Electronic Supplementary Information (ESI)

Mechanistic Insight into Cobalt-Mediated [2+2+2]-Cycloaddition Reactions with γ-Alkylidenebutenolide and γ- Alkylidenebuterolactam as 2 π Partners.

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Structures of intermediates III_{exo1}, III_{exo2} and III^{O}

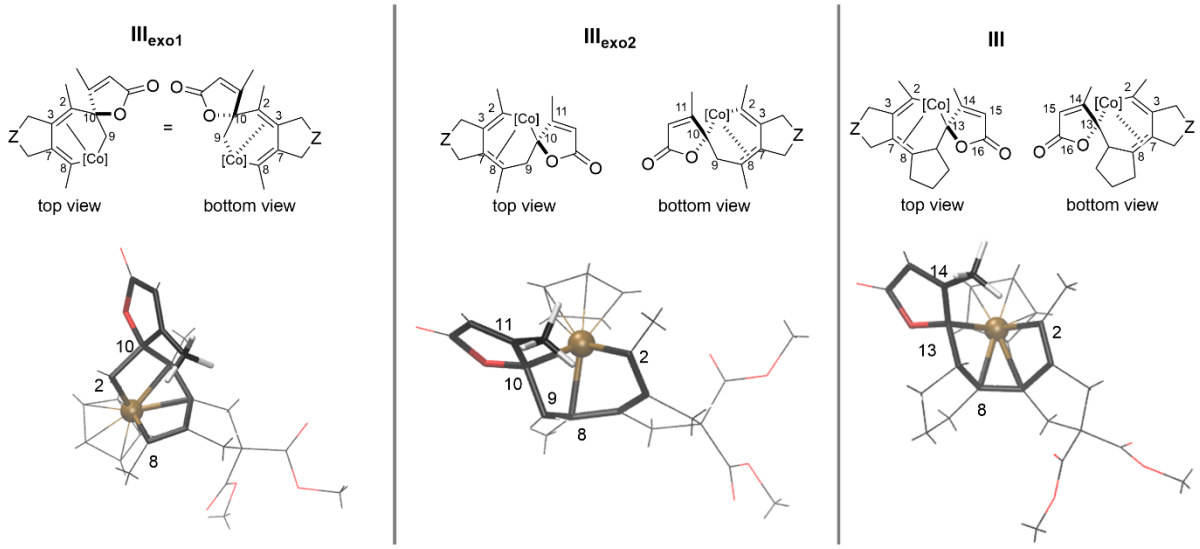


Figure S1: Optimized structures (bottom view) of **III_{exo1}**, **III_{exo2}** and **III^{O}**.

The optimized structures of **III_{exo1}**, **III_{exo2}** and **III^{O}** are shown in Figure S1. In **III_{exo1}**, the Co is bound to C9, which is external to the lactone, while C10 is already implicated in the bond with C2, thus in the spiro moiety. In both **III_{exo2}** and **III^{O}**, the carbon atom of the lactone ring (C10 in the intermolecular case and C13 in the intramolecular case) is connected to the Co. The next step could therefore be either the formation of the bond between C10 (or C13) and C2, leading to the spiro product, or the formation of the bond between C11 (or C14) and C2, leading to an intermediate of type **IV**.

Dimethyl-substituted γ-alkylidenebutenolide

Calculations were performed with the experimental γ-alkylidenebutenolide substrate, employed for the intermolecular reaction, which displays two methyl groups (instead of only one, as in Figure 3 in the article). The level of calculation is TPSS-D3/def2-TZVP. Solvent effects were added as computed by single point calculations on the optimized structures (COSMO model, toluene). Results are displayed in Figure S2, in terms of ΔG relative to $\mathbf{II_{exo}^{Me}}$ (T=383.15K).

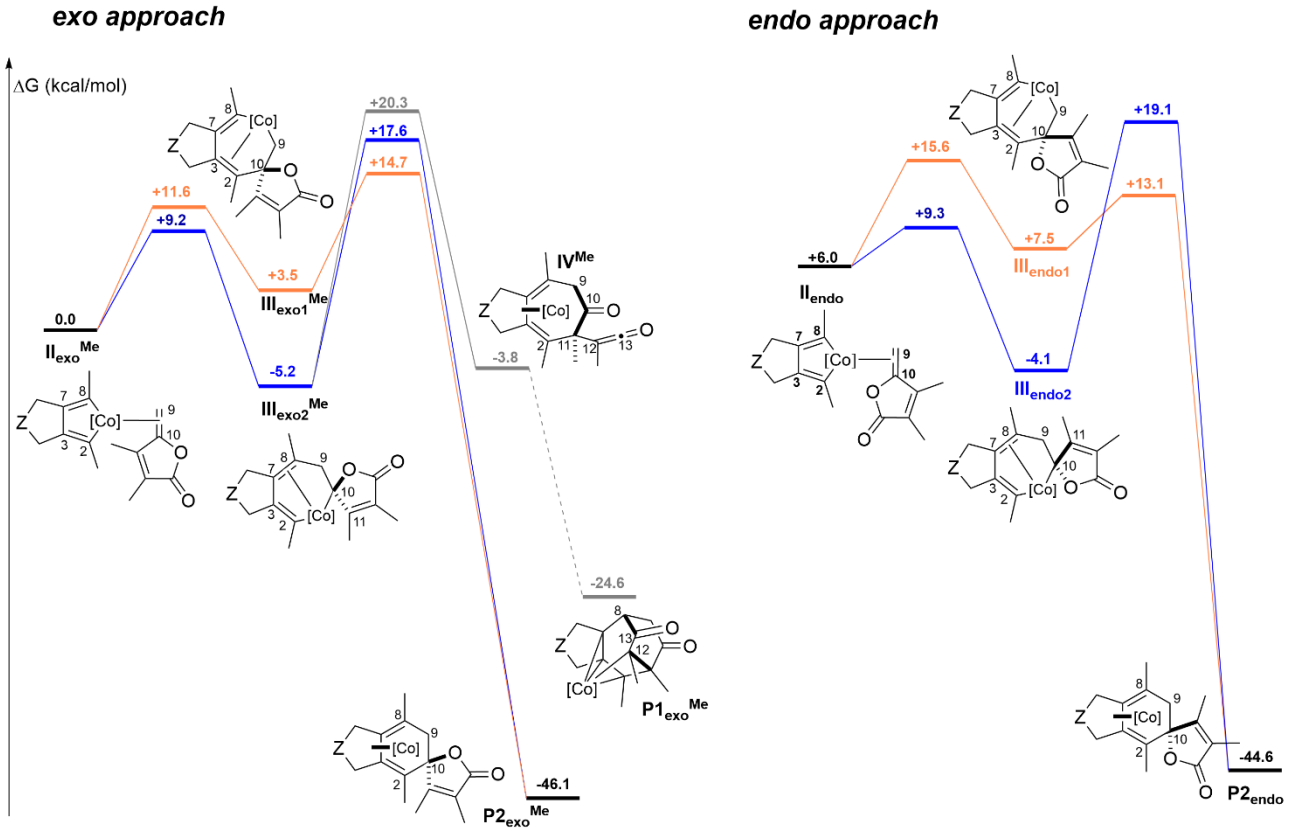


Figure S2. Computed *exo*- and *endo*- pathways. Z=C(CO_2Me)$_2$, [Co]=CpCo. ΔG are computed at the TPSS-D3/def2-TZVP level (T=383.15K). Solvent effects are added as single point calculations with the COSMO implicit model (toluene).

By comparing mono- to di-substituted cases, ΔG values of corresponding stationary points differ by about 1 kcal/mol (exemple: $\mathbf{III_{exo1}}$ at 2.5 kcal/mol vs $\mathbf{II_{exo1}^{Me}}$ at 3.5 kcal/mol). The only exceptions concern the transition states leading to **IV** *vs*. $\mathbf{IV^{Me}}$, and **IV** *vs*. $\mathbf{IV_{Me}}$: the hypothetical reaction leading to the diketone product is even more disfavored in the di-substituted than in the mono-substituted case. Therefore, we have not computed the complete path to the $\mathbf{P1_{exo}^{Me}}$ product.

The computed profiles with the disubstituted substrate are, indeed, sensibly the same as those obtained with the monosubstituted substrate. Significantly, trends are exactly the same: both for the *exo* and *endo* approaches, two insertion steps are possible. Although barriers for the insertion steps are less accessible from the lactone side (orange paths), the pathways through them are overall favored, with barriers for the reductive elimination lower than those computed for the blue paths. In conclusion, the di-substitution does not impact the overall mechanism of the transformation.

Lactam case: *E* isomer

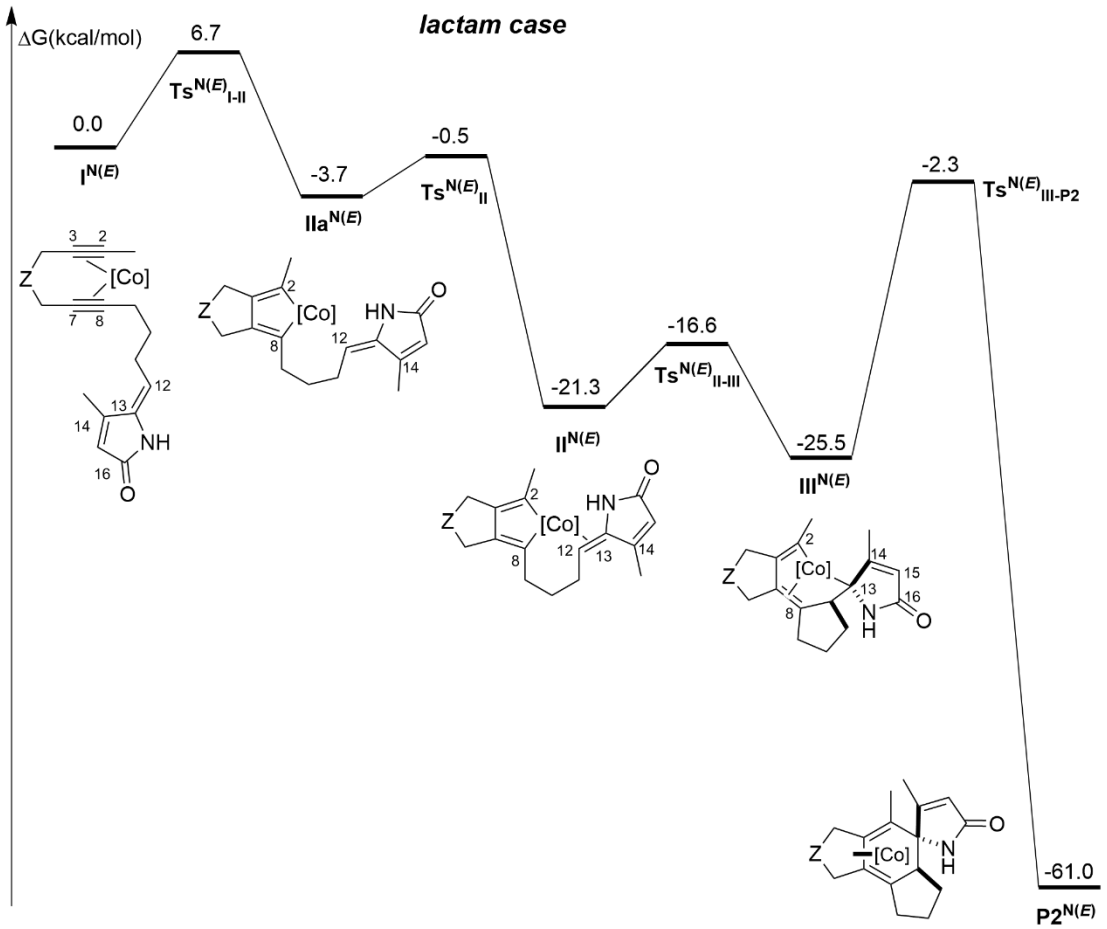


Figure S3. Computed pathway, for an *E*-lactam substrate, Z=C(CO_2Me)$_2$, [Co]=CpCo. ΔG are computed at the TPSS-D3/def2-TZVP level (T=383.15K). Solvent effects are added as single point calculations with the COSMO implicit model (toluene).

As the lactam substrate **8** exists in the Z and E form, calculations were also performed on an E isomer. Results for the pathway leading to the spirolactam product are reported in Figure S3. Barriers are comparable to those computed for the corresponding Z isomer (see Figure 5 in the article). The structure of intermediate **III**$^{N(E)}$ is depicted in Figure S4: the C(13) atom is closer to C(2) than C(14), which is clearly not correctly positioned to react and form the C(2)-C(14) bond, necessary to continue the reactivity towards a hypothetical Co(III) complex. Thus, the path to the Co(III) complex was not computed.

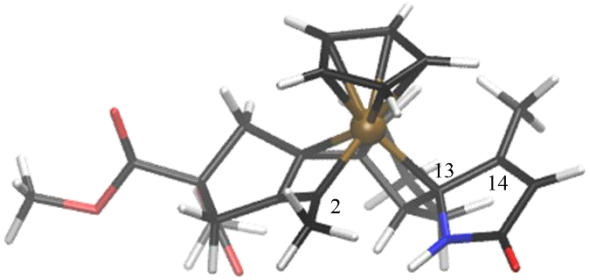


Figure S4. Computed structure of intermediate **III**$^{N(E)}$.

Lactam case: comparison between computational methods

The mechanistic profiles to the Co(III) and to the spirolactam complexes were computed at several level of theory: TPSS-D3/def2-TZVP; BP86-D3/def2-TZVP; and PBE0/def2-TZVP. In each case, structures were fully optimized and the nature of the stationary points were verified by frequency calculations. Solvent effects were added as computed by single point calculations on the optimized structures (COSMO model, toluene). Results are shown in Figure S5 and ΔG relative to $\mathbf{II^N}$ are reported in Table S1 (T=383.15K).

Table S1. ΔG (kcal/mol) are computed relative free-energies (Δ $E_{Toluene}$ + Δ(Chem. Pot.), T=383.15K) at different level of theory for the mechanistic profiles computed for the lactam case, see Figure S1.

System	**ΔG** TPSS-D3	**ΔG** BP86-D3	**ΔG** PBE0-D3
$\mathbf{I^N}$	0.0	0.0	0.0
$\mathbf{Ts^N_{I-II}}$	7.6	7.5	8.7
$\mathbf{IIa^N}$	-5.1	-5.6	-7.1
$\mathbf{Ts^N_{II}}$	-0.5	0.8	0.8
$\mathbf{II^N}$	-18.5	-21.6	-18.0
$\mathbf{Ts^N_{II-III}}$	-13.7	-16.4	-15.1
$\mathbf{III^N}$	-21.5	-24.1	-28.3
$\mathbf{Ts^N_{III-IV}}$	-1.7	-6.6	-4.0
$\mathbf{IV^N}$	-25.9	-30.3	-36.8
$\mathbf{Ts^N_{IV-V}}$	-11.3	-14.8	-19.4
$\mathbf{V^N}$	-14.2	-18.1	-22.4
$\mathbf{Ts^N_{V-P1}}$	0.3	-3.9	-3.9
$\mathbf{P1^N}$	-40.2	-43.8	-51.7
$\mathbf{Ts^N_{III-P2}}$	-2.7	-7.6	-8.4
$\mathbf{P2^N}$	-61.4	-65.4	-77.2

All computations deliver the same qualitative picture, predicting that the pathway to the Co(III) complex is less favored than the one to the spirocyclic lactam complex. However, relative energies are somewhat sensitive to the method used, notably the difference in energy between $\mathbf{III^N}$ and $\mathbf{II^N}$ is of -3.0 kcal/mol at the TPSS-D3 level and decreases to -10.3 kcal/mol at the PBE0-D3 level.

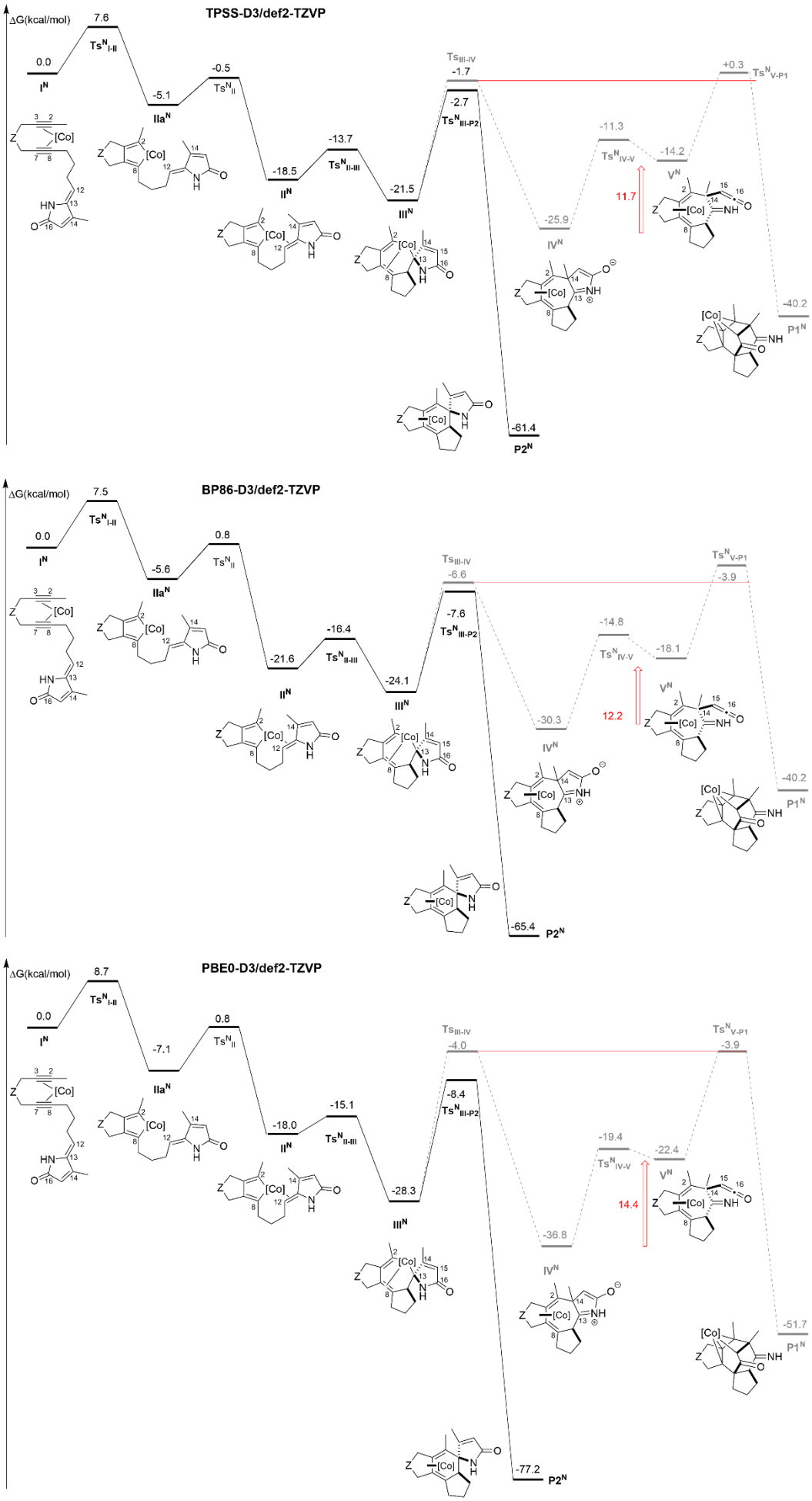


Figure S5. Computed pathways for the lactam case, Z=C(C(O)OMe)$_2$, [Co]=CpCo.

