408
28	8	0	3.668244	-0.422673	-0.131150
29	6	0	4.654045	-0.756039	0.859482
30	1	0	-3.590875	-2.548124	1.019065
31	1	0	-2.777730	-2.169359	-1.525457
32	1	0	0.602271	-2.800203	0.910784
33	1	0	-0.329687	-0.374636	-1.865196
34	1	0	-3.082062	0.613715	1.617893
35	1	0	-5.291754	1.494432	0.868966
36	1	0	-5.529040	2.461943	-1.408699
37	1	0	-3.560705	2.560317	-2.923519
38	1	0	-1.373969	1.711033	-2.174524

39	1	0	1.101412	2.076886	-1.592026
40	1	0	2.481235	4.098633	-1.327000
41	1	0	2.829685	5.092343	0.924424
42	1	0	1.780433	4.041318	2.918544
43	1	0	0.373602	2.003297	2.649273
44	1	0	-0.292057	-2.735232	-2.816121
45	1	0	1.051891	-3.159732	-1.754495
46	1	0	-0.330650	-4.261713	-1.903690
47	1	0	-1.076017	-2.036782	3.305718
48	1	0	-2.249501	-3.376715	3.328831
49	1	0	-0.510424	-3.715917	3.167444
50	1	0	5.535289	-0.171491	0.595254
51	1	0	4.299234	-0.491048	1.858926
52	1	0	4.879086	-1.825372	0.830681

TS12c

HF=-1603.8436123 NImag = 1 (-283.760)

Zero-point correction= 0.411233 (Hartree/Particle)

Thermal correction to Energy= 0.439426

Thermal correction to Enthalpy= 0.440371

Thermal correction to Gibbs Free Energy= 0.350799

Sum of electronic and zero-point Energies= -1603.432379

Sum of electronic and thermal Energies= -1603.404186

Sum of electronic and thermal Enthalpies= -1603.403242

Sum of electronic and thermal Free Energies= -1603.492813

B3LYP (PCM)/6-31G* HF=-1603.862063	M06-2X/6-31G* HF=-1603.285059	B3LYP/6-311+G** HF=-1604.213887	M06-2X/6-311+G** HF=-1603.664755
	M06-2X(PCM)/6-31G* HF=-1603.304138	B3LYP(PCM)/6-311+G** HF=-1604.235137	M06-2X(PCM)/6-311+G** HF=-1603.686338

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.022379	1.374268	-0.878195
2	6	0	-2.041464	0.934244	0.021785
3	6	0	-2.354033	0.828531	1.384636
4	6	0	-3.631964	1.156582	1.838227
5	6	0	-4.604134	1.597585	0.938073
6	6	0	-4.298036	1.705548	-0.419751
7	15	0	-0.381087	0.609143	-0.682244
8	6	0	0.634073	2.043510	-0.143081
9	6	0	1.060300	2.931424	-1.139778
10	6	0	1.804428	4.063834	-0.804570
11	6	0	2.126565	4.319451	0.529154
12	6	0	1.699549	3.442252	1.529348
13	6	0	0.954786	2.311275	1.195817
14	6	0	0.360210	-0.799275	0.272330
15	6	0	-0.374114	-1.889267	0.801725
16	6	0	-1.688251	-2.374178	0.309784
17	8	0	-2.466018	-3.073402	0.922771
18	7	0	0.082700	-2.600869	1.896140
19	8	0	1.259519	-2.357617	2.275066
20	8	0	-0.398464	0.502859	-2.183637
21	8	0	-1.918524	-1.937960	-0.956984
22	6	0	-3.198599	-2.277410	-1.507053
23	1	0	-3.199727	-1.860218	-2.514157
24	6	0	1.885893	-1.559467	-1.027781
25	6	0	2.508309	-0.400774	-1.592946
26	6	0	3.646991	-0.100484	-0.858807
27	6	0	3.780766	-1.085851	0.139937
28	7	0	2.791578	-1.988379	-0.022757