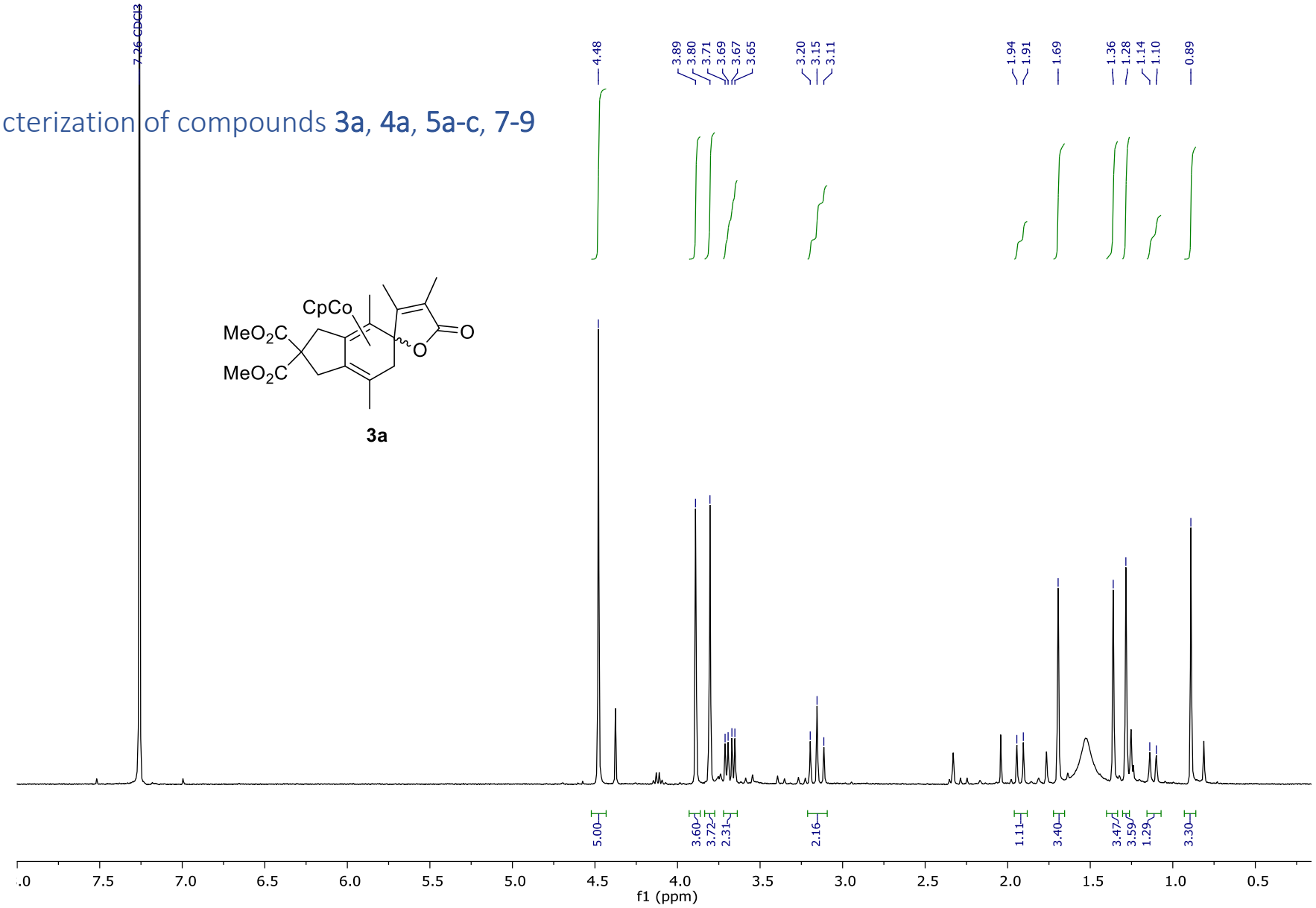


Figure S6. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

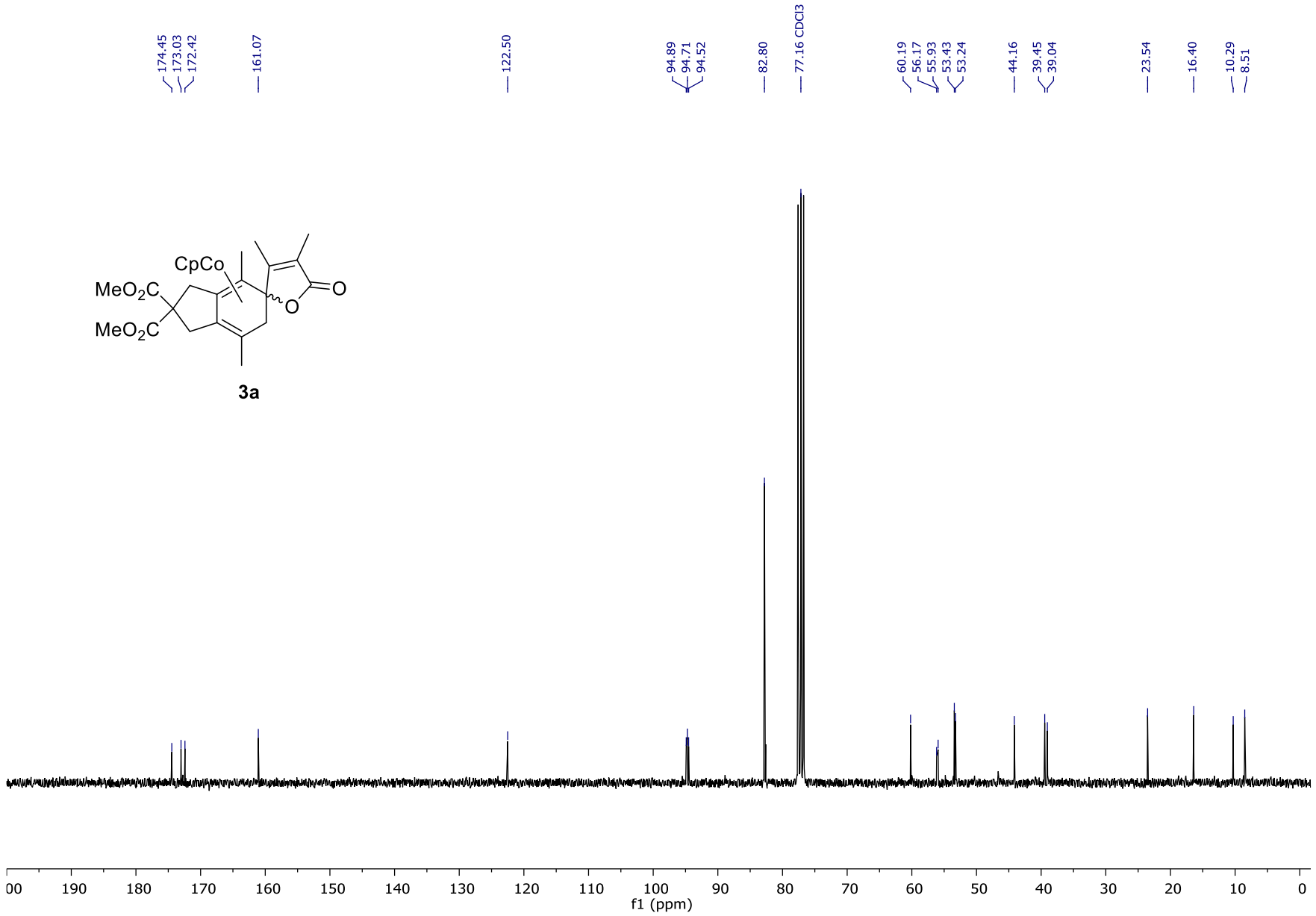


Figure S7. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

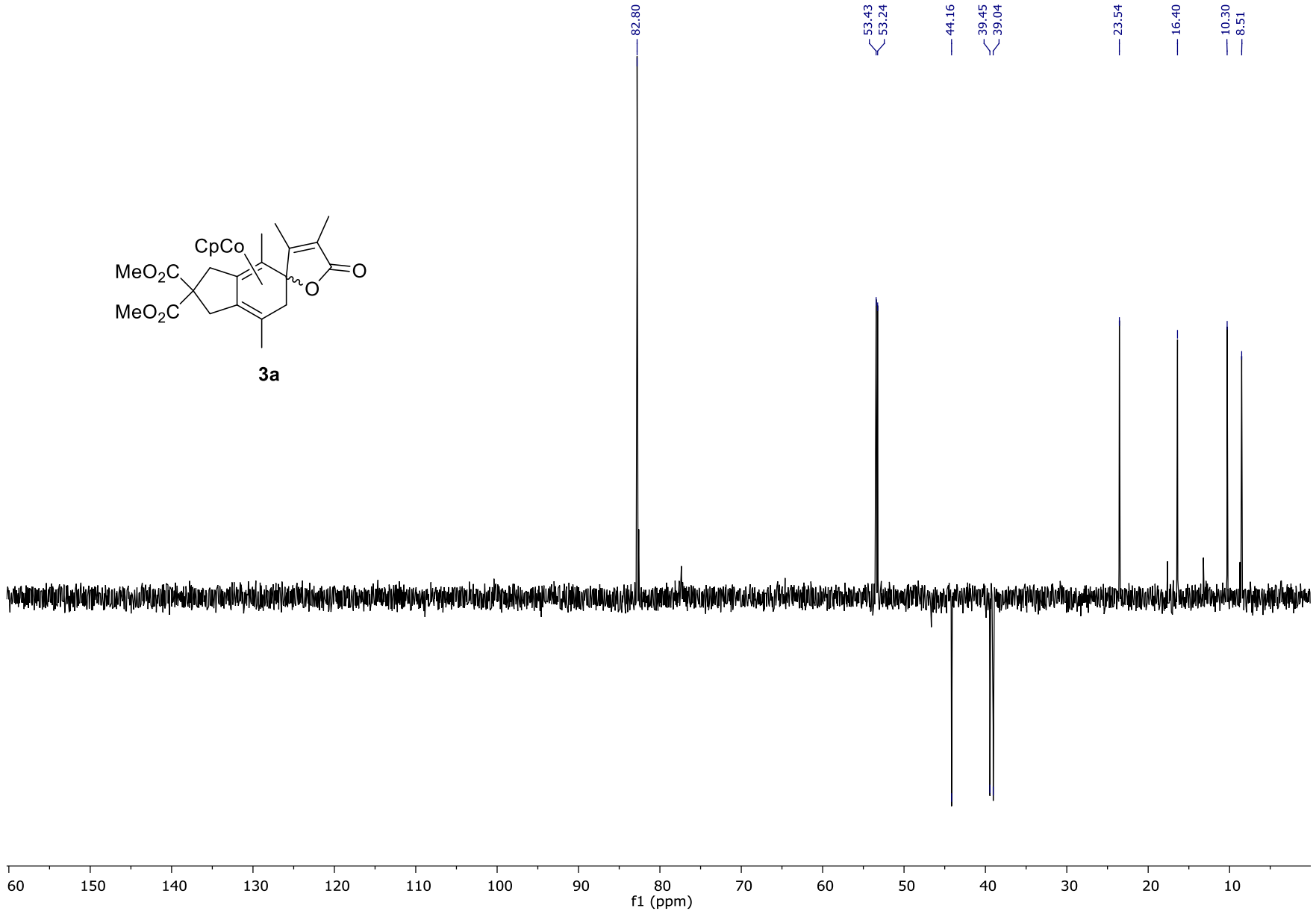


Figure S8. DEPT (75 MHz, $CDCl_3$) spectrum

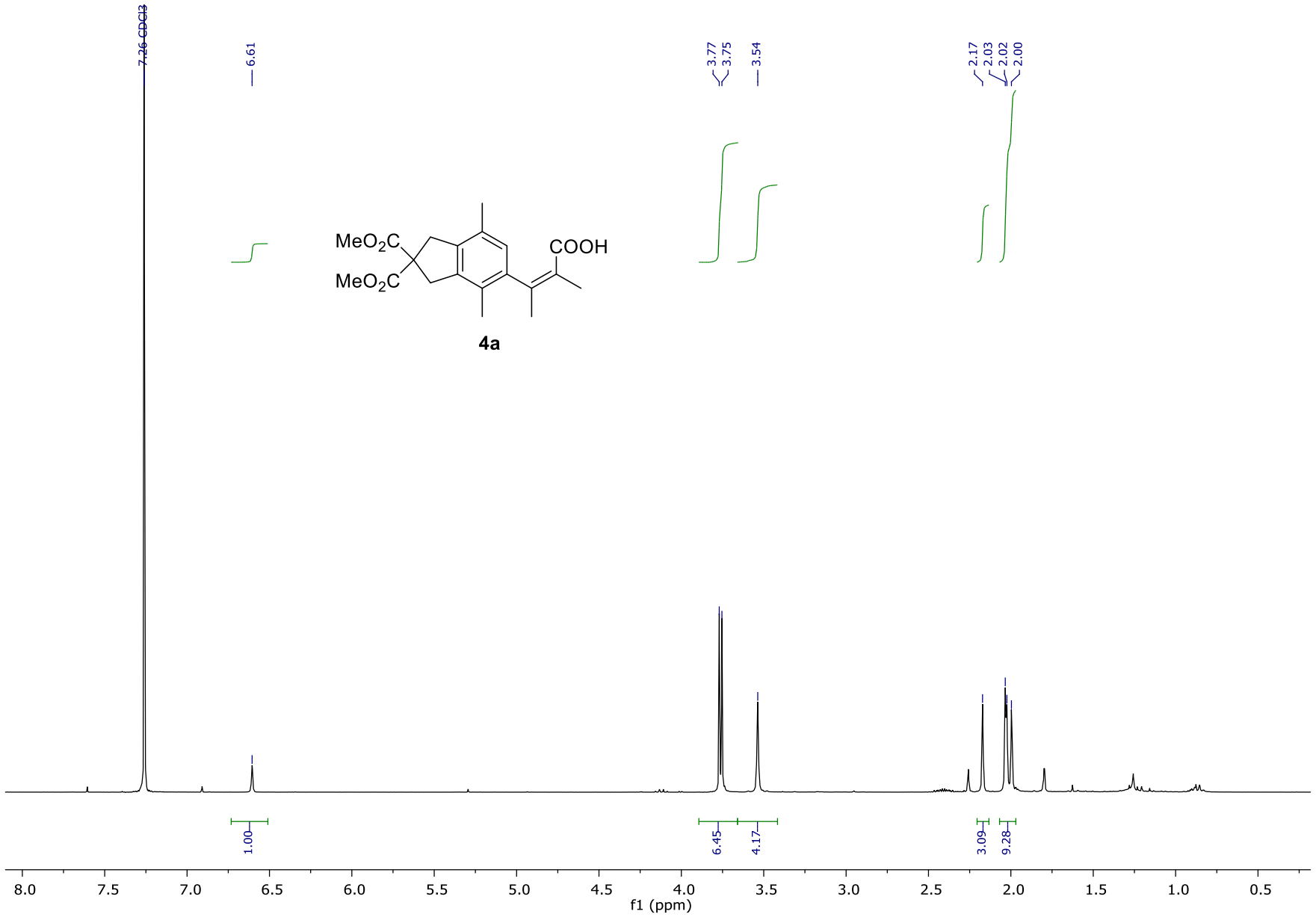


Figure S9. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

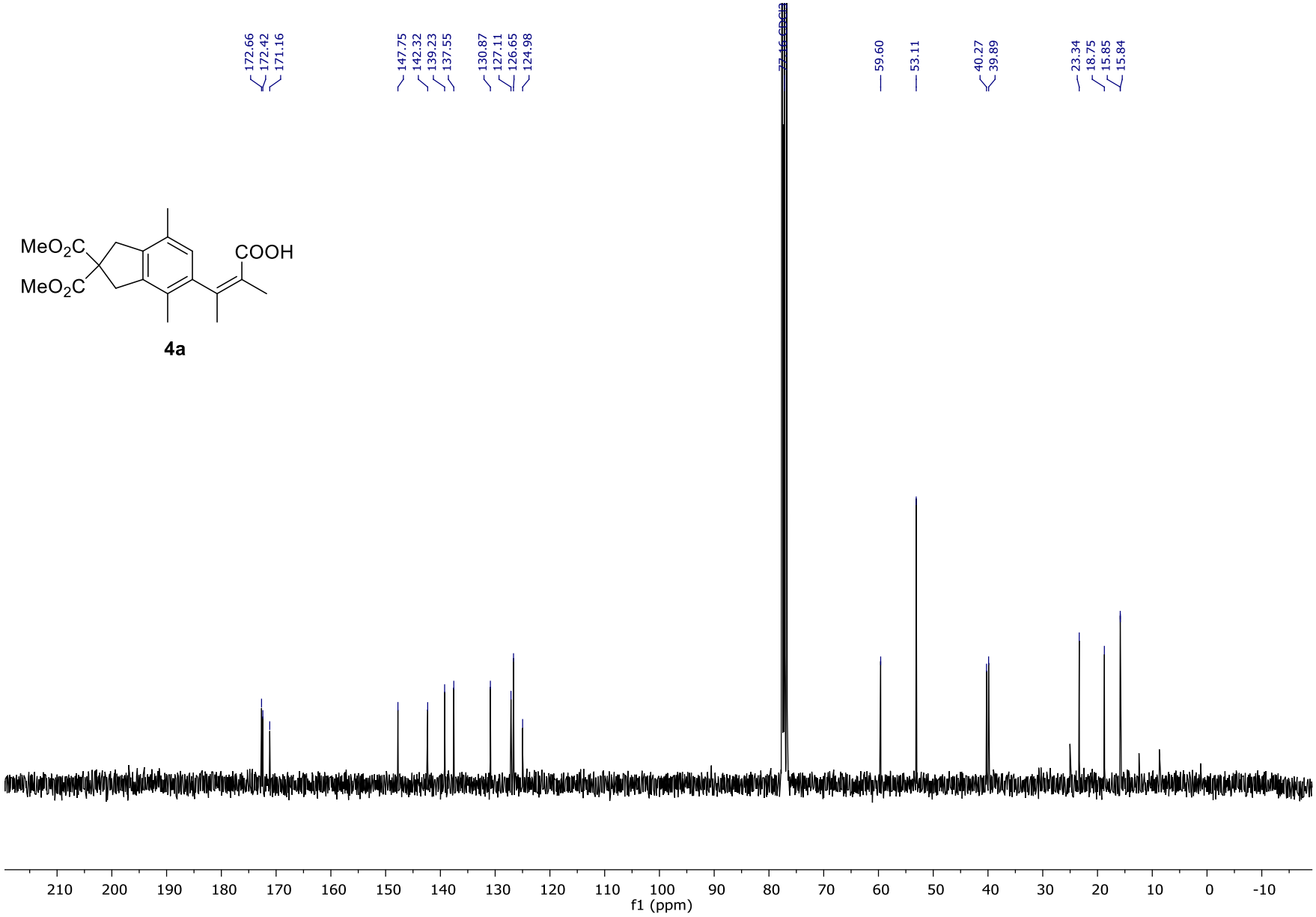


Figure S10. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

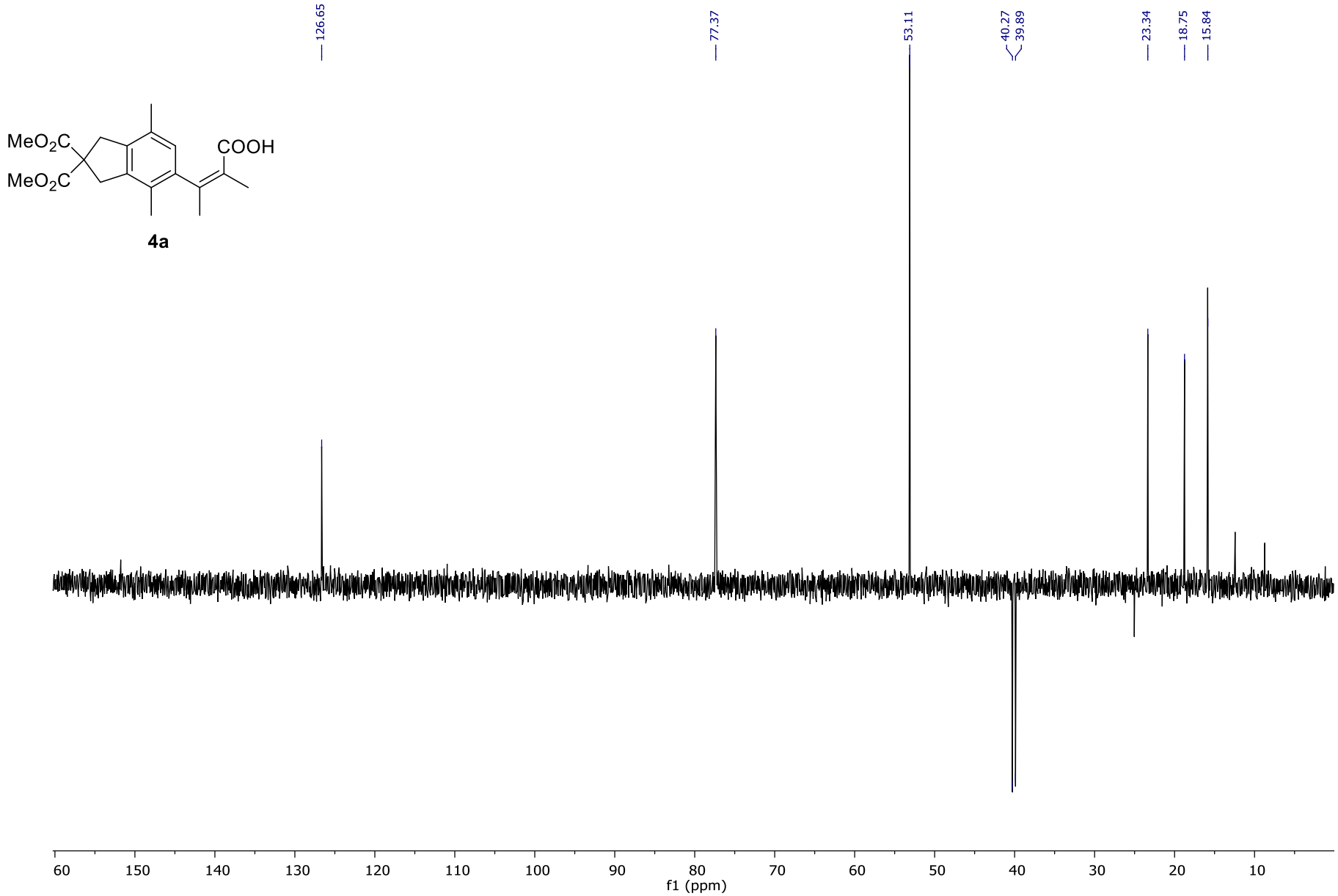


Figure S11. DEPT (75 MHz, $CDCl_3$) spectrum

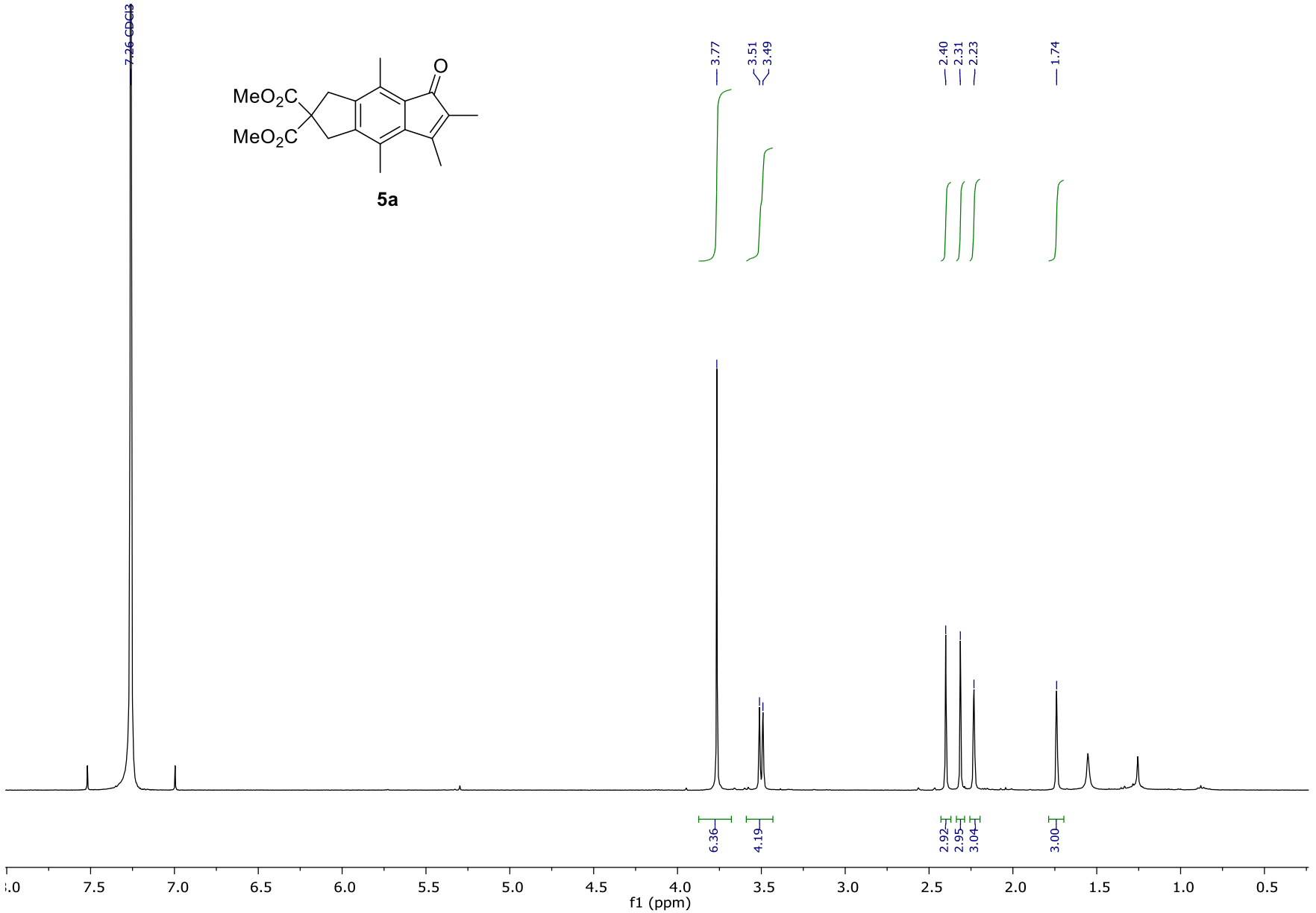


Figure S12. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

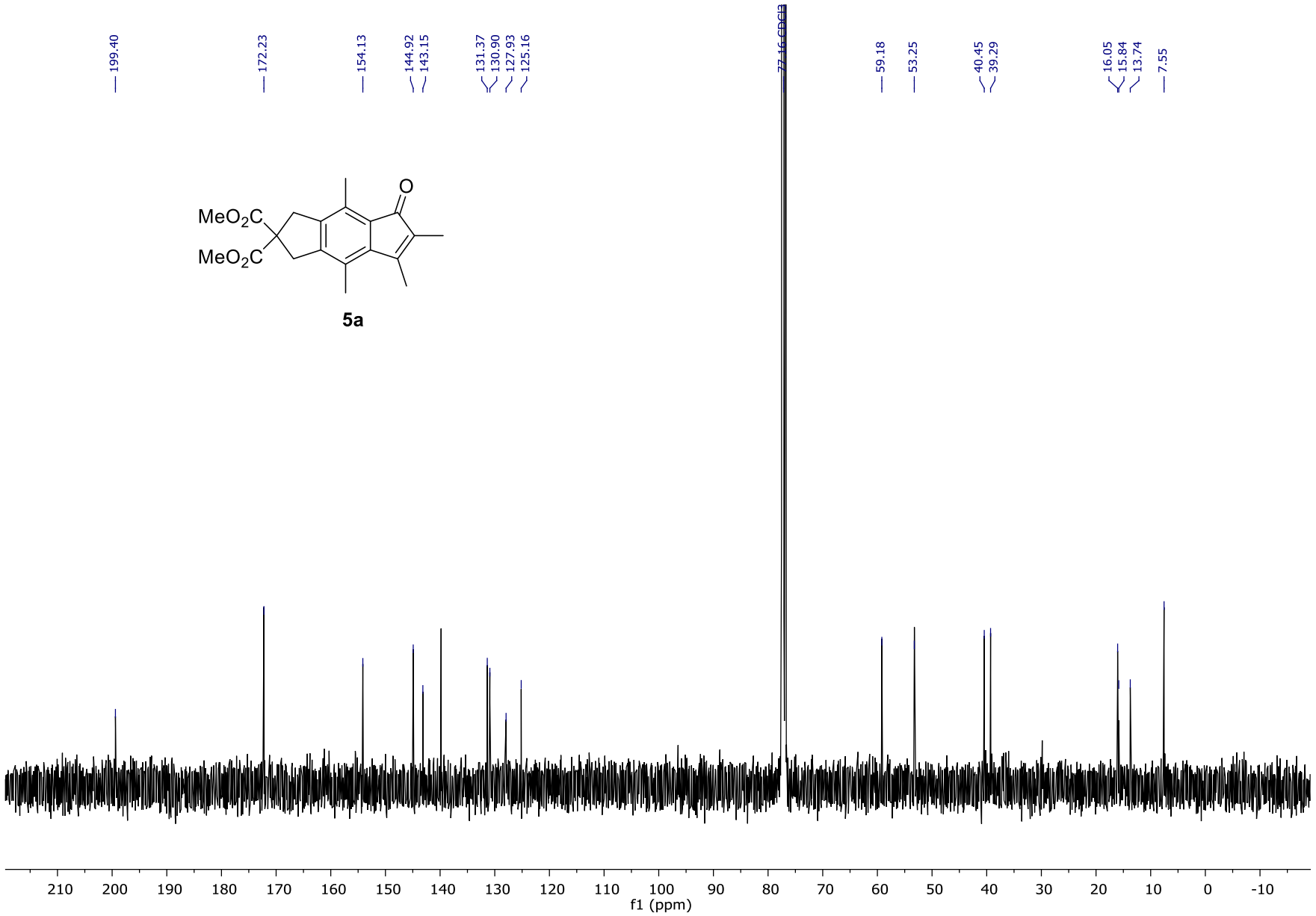


Figure S13. ^{13}C (75 MHz, $CDCl_3$) spectrum

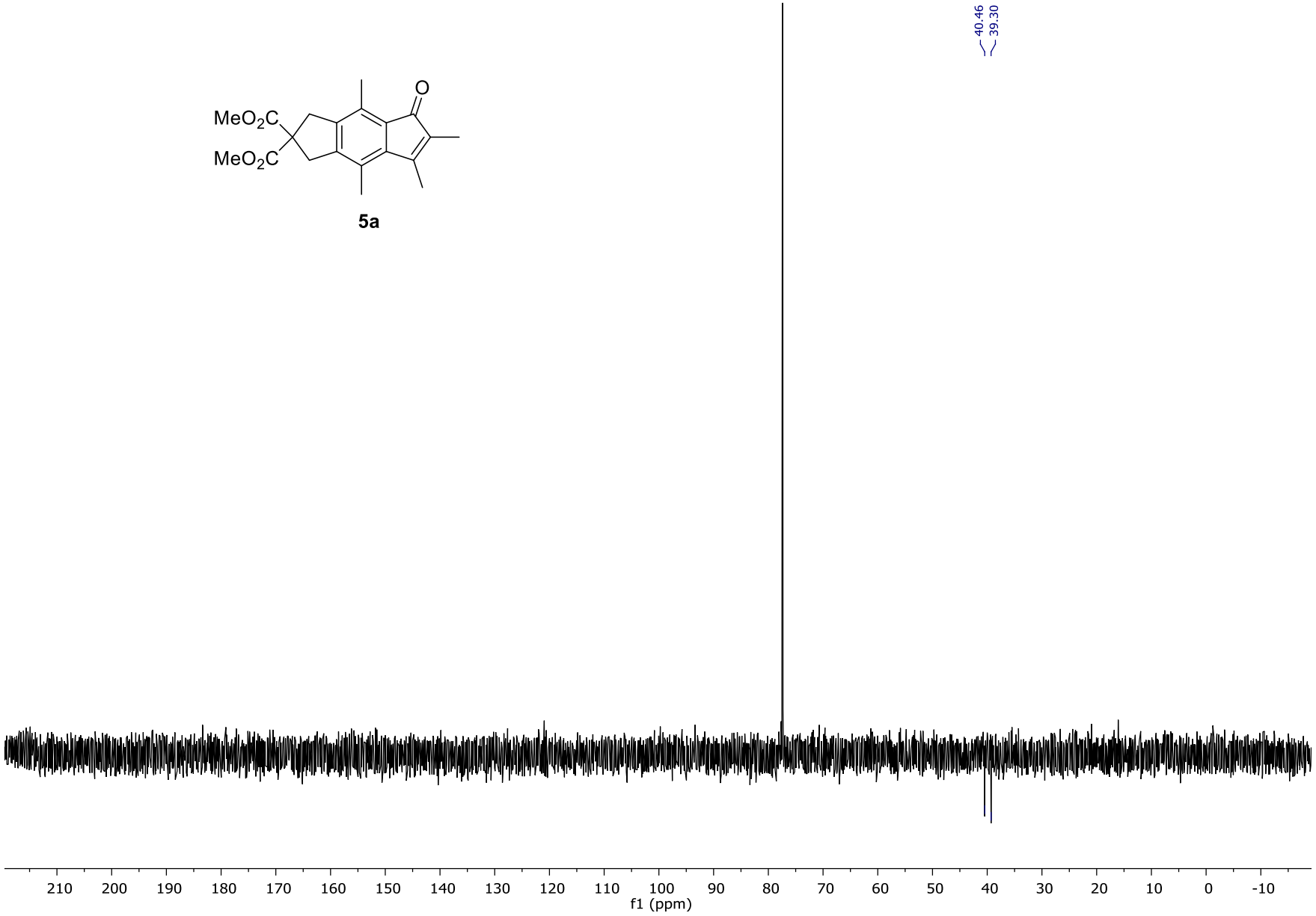


Figure S14. DEPT (75 MHz, $CDCl_3$) spectrum

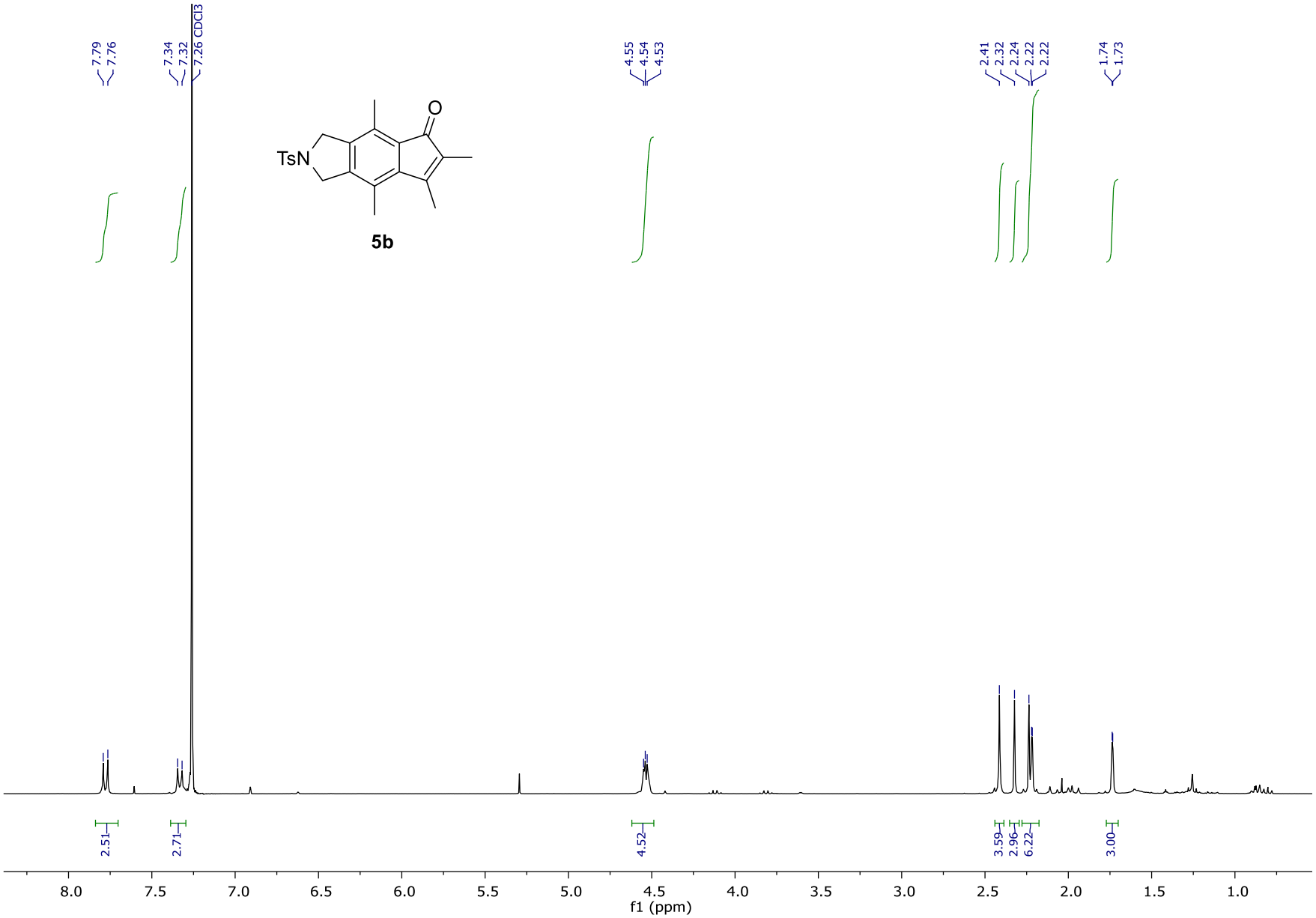


Figure S15. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

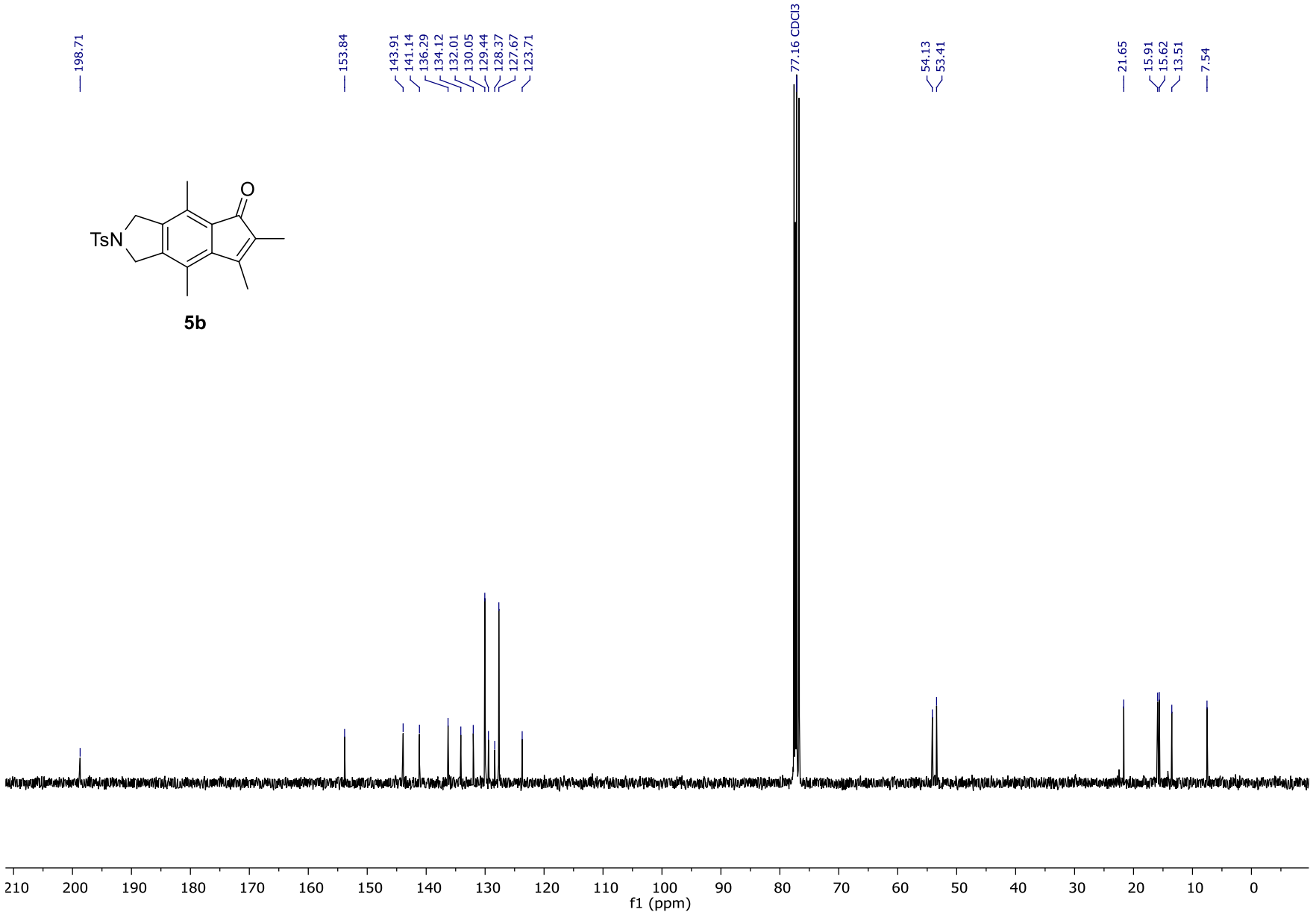


Figure S16. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

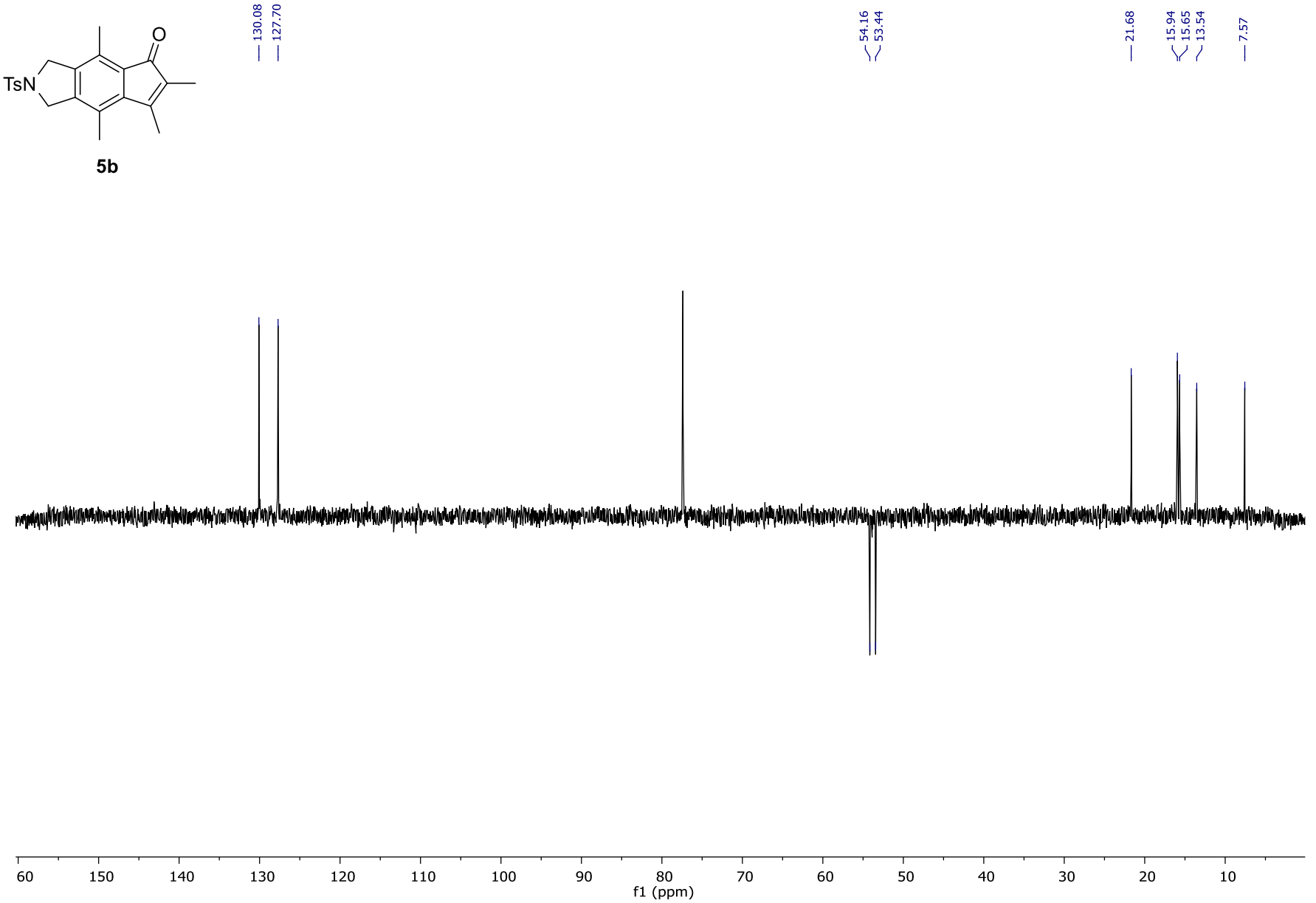


Figure S17. DEPT (75 MHz, $CDCl_3$) spectrum

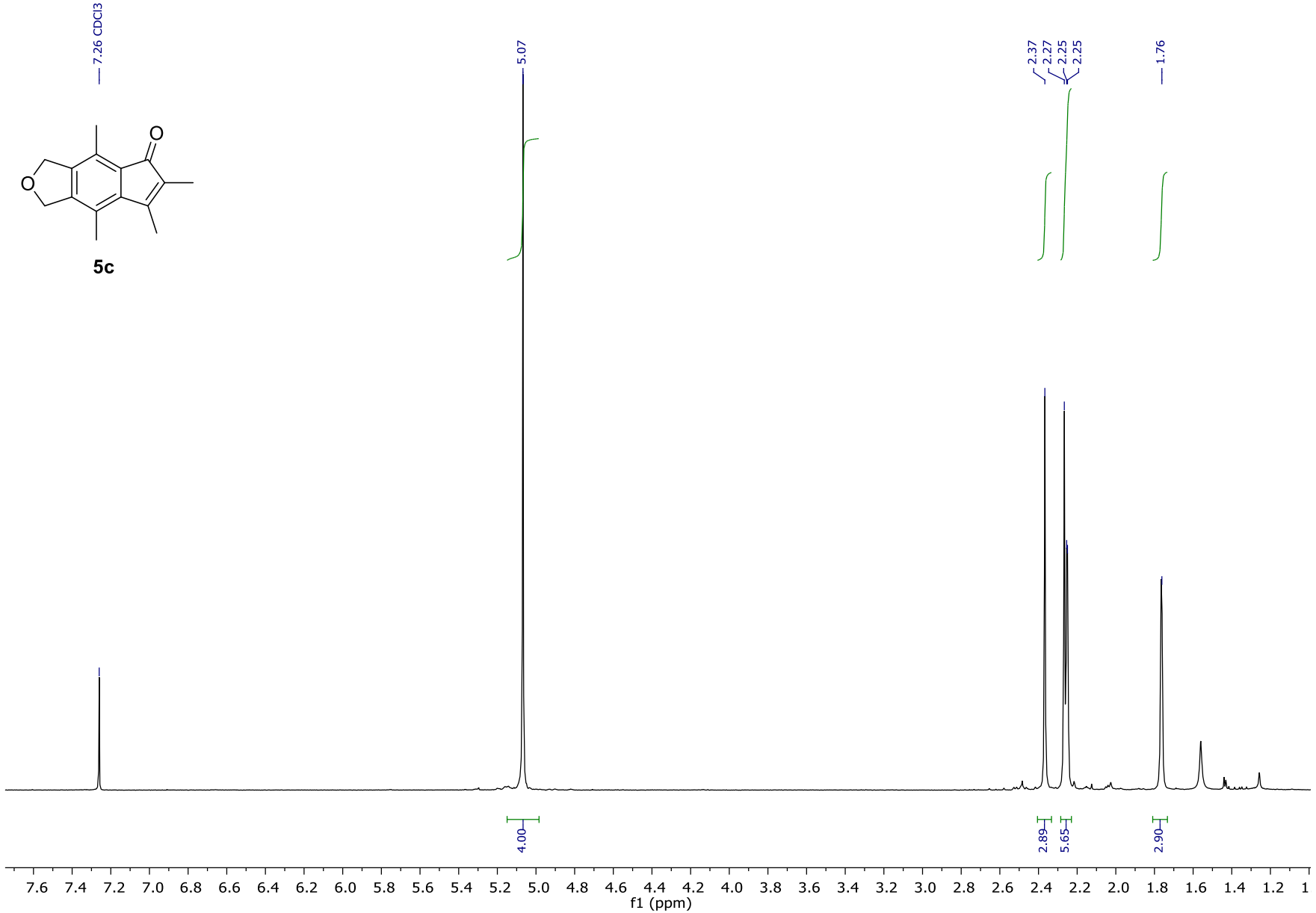


Figure S18. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

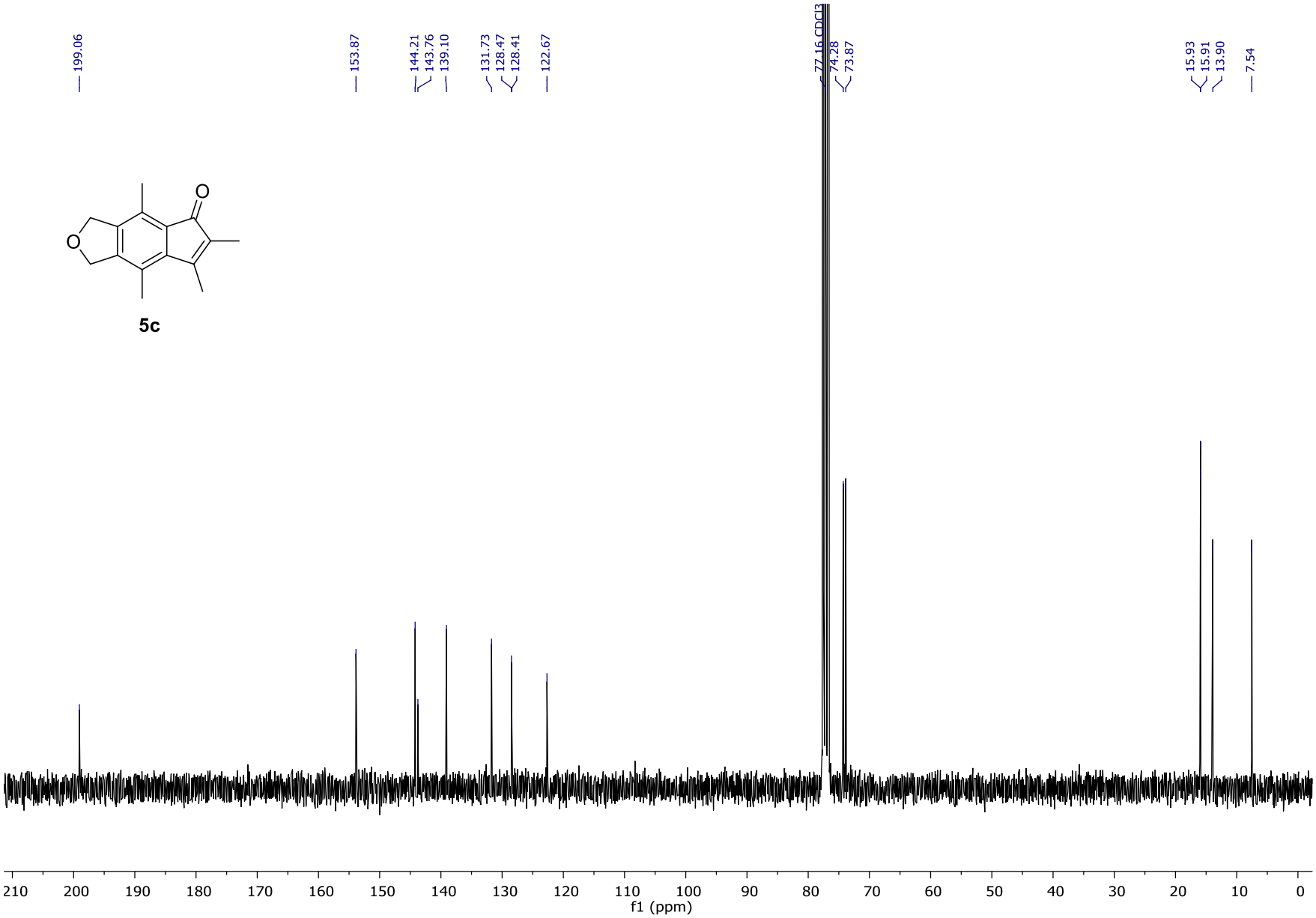


Figure S19. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

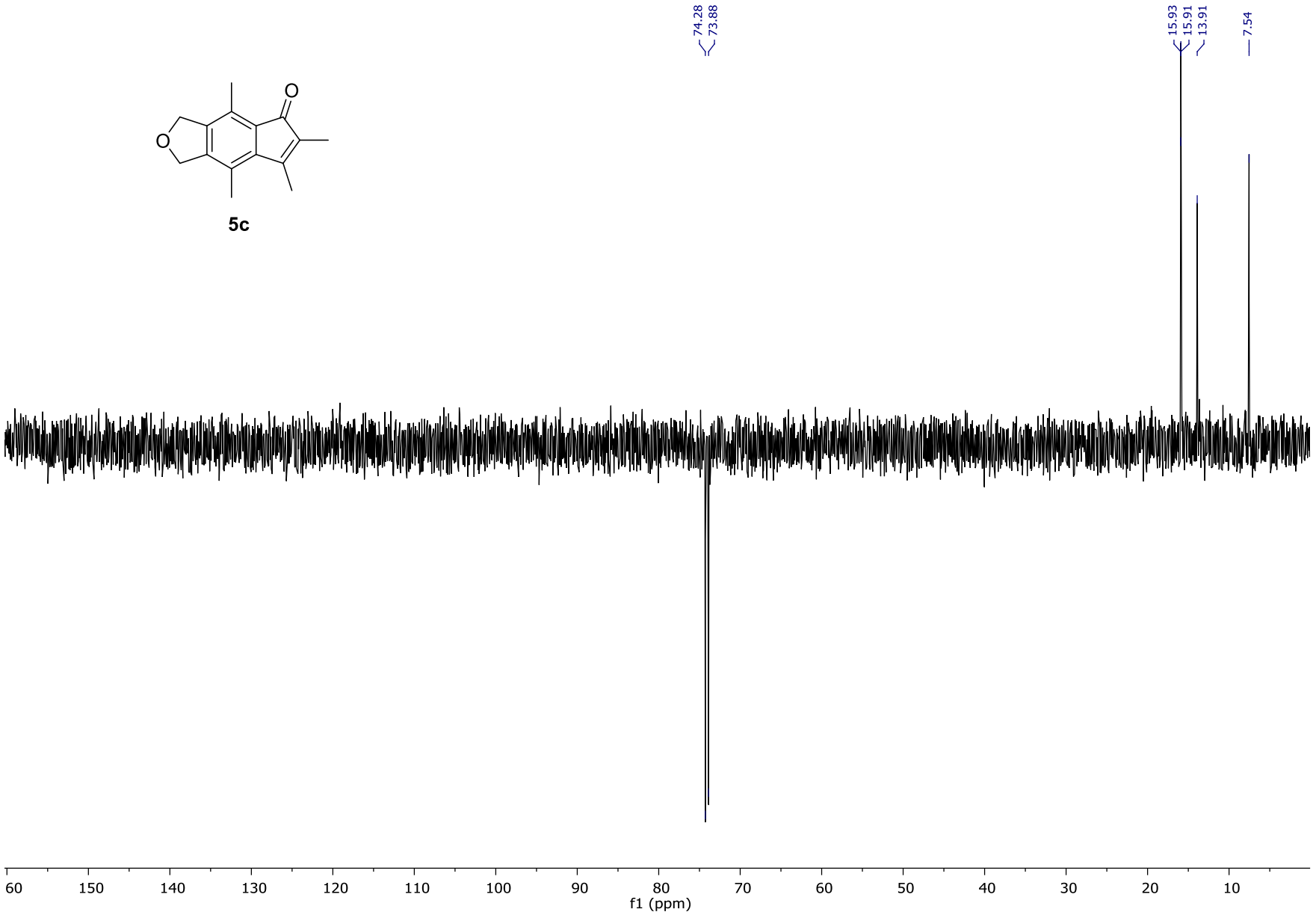


Figure S120. DEPT (75 MHz, $CDCl_3$) spectrum

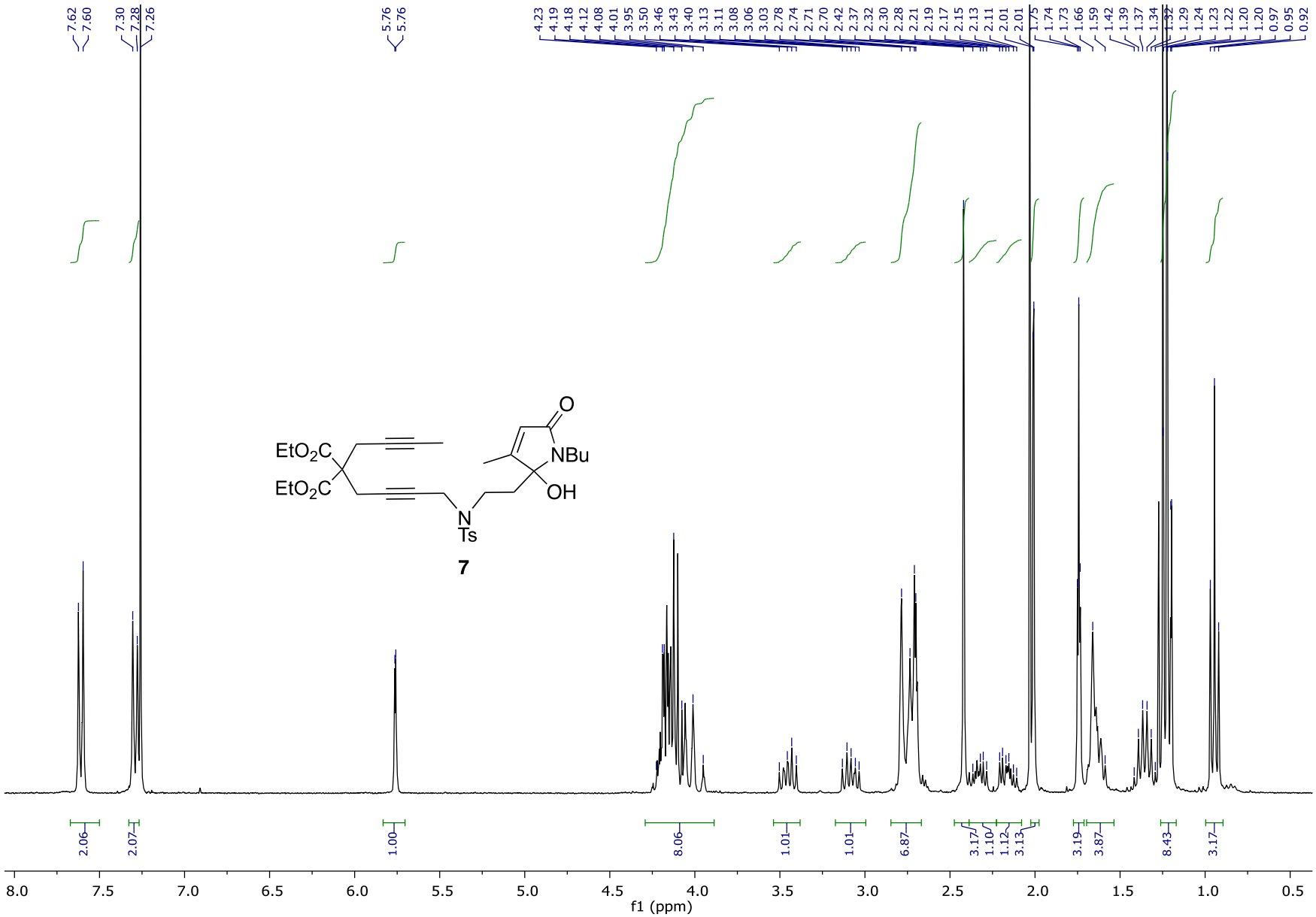


Figure S21. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

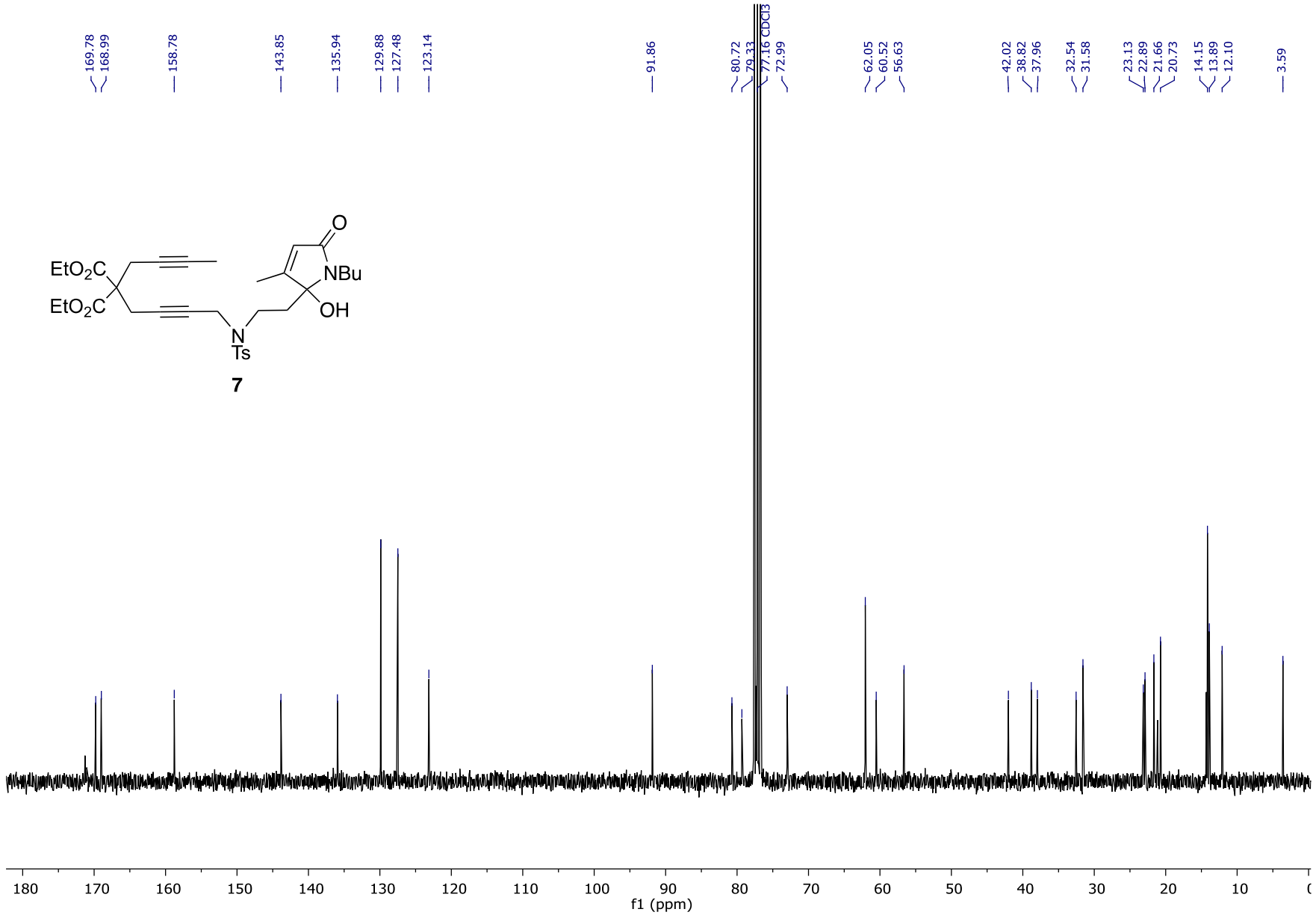


Figure S22. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

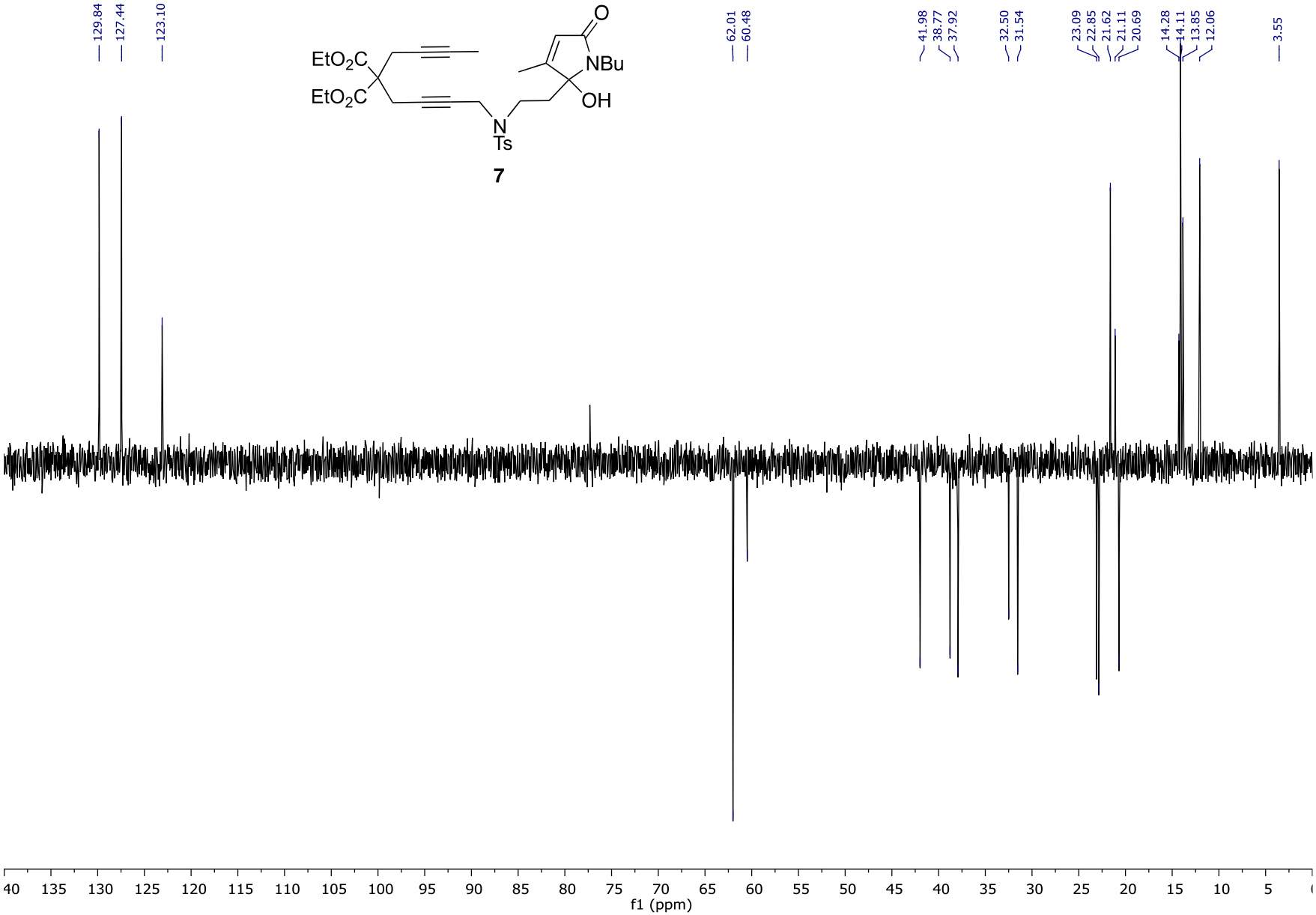
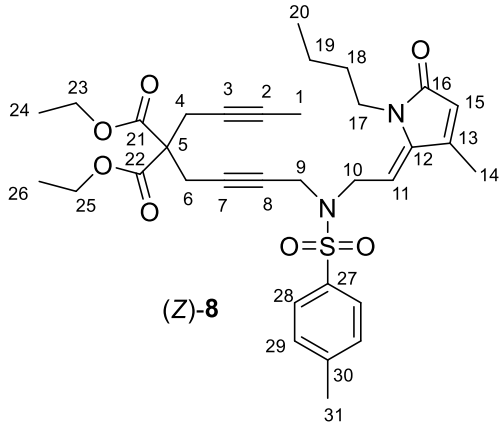


Figure S23. DEPT (75 MHz, $CDCl_3$) spectrum

Assignment of (Z)-8



(*Z*)-**8**