29	6	0	1.140539	-2.591961	-1.830519
30	6	0	4.779347	-1.199584	1.244829
31	1	0	2.476308	-2.574393	0.752158
32	1	0	4.315959	0.738166	-0.997850
33	1	0	2.108053	0.128247	-2.445690
34	1	0	1.122849	-0.463117	0.975947
35	1	0	0.802799	2.720381	-2.173437
36	1	0	2.131307	4.746266	-1.584783
37	1	0	2.705312	5.201315	0.791043
38	1	0	1.944493	3.639949	2.569494
39	1	0	0.624005	1.644051	1.987677
40	1	0	-1.616506	0.470107	2.096682
41	1	0	-3.868900	1.059992	2.894084
42	1	0	-5.598799	1.851694	1.294520
43	1	0	-5.053396	2.044130	-1.124021
44	1	0	-2.775865	1.441466	-1.933507
45	1	0	0.400804	-2.096251	-2.461782
46	1	0	1.837522	-3.155921	-2.462107
47	1	0	0.621877	-3.300523	-1.177067
48	1	0	5.352418	-0.274408	1.342827
49	1	0	4.282449	-1.406856	2.199537
50	1	0	5.485716	-2.018323	1.057074
51	1	0	-3.326369	-3.362743	-1.535021
52	1	0	-4.000719	-1.837967	-0.908347

TS12'c

HF=-1603.8266041 NImag = 1 (-256.180)

Zero-point correction= 0.412013 (Hartree/Particle)

Thermal correction to Energy= 0.439855

Thermal correction to Enthalpy= 0.440799

Thermal correction to Gibbs Free Energy= 0.352439

Sum of electronic and zero-point Energies= -1603.414591

Sum of electronic and thermal Energies= -1603.386749

Sum of electronic and thermal Enthalpies= -1603.385805

Sum of electronic and thermal Free Energies= -1603.474165

B3LYP (PCM)/6-31G* HF=-1603.845694	M06-2X/6-31G* HF=-1603.261199	B3LYP/6-311+G** HF=-1604.199039	M06-2X/6-311+G** HF=-1603.643091
	M06-2X(PCM)/6-31G* HF=-1603.281785	B3LYP(PCM)/6-311+G** HF=-1604.221144	M06-2X(PCM)/6-311+G** HF=-1603.666532

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.266312	0.467864	-1.934193
2	6	0	-1.874501	-0.868681	-1.616627
3	6	0	-2.765791	-1.222159	-0.529679
4	6	0	-3.562158	-0.144359	-0.218386
5	6	0	-3.204732	0.917724	-1.090941
6	6	0	-1.743573	-1.801373	-2.816283
7	6	0	-3.694091	2.327080	-1.097374
8	6	0	-0.002857	-0.905362	-0.989026
9	6	0	0.290315	-2.075580	-0.237068
10	7	0	0.766783	-3.131660	-0.989838
11	8	0	1.051034	-4.177936	-0.366573
12	15	0	0.533035	0.859805	-0.741393
13	8	0	0.179372	1.632489	-2.002961
14	6	0	-0.148755	1.734265	0.720784
15	6	0	-0.564304	3.054707	0.476163
16	6	0	-1.034175	3.853197	1.519707
17	6	0	-1.095926	3.341735	2.817356
18	6	0	-0.676450	2.034091	3.066703

19	6	0	-0.197659	1.231710	2.029328
20	6	0	2.341301	0.753568	-0.531796
21	6	0	2.961129	0.013087	0.486552
22	6	0	4.352266	0.006931	0.582262
23	6	0	5.126581	0.731243	-0.327654
24	6	0	4.510166	1.465287	-1.342000
25	6	0	3.118971	1.477435	-1.447366
26	6	0	0.039768	-2.305959	1.214526
27	8	0	0.646281	-1.795747	2.143878
28	8	0	-0.948368	-3.201309	1.410408
29	6	0	-1.134364	-3.640224	2.766869
30	1	0	-1.935266	-4.378965	2.726622
31	1	0	0.412644	-1.082029	-1.987514
32	1	0	2.623590	2.038048	-2.233765
33	1	0	5.110559	2.025621	-2.053702
34	1	0	6.210503	0.719097	-0.247588
35	1	0	4.832051	-0.571678	1.366787
36	1	0	2.371386	-0.566567	1.190719
37	1	0	-0.505677	3.444845	-0.535113
38	1	0	-1.343510	4.875878	1.319420
39	1	0	-1.460488	3.962533	3.631651
40	1	0	-0.713123	1.633516	4.076252
41	1	0	0.139448	0.225959	2.249967
42	1	0	-2.729669	-2.040839	-3.229295
43	1	0	-1.145702	-1.332539	-3.604866
44	1	0	-1.243658	-2.727679	-2.517950
45	1	0	-2.765445	-2.195442	-0.056800
46	1	0	-4.312848	-0.079249	0.558427
47	1	0	-1.618310	1.083309	-2.438890
48	1	0	-3.256350	2.891939	-0.265352
49	1	0	-3.432590	2.836746	-2.029089
50	1	0	-4.782637	2.352413	-0.979818
51	1	0	-0.213831	-4.093110	3.142787
52	1	0	-1.413419	-2.802471	3.411902

References and Notes

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