^{1}H NMR (300 MHz, Chloroform-*d*) δ 0.91 (t, *J* = 7.3 Hz, 3H, H20), 1.21 (t, *J* = 7.1 Hz, 6H, H24 and H26), 1.25 – 1.37 (m, 2H, H19), 1.45-1.56 (m, 2H, H18), 1.72 (br t, *J* = 2.4 Hz, 3H, H1), 1.97 (br d, *J* = 1.5 Hz, 3H, H14), 2.43 (s, 3H, H31), 2.67 (br q, *J* = 2.4 Hz, 2H, H4), 2.73 (br t, *J* = 2.1 Hz, 2H, H6), 3.69 (dd, *J* = 7.3 Hz, 2H, H17), 4.08 – 4.26 (m, 8H, H9, H10, 23 and H25), 4.98 (t, *J* = 7.0 Hz, 1H, H11), 5.85 (br q , *J* = 1.5 Hz, 1H, H15), 7.32 (d, *J* = 7.9 Hz, 2H, HAr), 7.70 (d, *J* = 7.9 Hz, 2H, HAr).

^{13}C NMR (75 MHz, $CDCl_3$) δ 3.6 (C1), 12.4 (C14), 13.9 (C20), 14.1 (2C, C24 and C26), 20.0 (C19), 21.7 (C31), 22.8 (C6), 23.0 (C4), 32.0 (C18), 37.3 (C9), 40.7 (C17), 43.4 (C10), 56.6 (C5), 62.0 (2C, C23 or C25), 73.0 (C2 or C3 or C7 or C8), 76.0 (C2 or C3 or C7 or C8), 79. 2 (C2 or C3 or C7 or C8), 81.3 (C2 or C3 or C7 or C8), 104.8 (C11), 120.5 (C15), 127.8 (2C, C28 or C29), 129.8 (2C, C28 or C29), 136.0 (C12 or C27 or C30), 141.9 (C12 or C27 or C30), 144.0 (C12 or C27 or C30), 148.5 (C13), 168.9 (2C, C21 and C22), 170.9 C16).

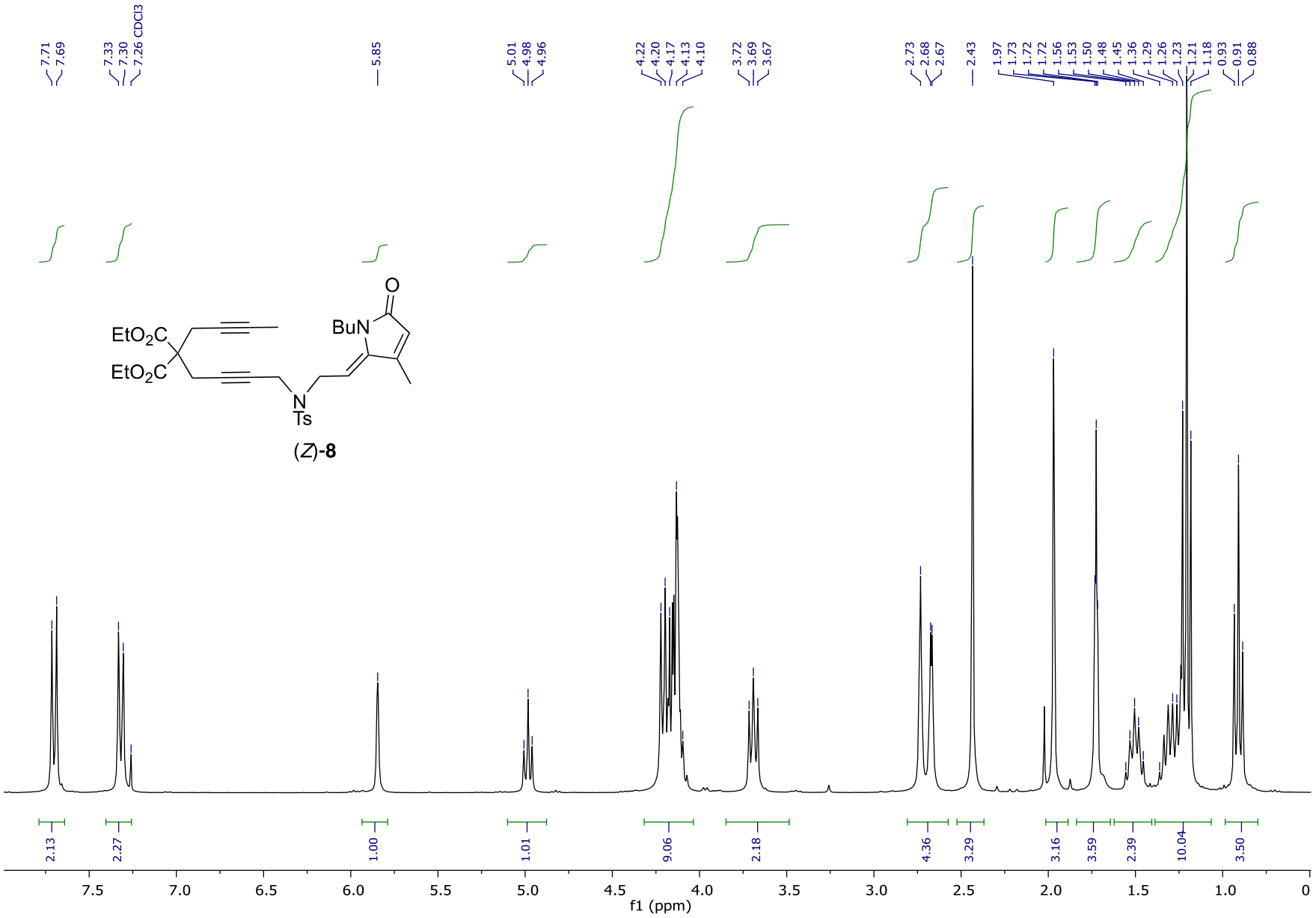


Figure S24. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

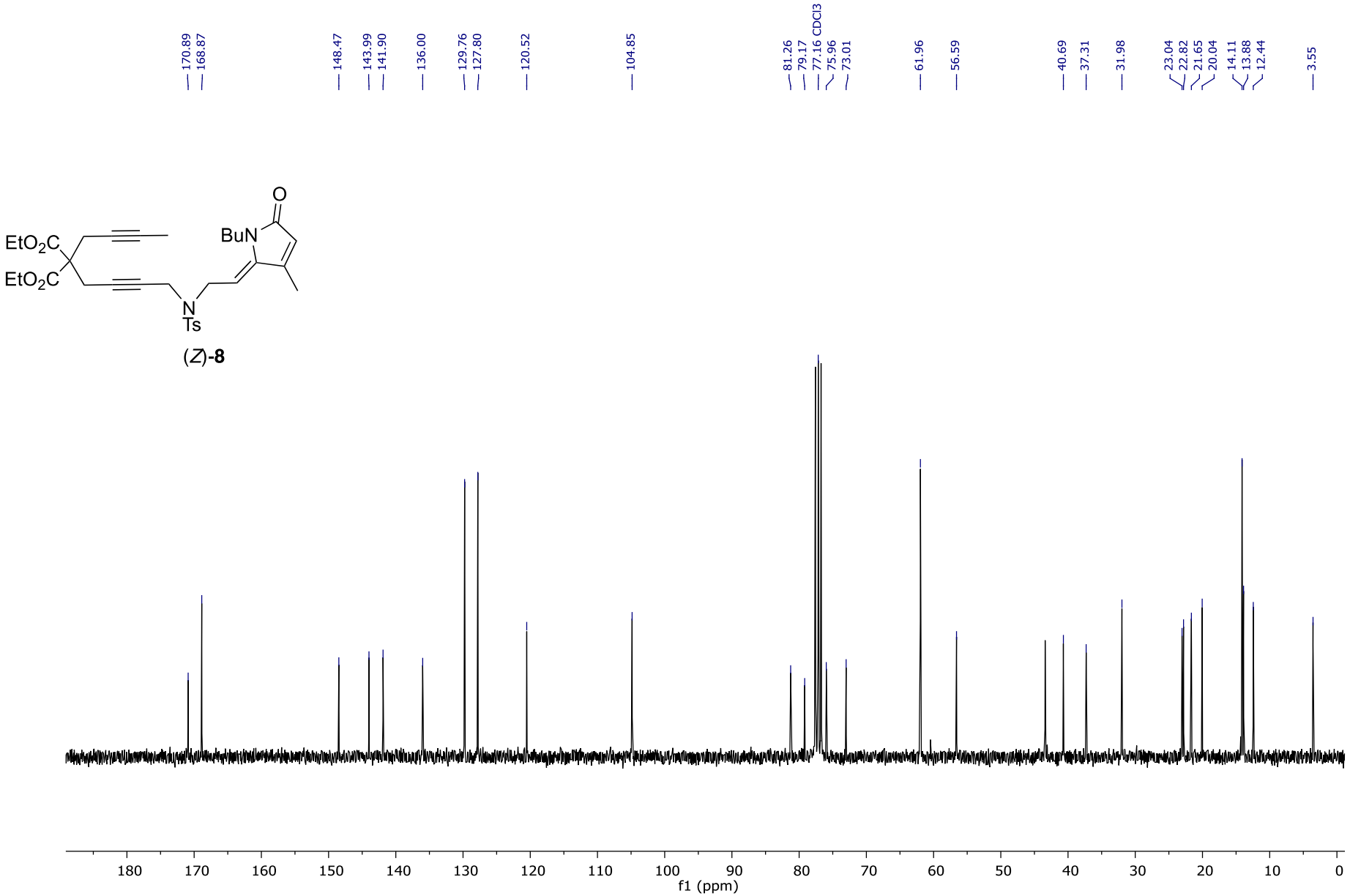


Figure S25. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

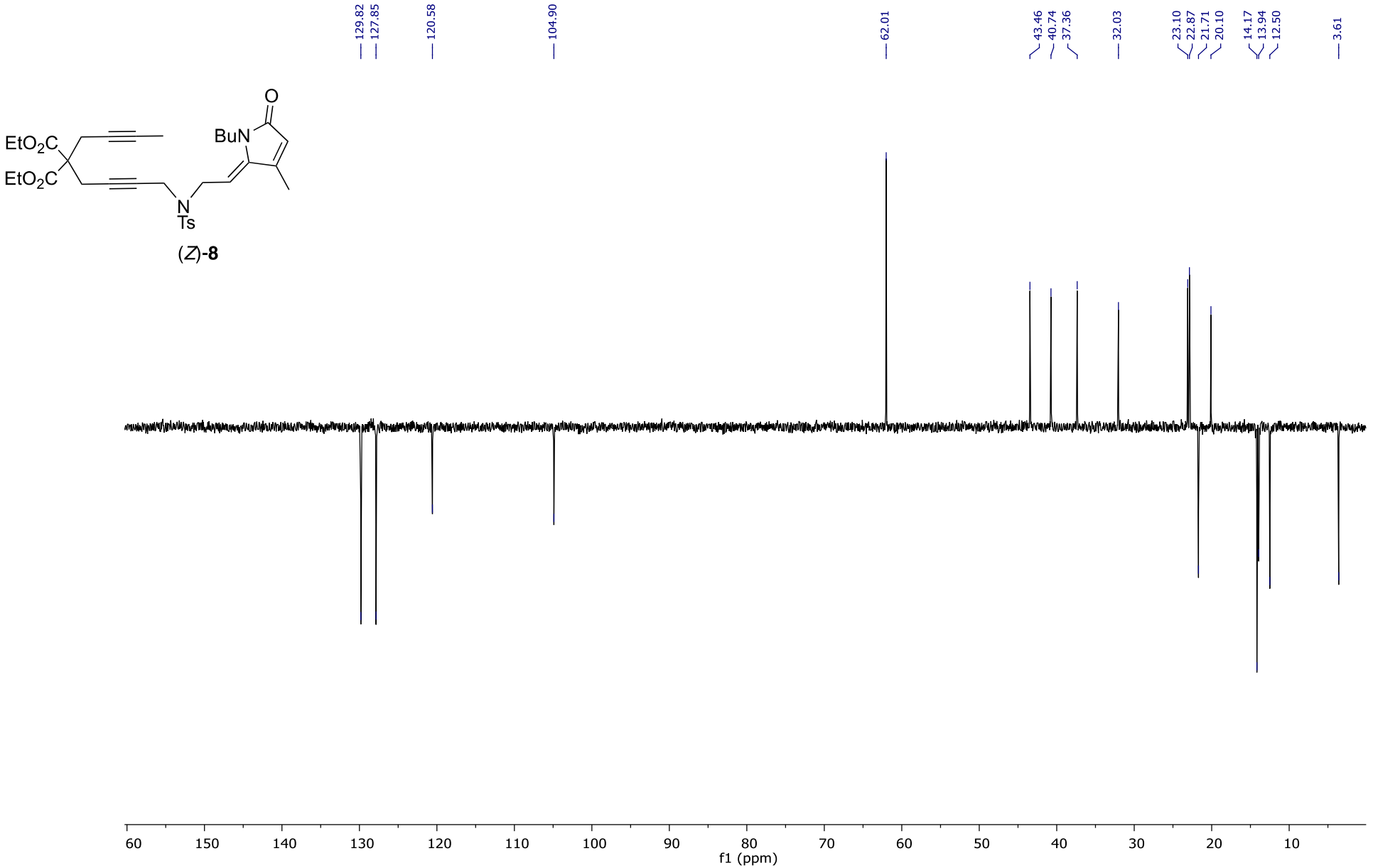


Figure S26. DEPT (75 MHz, $CDCl_3$) spectrum

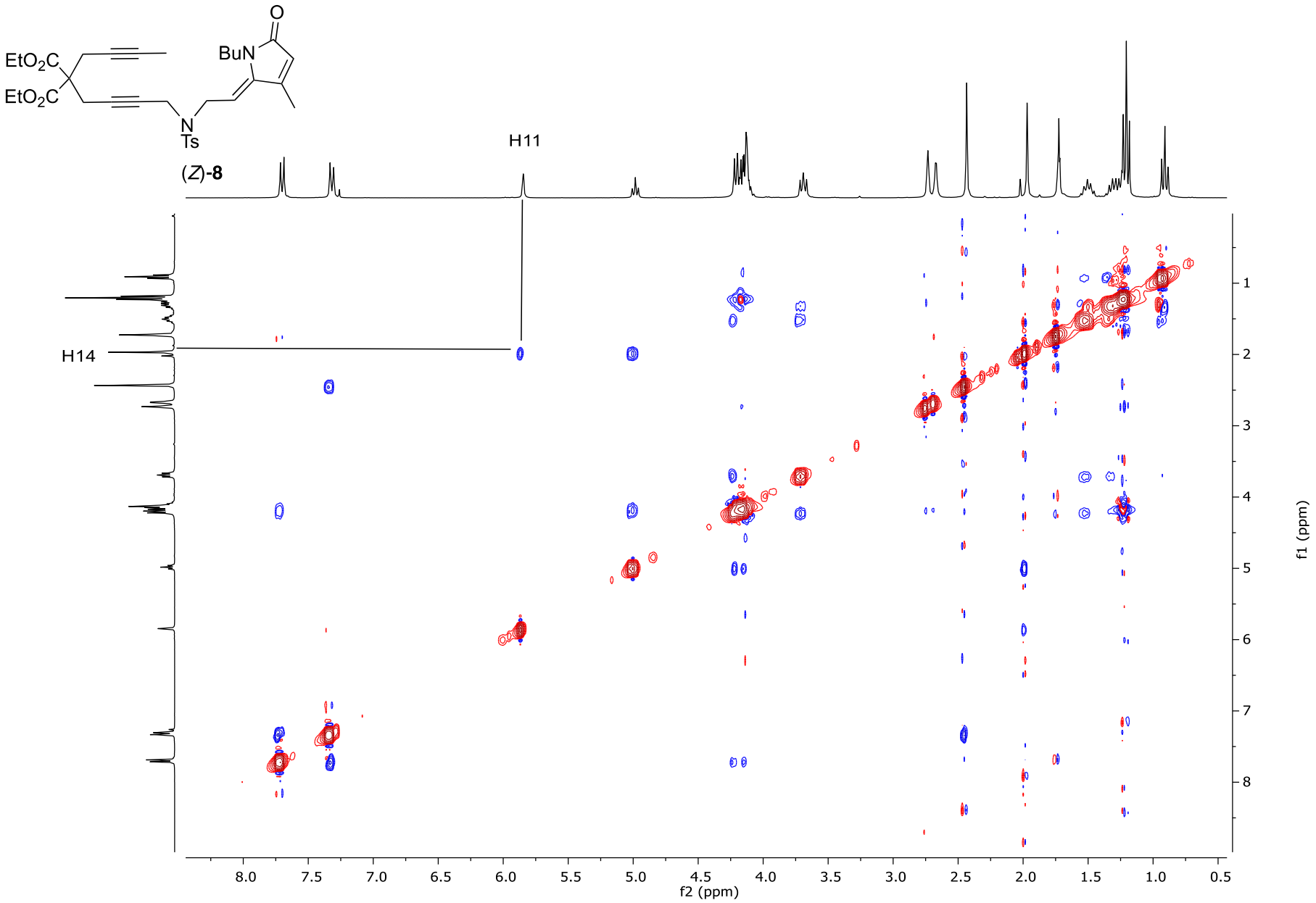
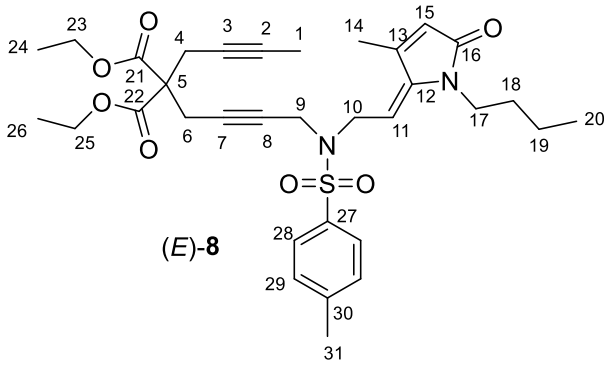


Figure S27. NOESY ($CDCl_3$) spectrum

Assignment of (*E*)-8



^{1}H NMR (300 MHz, Chloroform-*d*) δ 0.89 (t, *J* = 7.2 Hz, 3H, H20), 1.20 (t, *J* = 7.1 Hz, 6H, H24 and H26), 1.18 – 1.30 (m, 2H, H19), 1.34 – 1.47 (m, 2H, H18), 1.72 (t, *J* = 2.5 Hz, 3H, H1), 2.29 (br d, *J* = 1.6 Hz, 3H, H14), 2.43 (s, 3H, H31), 2.67 (br q, *J* = 2.5 Hz, 2H, H4), 2.74 (br t, *J* = 2.3 Hz, 2H, H6), 3.44 (t, *J* = 7.2 Hz, 2H, H17), 4.05 – 4.19 (m, 6H, H9, H23 and H25), 4.23 (d, *J* = 7.6 Hz, 2H, H10), 5.14 (t, *J* = 7.6 Hz, 1H, H11), 5.93 (br q, *J* = 1.6 Hz, 1H, H15), 7.28 – 7.37 (d, *J* = 7.9 Hz, 2H, HAr), 7.64 – 7.76 (d, *J* = 7.9 Hz, 2H, HAr)

^{13}C NMR (75 MHz, $CDCl_3$) δ 3.5 (C1), 13.9 (C20), 14.1 (2C, C24 and C26), 16.8 (C14), 20.2 (C19), 21.7 (C31), 22.8 (C6), 23.0 (C4), 30.8 (C18), 36.9 (C9), 38.6 (C17), 43.2 (C10), 56.5 (C5), 61.9 (2C, C23 and C25), 73.0 (C2 or C3 or C7 or C8), 76.1 (C2 or C3 or C7 or C8), 79.1 (C2 or C3 or C7 or C8), 81.1 (C2 or C3 or C7 or C8), 107.3 (C11), 124.7 (C15), 127.7 (2C, C28 or C29), 129.8 (2C, C28 or C29), 136.2 (C12 or C27, or C30), 142.2 (C12 or C27, or C30), 143.9 (C12 or C27, or C30), 145.7 (C13), 168.8 (2C, C21 and C22), 168.9 (C16)

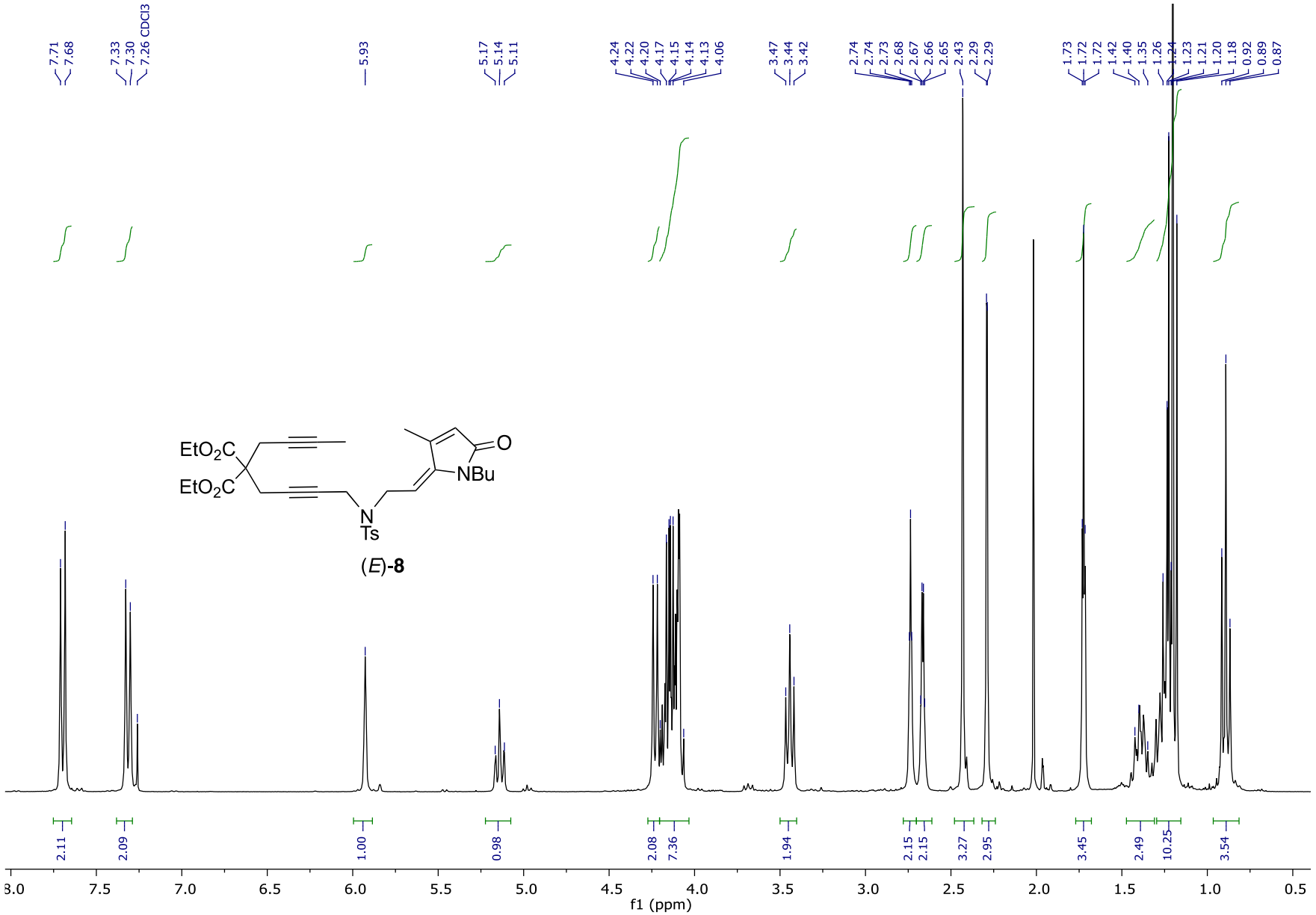


Figure S28. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

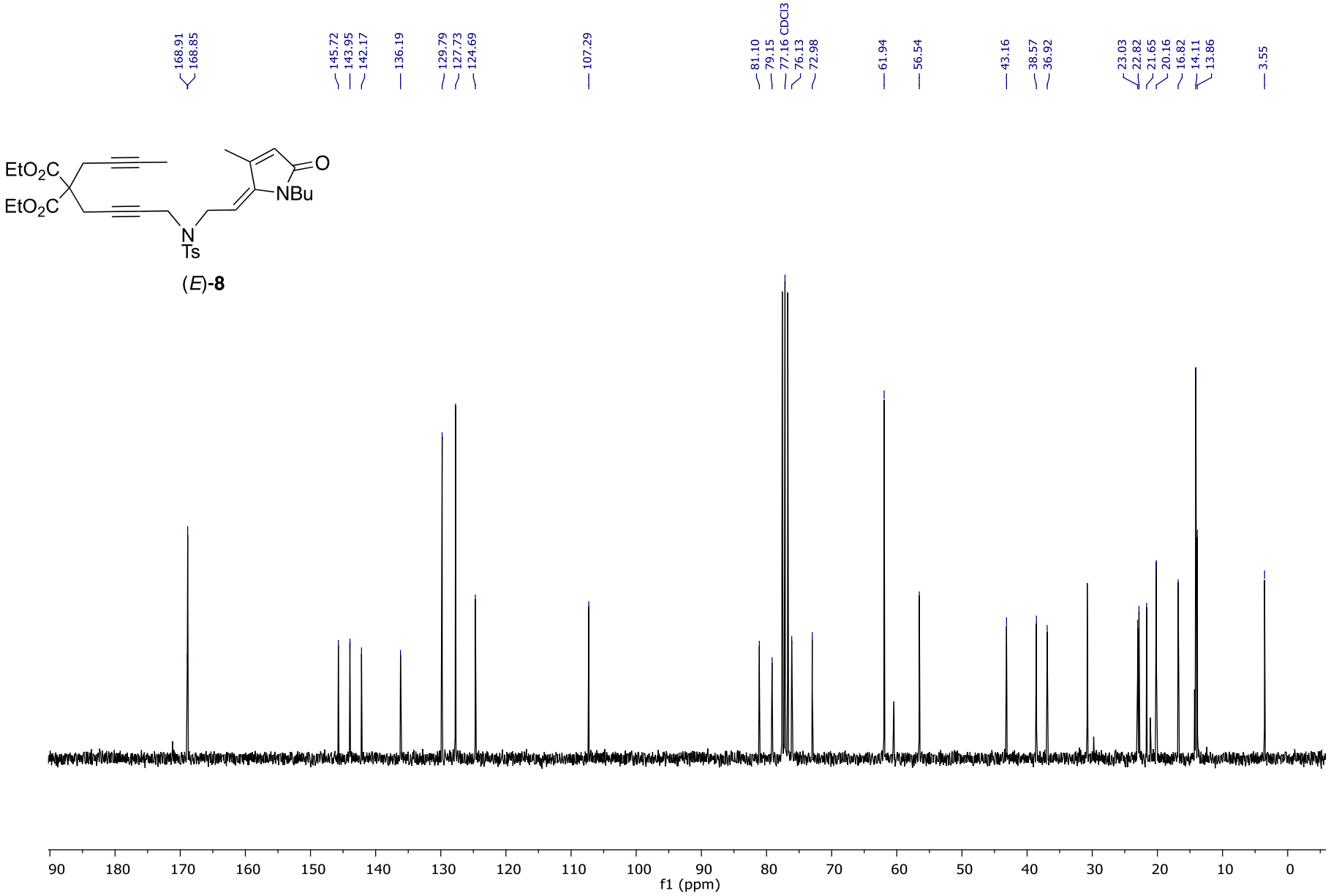


Figure S29. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

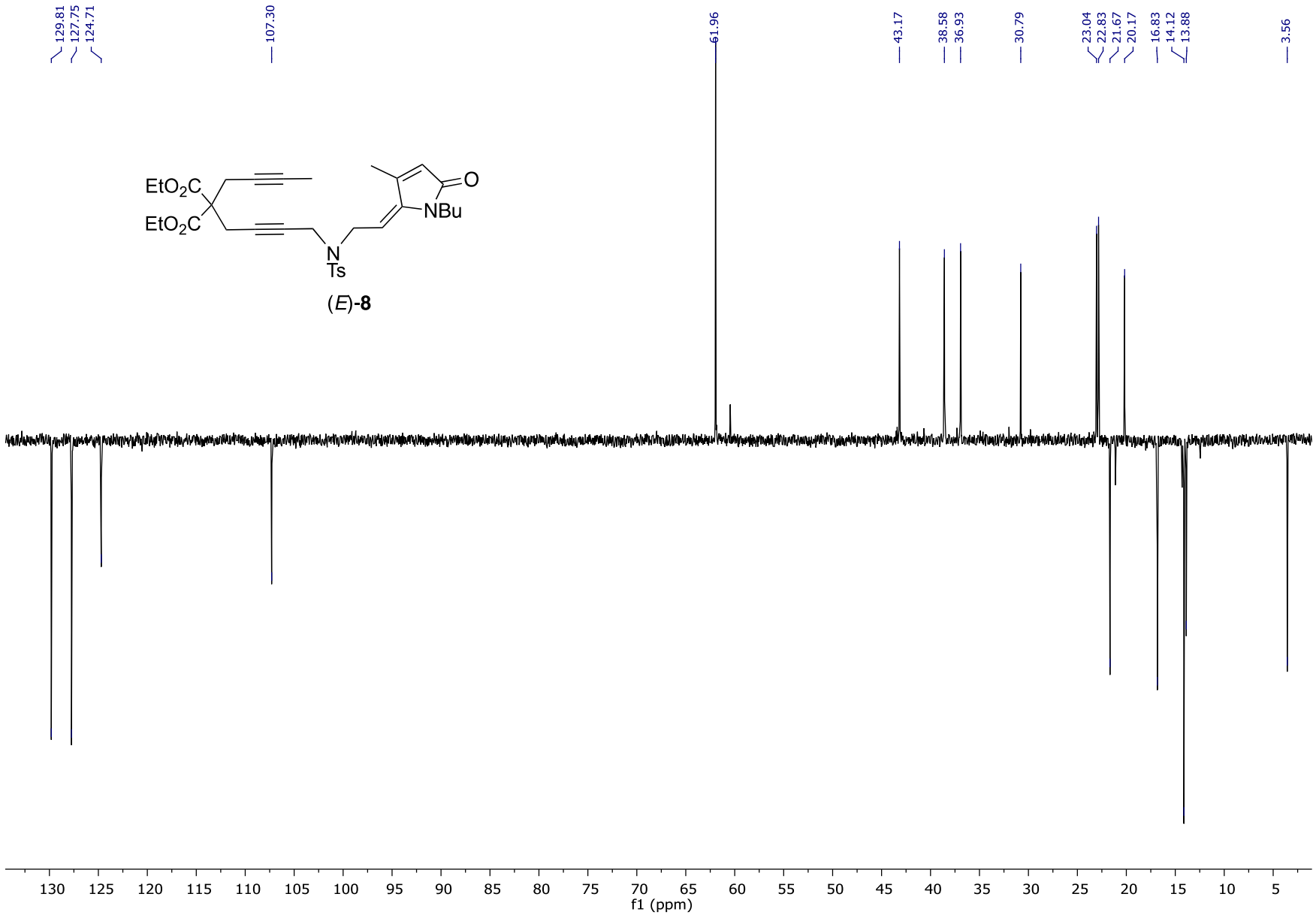


Figure S30. DEPT (75 MHz, $CDCl_3$) spectra

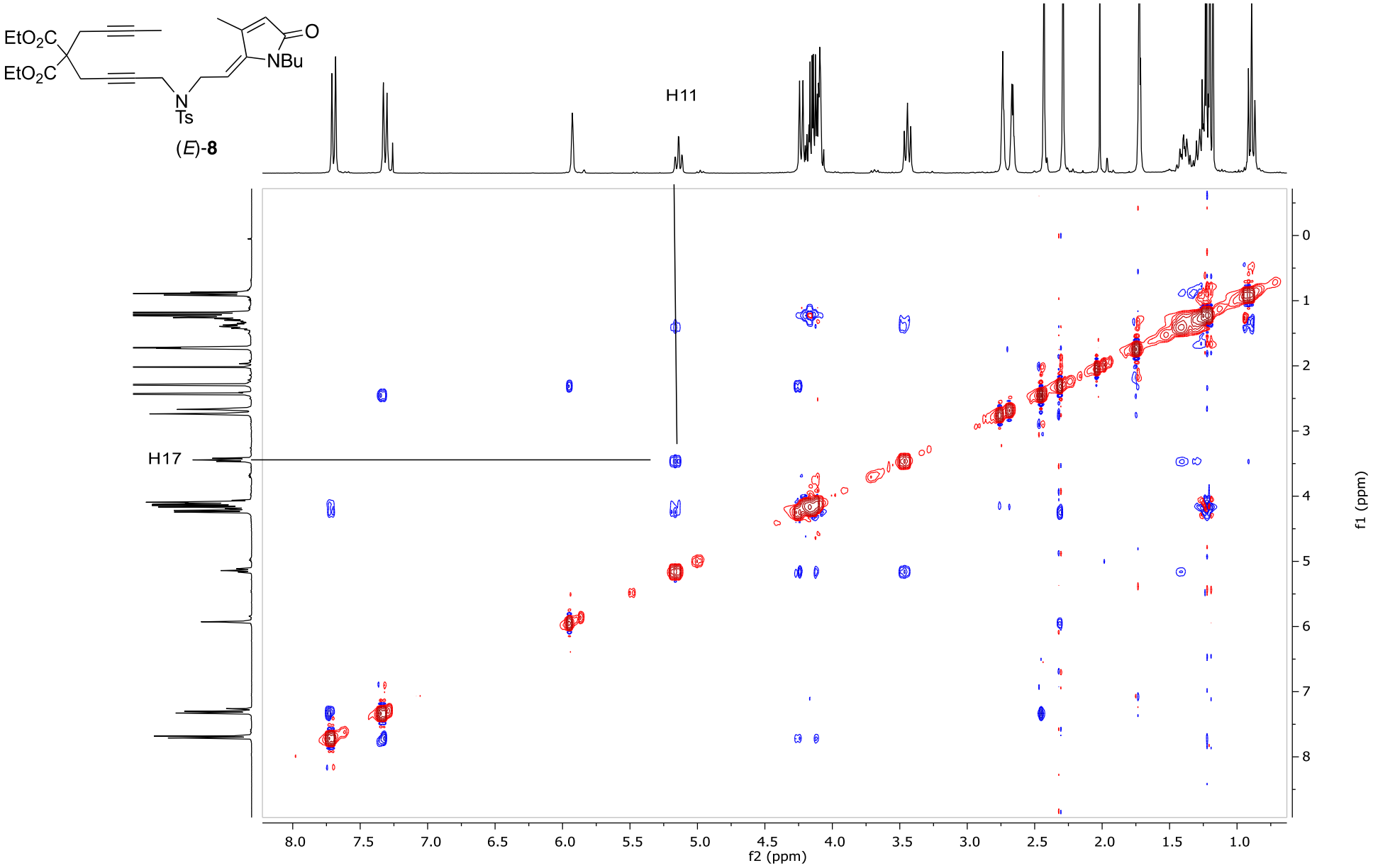
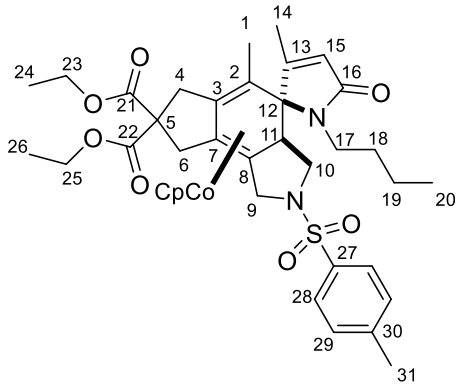


Figure S31. NOESY ($CDCl_3$) spectrum

Assignment of *cis*-9



^{1}H NMR (300 MHz, Chloroform-*d*) δ 0.69 (s, 3H, H1), 1.17 (t, *J* = 6.9 Hz, 3H, H20), 1.29 (t, *J* = 7.1 Hz, 3H, H24 or H26), 1.32-1.36 (m, 7H, H11, H14 and H24 or H26), 1.41 – 1.70 (m, 4H, H18 and H19), 2.20-2.35 (m, 1H, H17), 2.45 (s, 3H, H31), 3.10 – 3.66 (m, 9 H, H4, H6, H9, H10 and H17), 4.12 (s, 5H, Cp), 4.25 (q, *J* = 7.1, 2H, H23 or H25), 4.35 (br q, *J* = 7.1 Hz, 2H, H23 or H25), 5.59 (br q, *J* = 1.6 Hz, 1H, H15), 7.42 (d, *J* = 8.1 Hz, 2H, HAr), 7.82 (d, *J* = 8.1 Hz, 2H, HAr)

^{13}C NMR (75 MHz, Chloroform-*d*) δ 12.6 (C14), 14.2 (C24 or C26), 14.3 (2C, C24 or C26 and C20), 17.5 (C1), 21.6 (C18 or C19), 21.7 (C31), 30.2 (C17), 39.4 (C4 or C6), 40.1 (C4 or C6), 44.0 (C5), 48.7 (C11), 51.4 (C9 or C10), 53.6 (C9 or C10), 59.4 (C12), 60.5 (C2 or C3 or C7 or C8), 62.4 (C23 or C25), 62.6 (C23 or C25), 63.7 (C2 or C3 or C7 or C8), 84.0 (5C, Cp), 89.8 (C2 or C3 or C7 or C8), 95.2 (C2 or C3 or C7 or C8), 121.4 (C15), 127.9 (2C, C28 or C29), 130.0 (2C, C28 or C29), 134.0 (C27 or C30), 144.2 (C27 or C30), 160.6 (C2 or C3 or C7 or C8), 171.7 (C16 or C21 or C22), 172.2 (C16 or C21 or C22), 173.4 (C16 or C21 or C22)

one quaternary C carbon is in $CDCl_3$ peaks

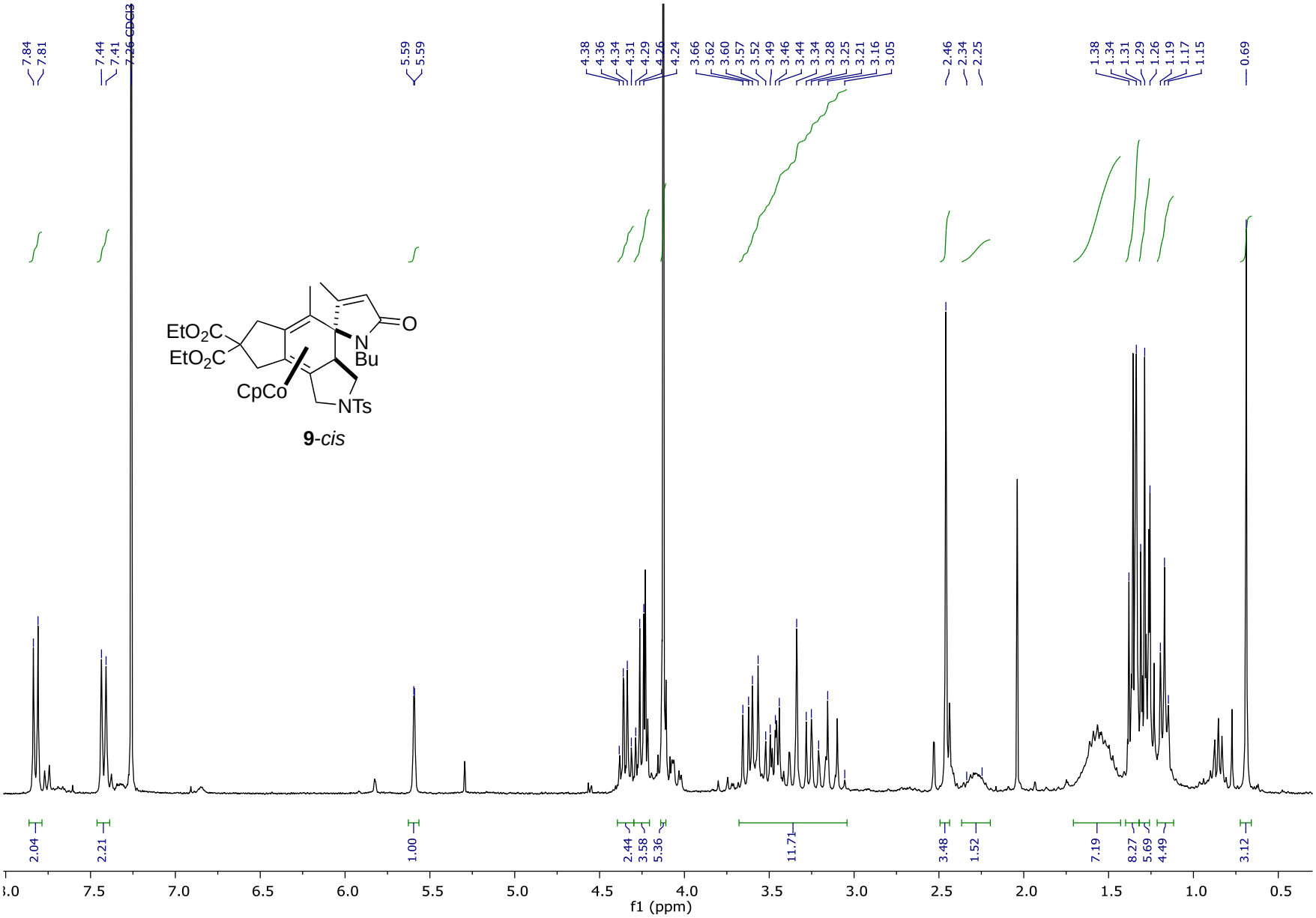


Figure S32. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum

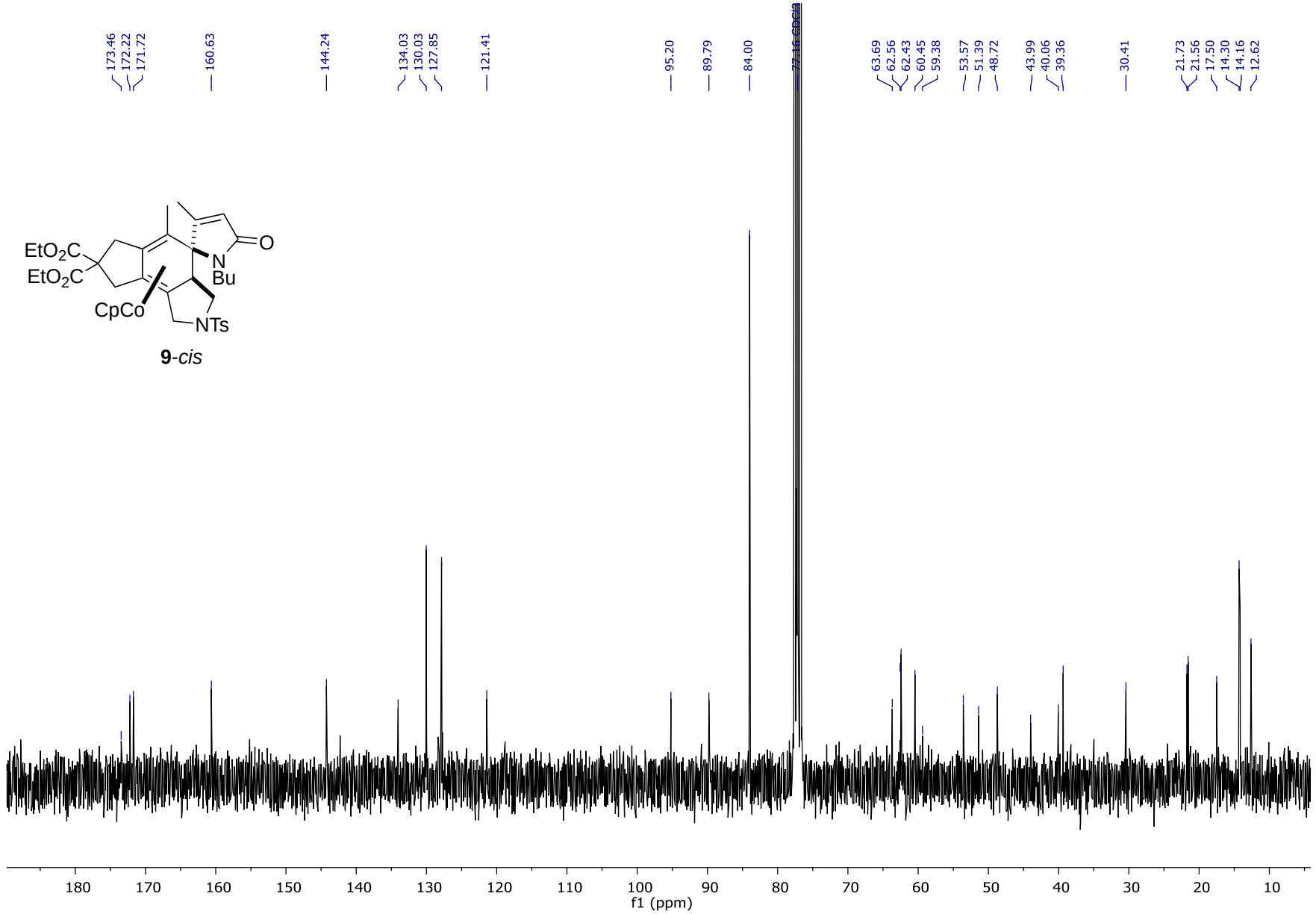


Figure S33. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

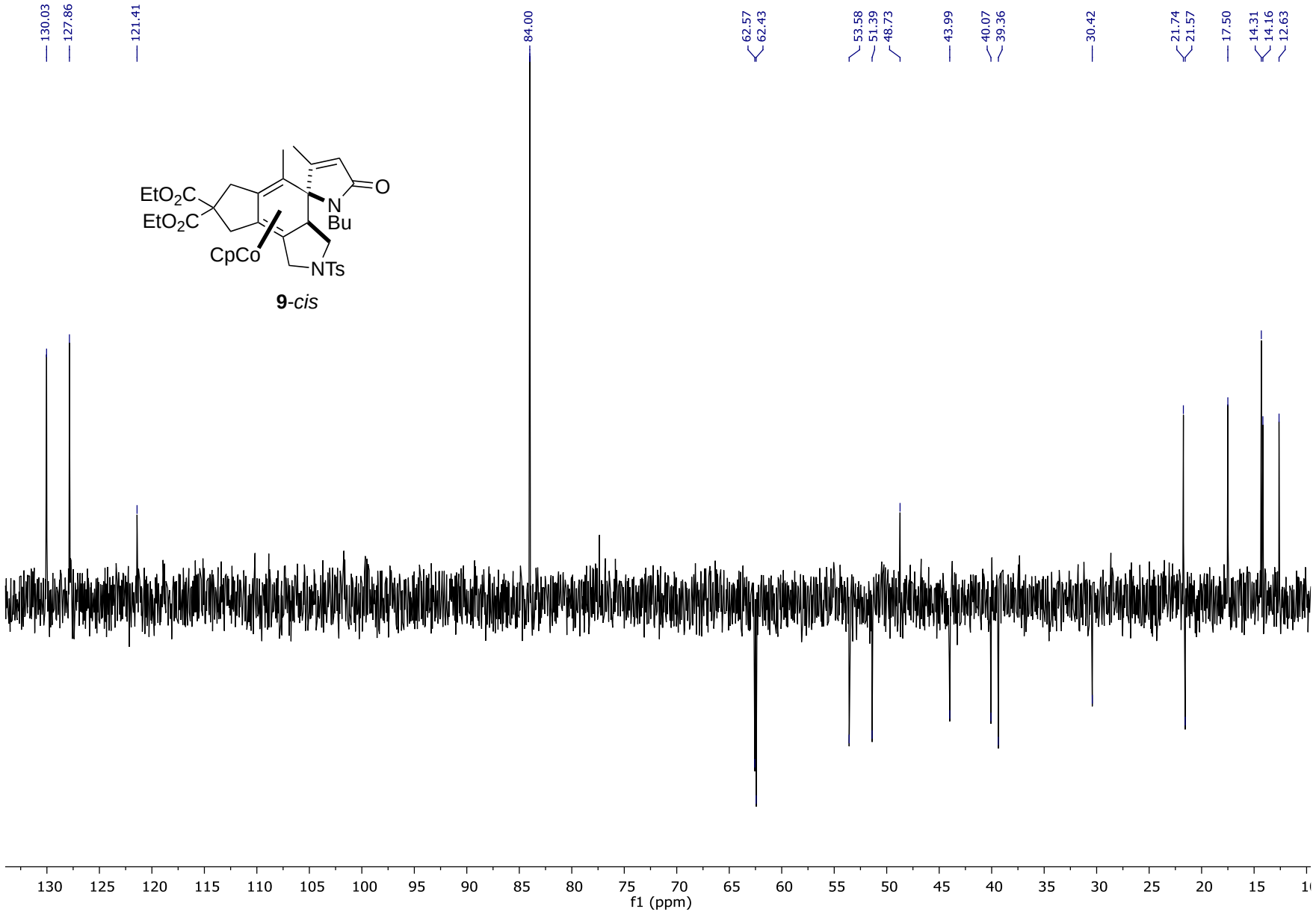


Figure S34. DEPT (75 MHz, $CDCl_3$) spectra

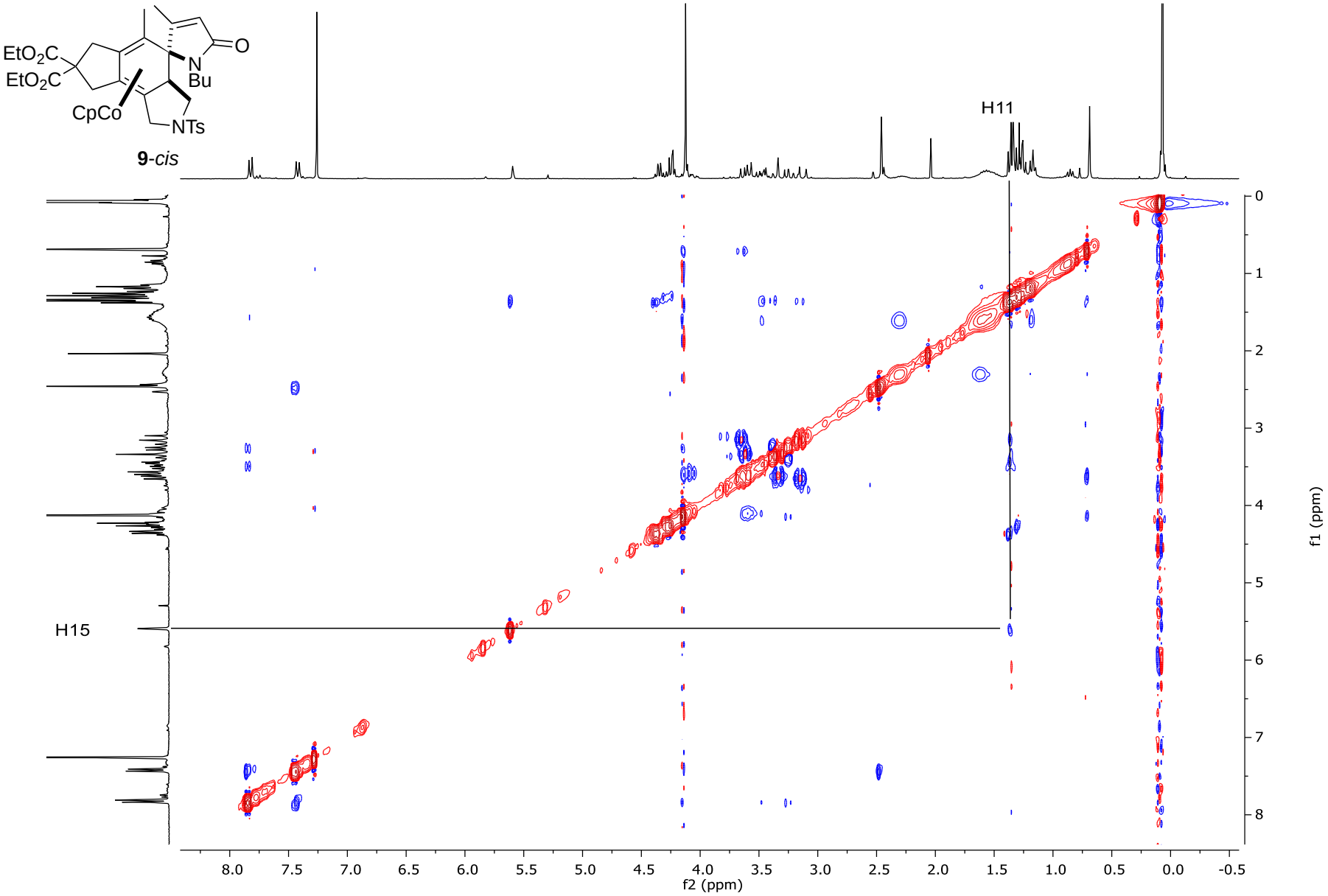
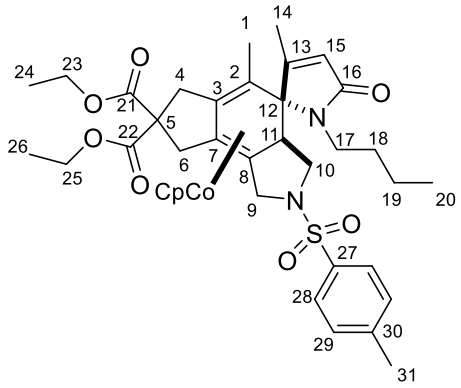


Figure S35. NOESY ($CDCl_3$) spectrum

Assignment of *trans*-9



^{1}H NMR (300 MHz, Chloroform-*d*) δ 0.77 (s, 3H, H1), 0.83 (t, *J* = 7.0 Hz, 3H, H20), 1.09 – 1.20 (m, 3H, H18 and H19), 1.20 – 1.27 (m, 1H, H11), 1.30 (t, *J* = 7.1 Hz, 3H, H24 or H26), 1.36 (t, *J* = 7.1 Hz, 3H, H24 or H26), 1.41 – 1.51 (m, 1H, H18 and H19), 2.26- 2.38 (m, 1H, H17), 2.43 (s, 3H, H31), 2.53 (br d, *J* = 1.5 Hz, 3H, H14), 2.60 – 2.73 (m, 1H, H17), 3.08 (d, *J* = 17.0 Hz, 1H, H4 or H6), 3.16 (br s, 2H, H9), 3.34 (br dd, *J* = 7.8 and 8.6 Hz, 1H, H10), 3.45 (d, *J* = 17.0 Hz, 1H, H4 or H6), 3.55 (d, *J* = 17.0 Hz, 1H, H4 or H6), 3.68 – 3.73 (m, 1H, H10), 3.73 (d, *J* = 17.0 Hz, 1H, H4 or H6), 4.23 (s, 5H, Cp), 4.23 – 4.39 (m, 4H, H23 and H25), 5.82 (br q, *J* = 1.5 Hz, 1H, H15), 7.39 (d, *J* = 8.3 Hz, 2H, HAr), 7.75 (d, *J* = 8.3 Hz, 2H, HAr)

^{13}C NMR (75 MHz, Chloroform-*d*) δ 13.9 (C20), 14.2 (C24 or C26), 14.3 (C24 or C26) , 17.8 (C14), 17.9 (C1), 20.5 (C18 or C19), 21.7 (C31), 30.8 (C18 or C19), 39.3 (C4 or C6 or C17), 39.7 (C4 or C6 or C17), 39.8 (C4 or C6 or C17), 49.4 (C11), 50.9 (C10), 53.2 (C9), 56.5 (C5 or C12), 59.8 (C5 or C12), 60.1 (C2 or C3 or C7 or C8), 62.4 (C23 or C25), 62.6 (C23 or C25), 77.5 (C2 or C3 or C7 or C8), 84.0 (5C, Cp), 89.7 (C2 or C3 or C7 or C8), 95.2 (C2 or C3 or C7 or C8), 126.3 (C15), 127.7 (2C, C28 or C29), 130.0 (2C, C28 or C29), 134.1 (C27 or C30), 144.1 (C27 or C30), 158.2 (C2 or C3 or C7 or C8), 169.6 (C21 or C22) , 171.7 (C21 or C22), 171.9 (C16

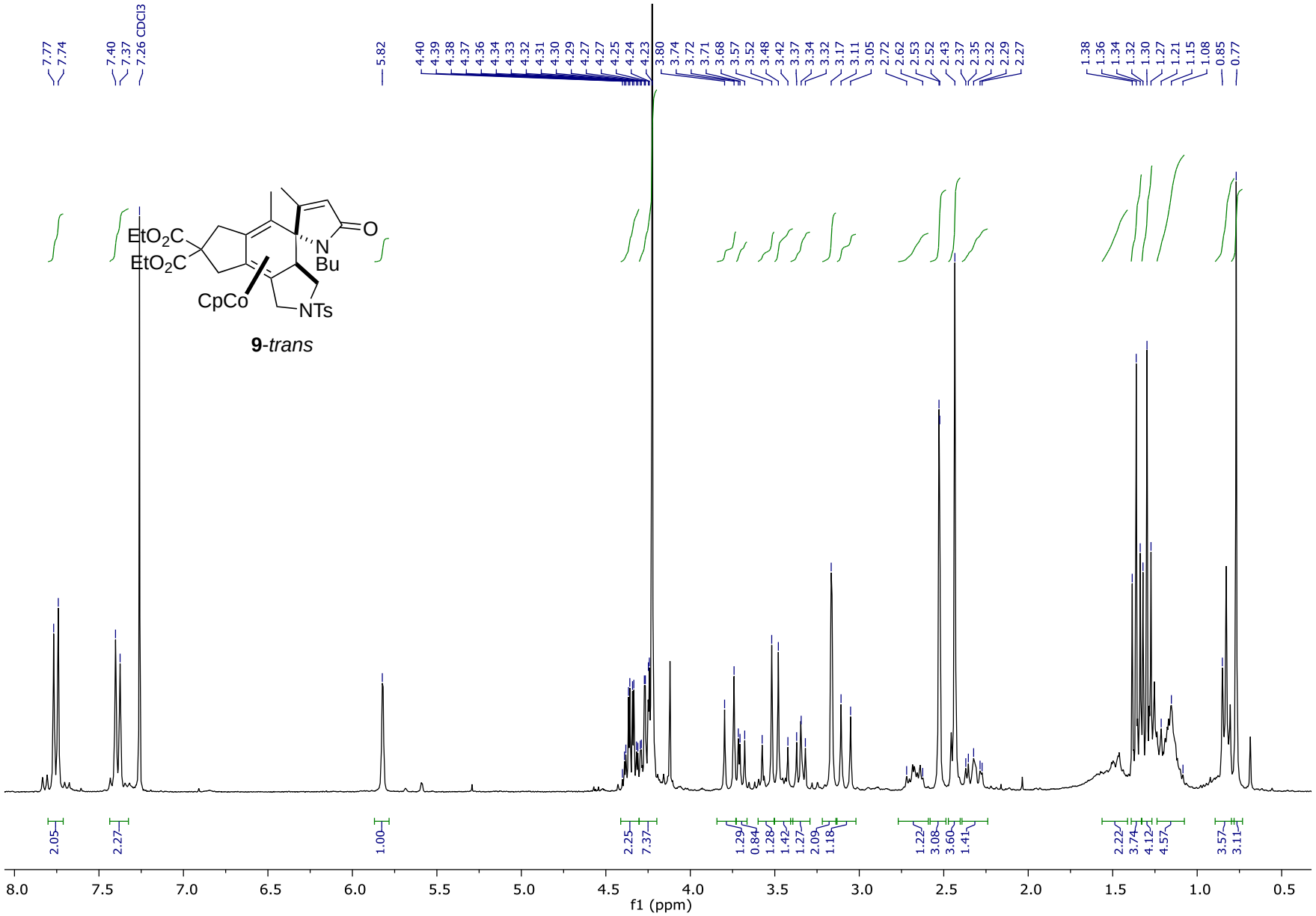
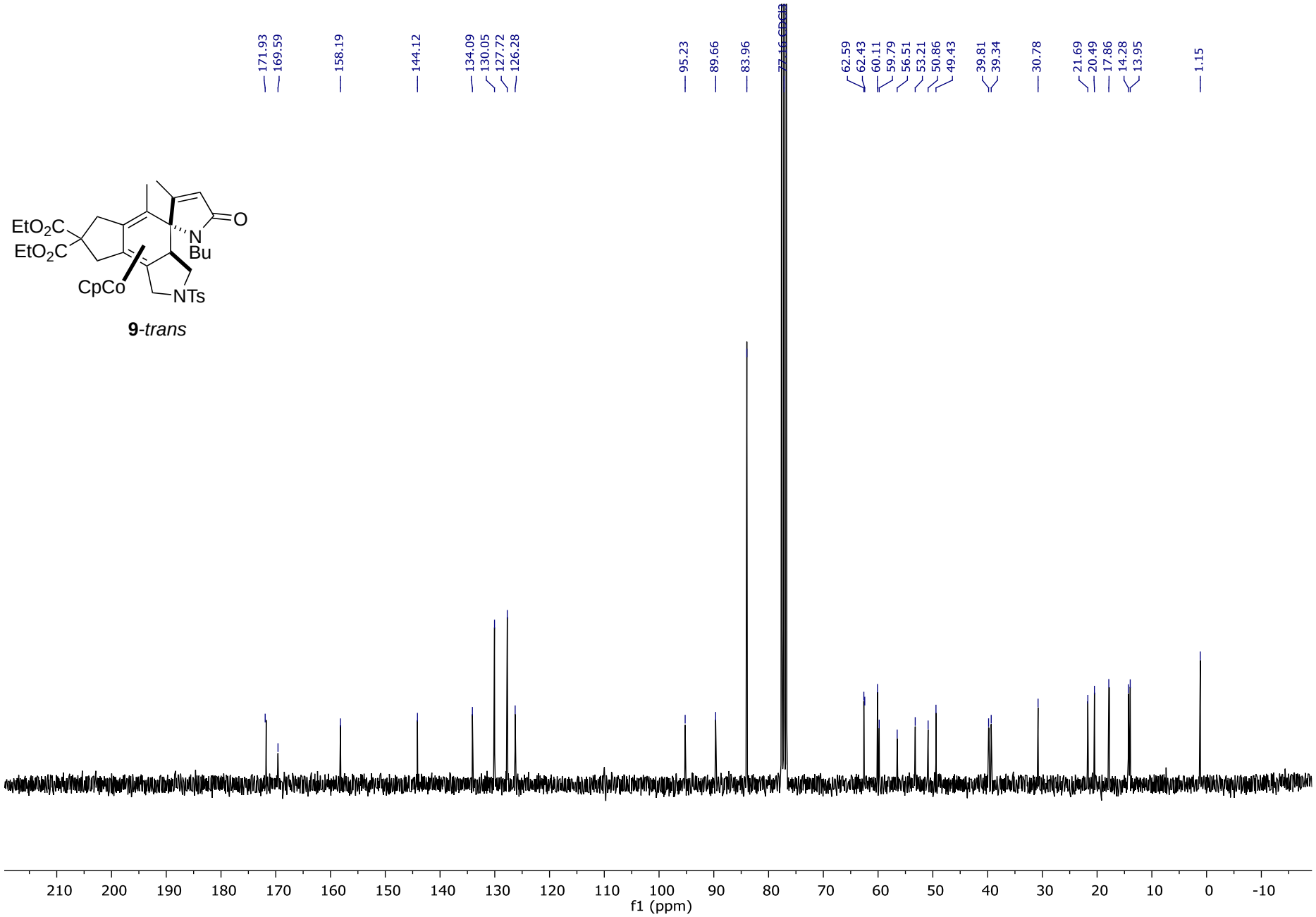


Figure S36. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum



9-*trans*

Figure S37. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum

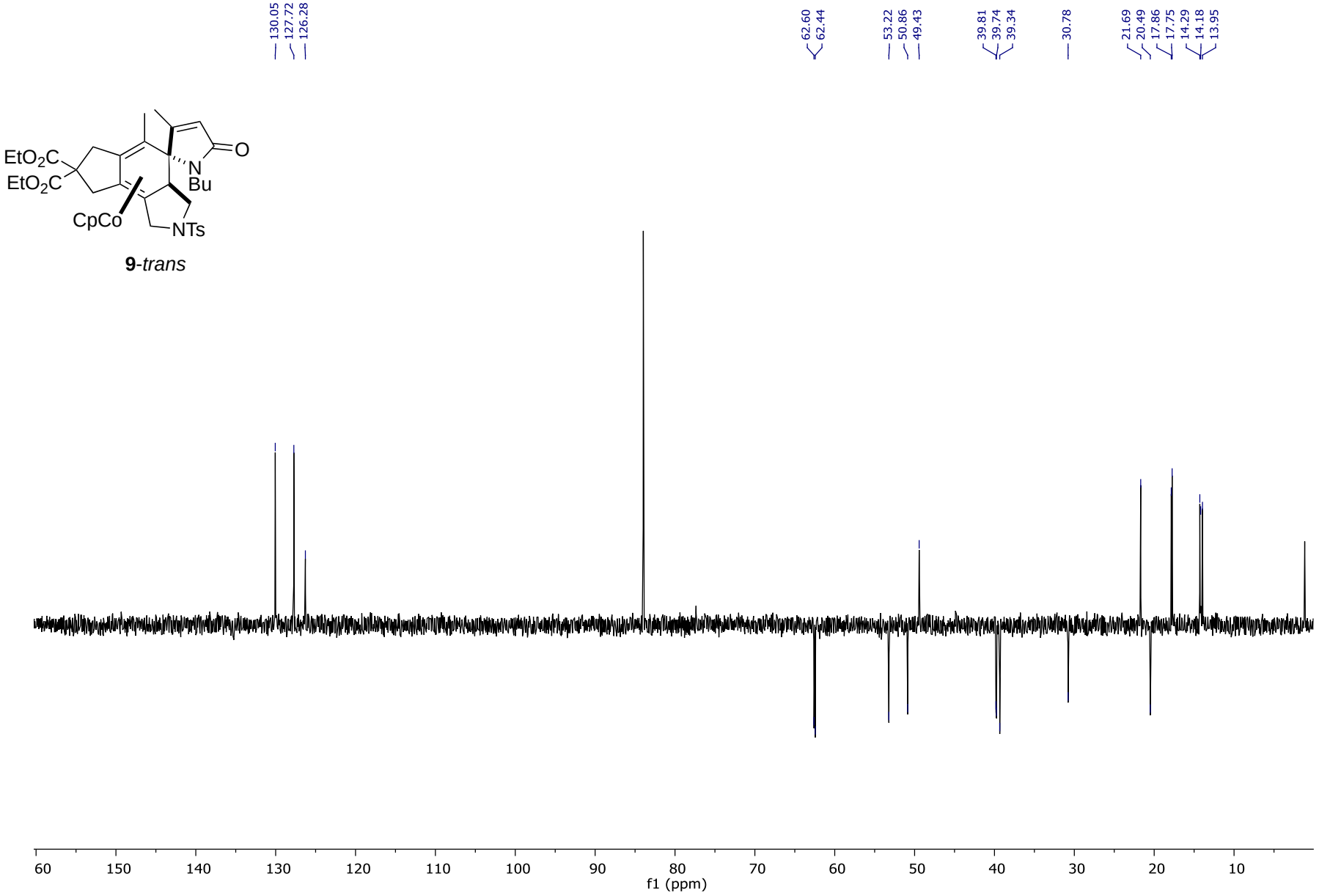


Figure S38. DEPT (75 MHz, $CDCl_3$) spectrum

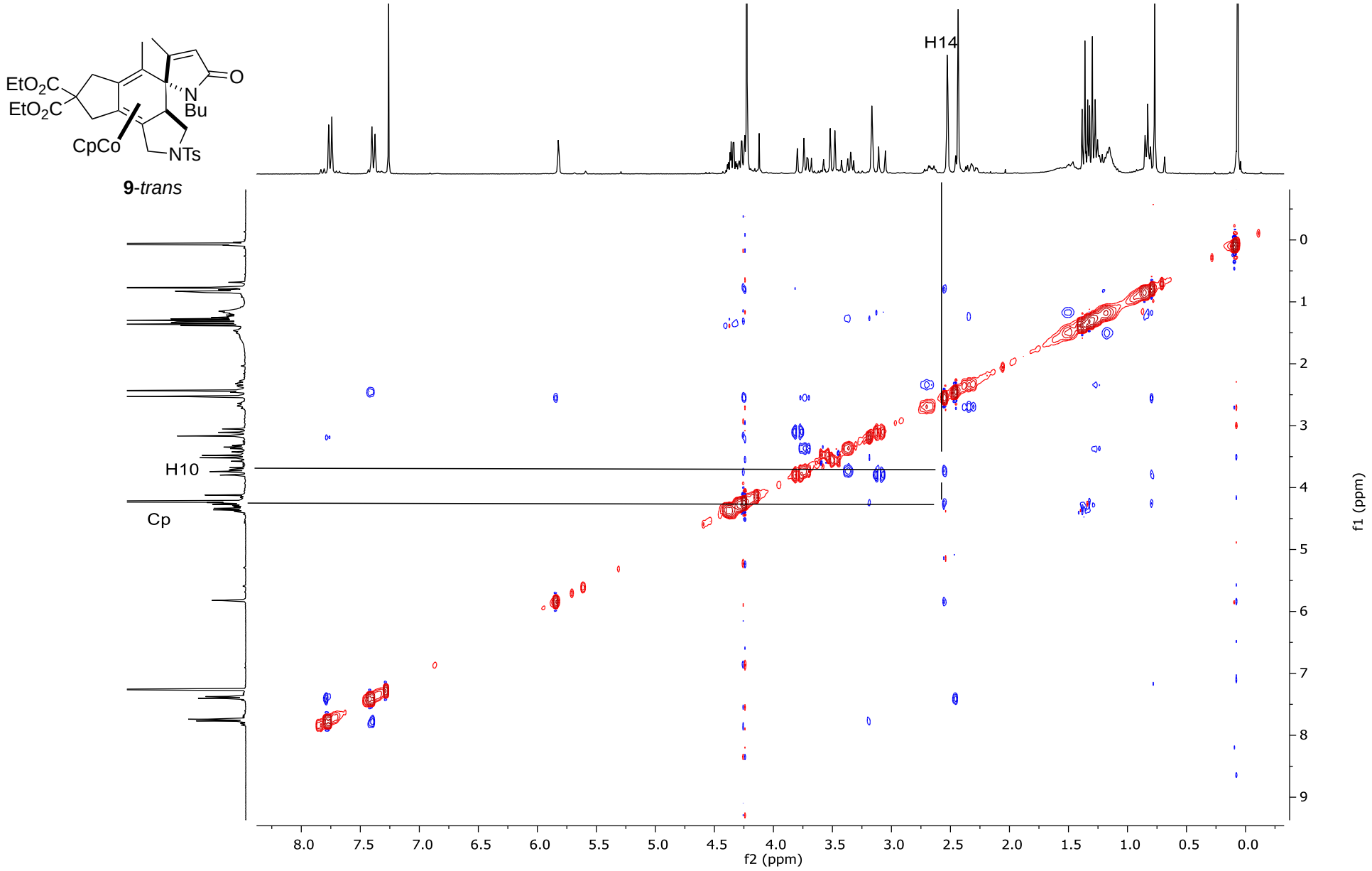


Figure S39. NOESY ($CDCl_3$) spectrum

List of coordinates

In the following we report the coordinates of the computed structures. Optimizations were performed at the TPSS-D3/def2-TZVP level. Solvent effects are added as single point calculations with the COSMO implicit model (toluene).

Table S2. List of computed energies. E (a.u., gas phase) is the total electronic energy. ZPE (a.u., gas phase) is the zero-point energy. "Chem. Pot." (kJ/mol, gas phase) is the chemical potential. $E_{Toluene}$ (a.u.) is the total electronic energy obtained by employing the COSMO model for reproducing solvent effects. ΔG (kcal/mol) are computed relative free-energies (Δ $E_{Toluene}$ + Δ(Chem. Pot.), T=383.15K).

System	E	ZPE	Chem. Pot.	$E_{Toluene}$	ΔG
Figure 3	**Exo approach**				
II_{exo}	-2765.815271	0.4546728	937.52	-2765.826211	0.00
$Ts_{II-IIIexo1}$	-2765.7956346	0.4524479	929.86	-2765.806506	10.53
III_{exo1}	-2765.8124604	0.4552817	941.67	-2765.823794	2.51
$Ts_{III-P2exo}$	-2765.794083	0.4539583	939.92	-2765.805258	13.72
$P2_{exo}$	-2765.8960570	0.458963	953.88	-2765.907425	-47.05
Ts_{III-IV}	-2765.7884839	0.4546732	945.57	-2765.801488	17.44
IV	-2765.8404165	0.457065	948.98	-2765.850328	-12.39
Ts_{IV-V}	-2765.8289044	0.4565329	951.74	-2765.838736	-4.46
V	-2765.8407002	0.4572427	952.39	-2765.850362	-11.60
Ts_{V-P1}	-2765.8120904	0.4565534	959.3	-2765.824133	6.51
$Ts_{II-IIIexo1}$	-2765.7956346	0.4524479	929.86	-2765.806506	10.53
$P1_{exo}$	-2765.8746457	0.4593094	961.92	-2765.887025	-32.33
$Ts_{II-IIIexo2}$	-2765.801029	0.4540872	933.7	-2765.812373	7.77
III_{exo2}	-2765.825935	0.4558109	939.64	-2765.837578	-6.63
$Ts_{III-P2exo2}$	-2765.790758	0.4541399	941.66	-2765.802013	16.17
Figure 3	**Endo approach**				
II_{endo}	-2765.8059	0.4546462	937.62	-2765.817732	5.3
$Ts_{II-IIIendo2}$	-2765.8007	0.4538618	936.45	-2765.813037	8.0
III_{endo2}	-2765.826293	0.4560525	945.74	-2765.838281	-5.6
$Ts_{III-P2endo2}$	-2765.787576	0.4549764	946.99	-2765.799371	19.1
$Ts_{II-IIIendo1}$	-2765.787986	0.4522329	927.39	-2765.799461	14.4
III_{endo1}	-2765.806205	0.4548385	941.99	-2765.817586	6.5
$Ts_{III-P2endo1}$	-2765.79766	0.4539963	944.76	-2765.809020	12.5
$P2_{endo}$	-2765.893745	0.4589252	956.41	-2765.905818	-45.4
Figure 5	**Lactam case**				
I^N	-2823.361213	0.5006682	1029.66	-2823.373231	0.0
Ts^N_{I-II}	-2823.343911	0.4991287	1018.97	-2823.357054	7.6
IIa^N	-2823.369751	0.5012422	1034.18	-2823.383076	-5.1
$^3IIa^N$	-2823.378198	0.5008928	1033.56	-2823.391060	-10.3
Ts^N_{II}	-2823.367272	0.5014843	1046.7	-2823.38046	-0.5
II^N	-2823.402673	0.5037944	1060.63	-2823.414563	-18.5
Ts^N_{II-III}	-2823.395071	0.5033413	1062.52	-2823.40751	-13.7

III^{N}	-2823.40571	0.5041444	1058.97	-2823.418728	-21.5
Ts$^{N}_{III-IV}$	-2823.373443	0.5023531	1060.79	-2823.387794	-1.7
IV^{N}	-2823.417291	0.5063455	1077.29	-2823.432685	-25.9
Ts$^{N}_{IV-V}$	-2823.397252	0.5046941	1071.09	-2823.407077	-11.3
V^{N}	-2823.40296	0.5059212	1073.5	-2823.412483	-14.2
Ts$^{N}_{V-P1}$	-2823.378837	0.5046874	1076.83	-2823.390645	0.3
P1^{N}	-2823.444015	0.5075289	1078.26	-2823.455881	-40.2
Ts$^{N}_{III-P2}$	-2823.37564	0.5020332	1056.09	-2823.387679	-2.7
P2^{N}	-2823.475736	0.5071147	1074.08	-2823.488052	-61.4
Figure 5	**Lactone case**				
I^{O}	-2843.236305	0.488355	999.53	-2843.247126	0.0
Ts$^{O}_{I-II}$	-2843.224289	0.487791	1000.64	-2843.235853	7.3
IIa^{O}	-2843.258288	0.489679	1017.13	-2843.268758	-9.4
Ts$^{O}_{II}$	-2843.242970	0.489706	1022.57	-2843.253098	1.8
II^{O}	-2843.281711	0.491502	1030.33	-2843.292266	-21.0
Ts$^{O}_{II-III}$	-2843.274674	0.490941	1030.85	-2843.285881	-16.8
III^{O}	-2843.286613	0.491564	1024.19	-2843.298556	-26.4
Ts$^{O}_{III-IV}$	-2843.254316	0.490437	1033.11	-2843.267276	-4.6
IV^{O}	-2843.306681	0.493364	1042.21	-2843.316289	-33.2
Ts$^{O}_{IV-V}$	-2843.292859	0.492386	1041.91	-2843.302186	-24.4
V^{O}	-2843.297224	0.493426	1037.86	-2843.306773	-28.3
Ts$^{O}_{V-P1}$	-2843.273323	0.492442	1045.44	-2843.285225	-12.9
P1^{O}	-2843.336703	0.495049	1046.26	-2843.348521	-52.5
Ts$^{O}_{III-P2}$	-2843.251196	0.489407	1024.49	-2843.262136	-3.5
P2^{O}	-2843.354146	0.494858	1044.2	-2843.365445	-63.6

List of coordinates

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$TS_{II\text{-}IIIexo1}$
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58
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H 1.5716201 -4.0050467 -1.8440133
C 0.5652566 -2.2790889 -2.8734234
H -0.2392356 -2.7504156 -3.4212906
C 1.9973359 -0.6808688 -2.0276392
H 2.4544122 0.2690092 -1.7844449
C 0.8856117 -0.8739298 -2.8762189
H 0.3326317 -0.0946846 -3.3828559
C -2.4179023 -0.7842945 -2.0482621
H -3.2611460 -0.1281786 -1.7974393
H -2.0416743 -0.4889326 -3.0350685
C -0.6709192 -2.9538091 0.0189066
H -1.7559517 -2.8680972 -0.0645438
C -0.1284495 -2.5767776 1.3941204
C -1.1059195 -2.4555303 2.5515964
O 0.7808460 -3.6341646 1.8240873
C -0.7750923 -3.3520523 3.4928150
C 0.4103317 -4.1090803 3.0693760
H -1.2718256 -3.5380821 4.4370582
C -2.2287690 -1.4758513 2.5801658
H -1.8377371 -0.4528860 2.6324763
H -2.8245454 -1.5325183 1.6630115
H -2.8739954 -1.6470276 3.4458737
C 2.0964312 -1.2645009 1.7245263
H 2.6986167 -0.4625717 1.2915466
H 2.0033806 -1.0759720 2.8037011
H 2.6237565 -2.2111728 1.6069959
O 1.0211450 -4.9957224 3.6213912
C -0.2075540 2.2517102 0.1704663
C 0.0694726 2.5201864 -1.3149032
O -0.7109460 2.3741488 -2.2301566
O 1.3458548 2.9537822 -1.4847492
C -0.2195485 3.5637712 0.9527396
O 0.0703859 3.6789080 2.1249455
O -0.6731866 4.5827696 0.1857116
C 1.6971885 3.2866886 -2.8517945
H 2.7239855 3.6477885 -2.8013764
H 1.6259476 2.3987327 -3.4851292
H 1.0245067 4.0595427 -3.2314483
C -0.7843419 5.8607006 0.8658613
H 0.1948837 6.1699934 1.2392580
H -1.1538917 6.5518822 0.1092556
H -1.4843770 5.7791041 1.7008749
H -2.7914960 -1.8123581 -2.1423156
H -0.3499114 -3.9612591 -0.2514299

$TS_{III\text{-}P2exo1}$
58
Energy = -2765.794083141
C 1.1347005 1.2081213 0.8334986
C -1.2650624 1.6780368 1.2368219
C -1.1024351 0.3357427 0.5907371

C 0.3195558 -0.0385439 0.5274702
C -1.7724708 -0.3524935 -0.3667450
C 0.8030466 -1.3757817 0.4642645
H 1.9491218 1.4023947 0.1339825
H 1.5688124 1.1438482 1.8393470
H -1.3022708 1.6082562 2.3340037
H -2.1225906 2.2521208 0.8830266
Co -0.1278850 -0.9158469 -1.2525060
C 1.4897476 -1.0916138 -2.5701472
H 2.4870643 -1.3716291 -2.2578934
C 0.4723764 -1.9864136 -2.9981343
H 0.5479063 -3.0637809 -3.0489017
C -0.6897647 -1.1975763 -3.2366702
H -1.6603666 -1.5702718 -3.5393209
C 0.9943414 0.2622036 -2.6653282
H 1.5542235 1.1522951 -2.4131901
C -0.3472037 0.2002239 -3.0752732
H -1.0213695 1.0378904 -3.1887071
C -3.1565532 -0.1389561 -0.8890566
H -3.8956949 -0.1088188 -0.0780083
H -3.1957783 0.8222655 -1.4149731
C -1.3635005 -2.2272385 -0.1739759
H -2.3337311 -2.2752403 0.3278599
C -0.1869765 -2.5098883 0.7716834
C -0.5014952 -2.7221965 2.2423715
O 0.4137753 -3.7720217 0.3589482
C -0.0992161 -3.9511876 2.5976753
C 0.4806034 -4.6413919 1.4359868
H -0.1659746 -4.4196604 3.5719017
C -1.1291108 -1.6703015 3.0913520
H -0.4603047 -0.8054006 3.1797351
H -2.0539509 -1.2985206 2.6344199
H -1.3469466 -2.0499686 4.0928315
C 2.2733814 -1.6684460 0.6304230
H 2.8800198 -0.8350346 0.2667133
H 2.5145098 -1.8240652 1.6922007
H 2.5572756 -2.5744913 0.0915024
O 0.9521791 -5.7497837 1.3306449
C 0.0877836 2.3634410 0.8277812
C -0.0702047 2.9733661 -0.5707535
O -1.0948718 3.0295007 -1.2159163
O 1.1166999 3.4653730 -1.0079486
C 0.4455284 3.4531652 1.8370308
O 1.1311112 3.2958734 2.8250245
O -0.1731271 4.6178203 1.5285674
C 1.0593436 4.1352416 -2.2937427
H 2.0780134 4.4718321 -2.4838621
H 0.7250113 3.4396799 -3.0672648
H 0.3680431 4.9799259 -2.2398138
C 0.0529695 5.7002842 2.4690370
H 1.1202855 5.9276452 2.5253618
H -0.5088155 6.5437732 2.0693558
H -0.3123988 5.4170594 3.4591723
H -3.4494030 -0.9252752 -1.5906038
H -1.3817303 -2.9507023 -0.9915859

P2$_{exo}$
58
Energy = -2765.896056973
C 0.9799178 0.9591930 0.9238883
C -1.3501121 1.4852341 0.1722130
C -1.0609398 0.0128275 0.0470640
C 0.2616680 -0.2869702 0.4792970
C -1.8068611 -1.0948509 -0.4653415
C 0.6709129 -1.6554267 0.3485302
H 1.9930847 1.0546702 0.5320553
H 1.0370125 0.9955559 2.0187535
H -2.0107092 1.6573455 1.0325654
H -1.8103333 1.9372316 -0.7082289
Co -0.0113329 -0.8608345 -1.3851563
C 1.5467642 -1.3699047 -2.6050737
H 2.4717807 -1.8066726 -2.2543710
C 0.3665769 -2.1010247 -2.9672298
H 0.2484995 -3.1751324 -2.9476379
C -0.6256895 -1.1344933 -3.3167606
H -1.6460808 -1.3530739 -3.6011589
C 1.2878788 0.0280993 -2.7595871
H 1.9870932 0.8258023 -2.5508145
C -0.0603319 0.1777640 -3.1930716
H -0.5717282 1.1150093 -3.3601512
C -3.1164574 -0.8389072 -1.1765286
H -3.9388923 -0.7306592 -0.4529528
H -3.0750874 0.0731499 -1.7788907
C -1.7451817 -2.4171901 0.2823688
H -2.4840511 -2.4342342 1.1004364
C -0.3308712 -2.7277813 0.8102537
C -0.2744339 -2.9476902 2.3112072
O 0.0939658 -4.0137166 0.2612171
C 0.1474137 -4.1960722 2.5588904
C 0.3904688 -4.8950165 1.2868619
H 0.3074686 -4.6712695 3.5186617
C -0.6129317 -1.8590208 3.2732590
H 0.1278765 -1.0524434 3.2105016
H -1.5831418 -1.4075623 3.0337347
H -0.6380234 -2.2281897 4.3012852
C 2.1274650 -2.0111284 0.5551662
H 2.7751174 -1.2112992 0.1867297
H 2.3509835 -2.1650246 1.6208371
H 2.3816640 -2.9356151 0.0311943
O 0.7790050 -6.0203695 1.0697142
C 0.0585632 2.1247708 0.4359090
C 0.5731317 2.8003154 -0.8412475
O -0.0886405 3.0842761 -1.8166084
O 1.8927516 3.0954617 -0.7268601
C -0.0867901 3.1865779 1.5339801
O -0.0503956 2.9583160 2.7248260
O -0.3295602 4.4094285 1.0113138
C 2.4443072 3.8427334 -1.8409390
H 3.4962335 3.9843885 -1.5949367
H 2.3296849 3.2780564 -2.7695394
H 1.9277552 4.8012633 -1.9347398
C -0.5492831 5.4626993 1.9867663
H 0.3332186 5.5720483 2.6216019
H -0.7245798 6.3611457 1.3962854
H -1.4170211 5.2218410 2.6055306
H -3.3740463 -1.6751489 -1.8351438
H -2.0147559 -3.2284821 -0.3999293

Ts$_{III-IV}$
58
Energy = -2765.788483876
C -0.9421181 1.6963721 1.2176123
C -0.3779544 1.8146859 -1.1975526
C -0.6868120 0.3715220 -0.8132616
C -0.8058949 0.3070934 0.6418457
C -0.7903460 -0.6407562 -1.8090581
C -0.4649646 -0.8581628 1.2753723
H -0.4447326 1.8215680 2.1811546
H -2.0034709 1.9406059 1.3561355
H -1.1545989 2.1852500 -1.8776508
H 0.5842242 1.9332846 -1.7007560
Co 0.5801338 -1.2412906 -0.3939636
C 2.0964268 -2.4175788 0.3092957
H 1.9414047 -3.2039341 1.0355898
C 2.0127888 -2.5589639 -1.1101017
H 1.7320039 -3.4587797 -1.6370825
C 2.2569326 -1.2781901 -1.6762035
H 2.2197723 -1.0382233 -2.7302837
C 2.4926099 -1.0550072 0.5906599
H 2.6329717 -0.6369962 1.5780175

C	2.5922588	-0.3567411	-0.6219408
H	2.8008633	0.6972369	-0.7390750
C	-0.4769568	-0.2547107	-3.2396551
H	-1.3867110	0.1228030	-3.7309692
H	0.2925198	0.5160081	-3.3195765
C	-1.5705740	-1.9406225	-1.6667321
H	-2.6628232	-1.8031382	-1.6215758
C	-0.9711966	-2.5731060	-0.4366413
C	-1.6566078	-2.4385286	0.8879652
O	-0.5337026	-3.8893138	-0.5582393
C	-1.3457750	-3.6074560	1.5887672
C	-0.6344581	-4.5189586	0.7511439
H	-1.6714500	-3.8726925	2.5853500
C	-3.0007311	-1.7567357	1.0677494
H	-3.0834653	-0.8405652	0.4776205
H	-3.7981442	-2.4480555	0.7665093
H	-3.1610525	-1.5019612	2.1203603
C	-0.0764660	-0.9856971	2.7103832
H	0.6856170	-0.2462097	2.9923247
H	-0.9439285	-0.8398925	3.3684505
H	0.3124924	-1.9910530	2.9057944
O	-0.1777621	-5.6338309	0.8947836
C	-0.3622903	2.6366184	0.1283881
C	1.0660855	3.0767893	0.4762700
O	2.0599675	2.8915941	-0.1938834
O	1.0773437	3.7211582	1.6661391
C	-1.2313406	3.8884699	-0.0475281
O	-2.3853104	4.0005844	0.3038424
O	-0.5485837	4.8455510	-0.7177686
C	2.3774633	4.2147088	2.0827891
H	2.2005428	4.7050636	3.0392948
H	3.0764738	3.3816667	2.1905045
H	2.7613258	4.9198681	1.3416135
C	-1.2981091	6.0601847	-0.9887228
H	-1.6247775	6.5123298	-0.0492868
H	-0.6015248	6.7093764	-1.5177692
H	-2.1695876	5.8301069	-1.6063681
H	-0.1463991	-1.1314847	-3.8042179
H	-1.3494788	-2.5758404	-2.5288585

IV

58

Energy = -2765.840416541

C	1.1888742	1.1644311	-0.7219996
C	2.2251226	0.1084595	-0.2295492
C	1.5480294	-1.2687976	-0.4777596
C	0.0705559	-0.9650240	-0.5737064
C	-0.1408295	0.4398703	-0.6972403
C	-1.0275431	-1.8746190	-0.4207279
C	-1.4592590	1.0165702	-0.6657169
H	1.2315460	2.0573585	-0.0978261
H	1.4087091	1.4579095	-1.7573802
H	1.9020329	-1.6662882	-1.4375284
H	1.8044909	-1.9913231	0.2969916
Co	-1.1026379	-0.2917062	0.8808683
C	-2.0913814	0.8107072	2.2996692
H	-2.6418057	1.7148665	2.0818314
C	-2.6230339	-0.5138068	2.2379675
H	-3.6366106	-0.7889238	1.9824573
C	-1.5445589	-1.4043237	2.5485414
H	-1.6060475	-2.4834766	2.5615486
C	-0.7064333	0.7410636	2.6602704
H	-0.0262969	1.5748450	2.7604996
C	-0.3703965	-0.6333324	2.8175937
H	0.6016932	-1.0327409	3.0712660
C	-2.2049823	-1.9423362	-1.3956815
H	-1.8493816	-2.0603973	-2.4302913
C	-3.1079582	-0.7409013	-1.3014163
C	-2.5735628	0.6247881	-1.7036712
O	-4.2627736	-0.8547043	-0.9075482
C	-3.7472907	1.5680530	-1.6830844
C	-4.9648046	1.2836749	-1.2332519
H	-3.6338413	2.5725809	-2.0788213
C	-1.9541434	0.5919103	-3.1262818
H	-1.0842479	-0.0712511	-3.1624077
H	-2.6935440	0.2664652	-3.8649838
H	-1.6214154	1.5994483	-3.3961315
C	-1.4894193	2.4941260	-0.3019890
H	-0.7466951	2.7208025	0.4664086
H	-1.2744629	3.1222018	-1.1803361
H	-2.4748374	2.7841030	0.0676968
O	-6.0913676	1.3088559	-0.8997323
C	3.5092753	0.2410284	-1.0584539
C	2.5609566	0.3572827	1.2463666
O	4.3937139	1.0775930	-0.4697139
O	3.2041994	-0.7131994	1.7778700
O	2.3372570	1.3738001	1.8680180
O	3.6951975	-0.2867190	-2.1344704
C	5.6135034	1.3114074	-1.2223444
H	5.3739203	1.7584649	-2.1900993
H	6.1972873	1.9950506	-0.6071319
H	6.1423850	0.3678461	-1.3766936
C	3.6766175	-0.5220851	3.1356720
H	2.8396241	-0.2936087	3.8000684
H	4.1481489	-1.4658309	3.4081224
H	4.3952255	0.3008968	3.1639888
H	-2.8188193	-2.8123842	-1.1513699
C	-0.6861938	-3.2593262	0.1090707
H	-0.3261035	-3.9076659	-0.7045675
H	0.0869816	-3.2229553	0.8808001
H	-1.5726683	-3.7387340	0.5363205

TSIV-V

58

Energy = -2765.828904397

C	-0.3238901	-1.4077744	1.1105378
C	1.2339903	-1.4847896	1.1150599
C	1.7019224	0.0003063	1.1528751
C	0.5221285	0.7877952	0.6373905
C	-0.6439784	-0.0219027	0.5843316
C	0.4808014	2.1365361	0.1576684
C	-1.8664456	0.4342297	-0.0453449
H	-0.7411966	-2.2321333	0.5330483
H	-0.7015486	-1.4803998	2.1388515
H	1.8920079	0.2845557	2.1958558
H	2.6213586	0.1530840	0.5880037
Co	-0.2265996	0.7674460	-1.1995422
C	-1.0469849	0.1310387	-2.9794254
H	-2.0500348	-0.2554030	-3.0866039
C	-0.6800559	1.5132281	-3.0588302
H	-1.3423128	2.3414359	-3.2655904
C	0.7284784	1.5794505	-2.8250518
H	1.3175338	2.4851249	-2.7905994
C	0.1218144	-0.6454276	-2.7171454
H	0.1547324	-1.7168397	-2.5800937
C	1.2243939	0.2527582	-2.6173902
H	2.2508189	-0.0108863	-2.4013625
C	-0.4793344	3.1440871	0.7681388
H	-0.3434228	3.1554857	1.8643983
C	-1.9707765	3.0232046	0.5447314
C	-2.6863116	1.6487386	0.4579595
O	-2.6392861	4.0429725	0.5250557
C	-3.9284244	1.9033901	-0.3979309
C	-4.0014927	1.7315763	-1.6970251
H	-4.7160693	2.5177212	0.0282701
C	-3.1519837	1.3649564	1.9196854
H	-2.2806524	1.2518171	2.5730659
H	-3.7704796	2.1885227	2.2898121
H	-3.7368889	0.4417331	1.9524680
C	-2.7556886	-0.7451669	-0.4579652

H	-2.1407844	-1.5686076	-0.8267994
H	-3.3458845	-1.1152020	0.3926245
H	-3.4651151	-0.4911513	-1.2445440
O	-4.1131411	1.5312513	-2.8493522
C	1.7017146	-2.2172328	2.3794022
C	1.7171914	-2.2478129	-0.1238488
O	2.1980388	-3.4449205	2.1108665
O	3.0045701	-1.9463752	-0.4223401
O	1.0633257	-3.0573978	-0.7481866
O	1.6063794	-1.7590981	3.4988328
C	2.6181267	-4.2056789	3.2745976
H	1.7695273	-4.3570654	3.9458355
H	2.9788290	-5.1532492	2.8763670
H	3.4109988	-3.6704274	3.8025150
C	3.5671782	-2.7189018	-1.5133443
H	2.9958981	-2.5495253	-2.4293887
H	4.5906857	-2.3596908	-1.6173730
H	3.5453610	-3.7824220	-1.2631304
H	-0.2252788	4.1524095	0.4271182
C	1.8280179	2.7882607	-0.1215864
H	2.2874930	3.1465282	0.8127642
H	2.5266952	2.0950379	-0.5976963
H	1.7103867	3.6584154	-0.7758009

V

58

Energy = -2765.840700216

C	1.1978557	1.0966258	-0.6477916
C	2.1902393	0.0127870	-0.1209831
C	1.4758626	-1.3527165	-0.3410754
C	0.0183253	-1.0094508	-0.5380335
C	-0.1424313	0.4007718	-0.6990588
C	-1.1286180	-1.8655609	-0.4040007
C	-1.4598142	0.9875474	-0.7766182
H	1.2233175	1.9790326	-0.0064764
H	1.4738414	1.4078289	-1.6644656
H	1.8686610	-1.8121767	-1.2565315
H	1.6615620	-2.0435677	0.4818942
Co	-1.1968575	-0.2602636	0.8392705
C	-2.1769662	0.8766091	2.2472214
H	-2.7445445	1.7663573	2.0153164
C	-2.6933706	-0.4567511	2.2419129
H	-3.7140500	-0.7476925	2.0437450
C	-1.6016535	-1.3236278	2.5594100
H	-1.6516161	-2.4018462	2.6129945
C	-0.7871589	0.8330969	2.5837461
H	-0.1108084	1.6737383	2.6439956
C	-0.4322278	-0.5319197	2.7757070
H	0.5502897	-0.9117215	3.0183866
C	-2.2657126	-1.9020450	-1.4258690
H	-2.2308164	-2.8532577	-1.9734026
C	-2.1442629	-0.8084878	-2.4558643
C	-2.3723368	0.6414814	-1.9806637
O	-1.8811658	-1.0628980	-3.6195049
C	-3.8601924	0.7532289	-1.6589269
C	-4.4035534	0.8435039	-0.4645528
H	-4.5658033	0.7642799	-2.4869385
C	-2.0677667	1.5893442	-3.1657976
H	-1.0001782	1.5629222	-3.4045294
H	-2.6144211	1.2618651	-4.0535911
H	-2.3625790	2.6123994	-2.9243777
C	-1.5170141	2.4727587	-0.4191043
H	-0.9747985	2.6683295	0.5079103
H	-1.0655520	3.0942947	-1.2036310
H	-2.5500145	2.8094732	-0.2894342
O	-4.9473746	0.9576057	0.5692226
C	3.4915867	0.0851087	-0.9326482
C	2.5319418	0.2826925	1.3494831
O	4.3158033	1.0377152	-0.4368353
O	3.1869674	-0.7790163	1.8857288
O	2.3015442	1.3003563	1.9665290
O	3.7400754	-0.5727386	-1.9194376
C	5.5497321	1.2271826	-1.1782169
H	5.3255013	1.5295462	-2.2040065
H	6.0816562	2.0135576	-0.6439307
H	6.1243116	0.2977888	-1.1892419
C	3.6543921	-0.5798314	3.2441997
H	2.8113597	-0.3745178	3.9089181
H	4.1484162	-1.5126640	3.5141862
H	4.3521998	0.2606587	3.2760089
H	-3.2286154	-1.8403513	-0.9070132
C	-0.8872121	-3.2511163	0.1734909
H	-0.5202976	-3.9303988	-0.6100227
H	-0.1547572	-3.2407107	0.9846520
H	-1.8209005	-3.6751597	0.5586460

$Ts_{V\text{-}P1}$

58

Energy = -2765.812090389

C	-0.3238023	-1.5985640	0.6587505
C	1.2379362	-1.5871144	0.7438135
C	1.6646395	-0.0914782	0.8423012
C	0.4149728	0.6996653	0.5380750
C	-0.7214700	-0.1561962	0.4465675
C	0.2698481	2.1496144	0.6543676
C	-1.9852651	0.3594445	0.0043617
H	-0.6498327	-2.2880541	-0.1216258
H	-0.7618744	-1.9416981	1.6045224
H	1.9901914	0.1131035	1.8698480
H	2.5023392	0.1407193	0.1832963
Co	-0.4323223	0.8760736	-1.2355918
C	-1.2725349	0.3660781	-3.0842185
H	-2.3152303	0.1212863	-3.2297168
C	-0.7050198	1.6576284	-3.1550098
H	-1.2254795	2.5834282	-3.3495411
C	0.6968087	1.5468995	-2.8320047
H	1.3758894	2.3833605	-2.7457374
C	-0.2384671	-0.5552003	-2.7099159
H	-0.3471825	-1.6174244	-2.5436971
C	0.9860995	0.1804733	-2.5896676
H	1.9481606	-0.2281265	-2.3130970
C	-0.5312860	2.5337268	1.9030136
H	-0.0045761	2.2002335	2.8073630
C	-1.9328803	1.9450407	1.9484031
C	-2.5791285	1.6973171	0.5622719
O	-2.5100627	1.7270597	2.9982126
C	-2.2183681	2.8540242	-0.3278265
C	-0.9189899	3.1103633	-0.6874906
H	-2.9729541	3.6045839	-0.5607466
C	-4.1037712	1.6311497	0.7538289
H	-4.3876725	0.8241682	1.4317817
H	-4.4424474	2.5700936	1.2011317
H	-4.6153502	1.5054259	-0.2038158
C	-2.9860792	-0.6616614	-0.4985324
H	-2.4790809	-1.4754785	-1.0232903
H	-3.5586155	-1.0977222	0.3311107
H	-3.7012127	-0.2090499	-1.1890253
O	-0.3047321	3.9813033	-1.2877788
C	1.6672211	-2.3534143	2.0062577
C	1.8507253	-2.3022683	-0.4647854
O	1.5937639	-3.6875660	1.7941818
O	3.1961931	-2.1379696	-0.4731150
O	1.2537562	-2.9453868	-1.3022920
O	1.9739626	-1.8529435	3.0655027
C	1.9130531	-4.5111365	2.9479526
H	1.2151505	-4.2981950	3.7611957
H	1.8088969	-5.5375982	2.5985819
H	2.9340194	-4.3071574	3.2792234
C	3.8892799	-2.8333902	-1.5426393
H	3.5408236	-2.4717763	-2.5134278

H 4.9434174 -2.6028734 -1.3932839
H 3.7040487 -3.9075810 -1.4671921
H -0.6272977 3.6257477 1.9483216
C 1.5664546 2.9213520 0.5100998
H 2.2142568 2.7200911 1.3743609
H 2.0980057 2.6253692 -0.3982490
H 1.3780852 3.9941964 0.4529351

P1$_{exo}$
58
Energy = -2765.874645694
C 1.1817398 1.1080709 -0.4681883
C 2.0350422 -0.0183765 0.1915327
C 1.1555946 -1.3028982 0.1734649
C -0.2050577 -0.8956210 -0.3702474
C -0.1880008 0.5027646 -0.6768371
C -1.0691194 -1.9576519 -1.0592457
C -1.3672560 1.2404081 -0.9923214
H 1.1960807 2.0024926 0.1570889
H 1.5937838 1.3864453 -1.4467069
H 1.6248402 -2.0284050 -0.4968644
H 1.1035672 -1.7694732 1.1589098
Co -1.4928488 0.3126705 0.8190475
C -2.1175134 1.7903947 2.1446546
H -2.5080028 2.7567625 1.8557956
C -2.8765071 0.5955611 2.3061871
H -3.9434788 0.4971308 2.1642596
C -1.9785479 -0.4707403 2.6545824
H -2.2522250 -1.5063899 2.8026195
C -0.7464102 1.4775510 2.3972345
H 0.0923967 2.1560314 2.3422717
C -0.6674695 0.0870767 2.7151574
H 0.2389161 -0.4593387 2.9384004
C -1.2843332 -1.6140855 -2.5500026
H -0.3371744 -1.6226681 -3.1027081
C -1.9744826 -0.2816204 -2.8077153
C -2.5561065 0.4448682 -1.5843448
O -2.0104799 0.2114933 -3.9228760
C -2.9167487 -0.4542619 -0.3957095
C -2.4381262 -1.8290134 -0.3453340
H -3.9363295 -0.3269849 -0.0343909
C -3.7426140 1.3198905 -1.9872717
H -3.4771476 1.9992396 -2.8003052
H -4.5616829 0.6808683 -2.3318807
H -4.0975442 1.8976707 -1.1273182
C -1.2822252 2.7276640 -1.2189455
H -0.5020972 3.1784713 -0.6001805
H -1.0501349 2.9380110 -2.2726751
H -2.2276448 3.2228884 -0.9856755
O -2.9826349 -2.7606474 0.2450322
C 3.2909129 -0.2277144 -0.6726479
C 2.4942383 0.3844307 1.5947964
O 4.2295920 0.7007679 -0.3783746
O 3.0695302 -0.6731455 2.2182867
O 2.3908267 1.4809912 2.1031237
O 3.4151490 -1.0595002 -1.5448355
C 5.4302656 0.6408425 -1.1937591
H 5.1748621 0.7996423 -2.2442276
H 6.0660505 1.4417208 -0.8182799
H 5.9107421 -0.3334944 -1.0777224
C 3.5981832 -0.3883083 3.5396593
H 2.7946940 -0.0555092 4.2016410
H 4.0244937 -1.3301782 3.8830072
H 4.3612515 0.3910877 3.4739129
H -1.9217584 -2.3861685 -3.0053299
C -0.5304257 -3.3827279 -0.9180195
H 0.3860443 -3.5221809 -1.5002009
H -0.3313140 -3.6296149 0.1281328
H -1.2853552 -4.0871902 -1.2776569

TS$_{II-IIIexo2}$
58
Energy = -2765.801029417
C 1.3164481 2.2966336 -0.4631730
C -1.0777934 2.3857836 -1.0585376
C -0.6451338 0.9503810 -0.8867168
C 0.7644808 0.8910735 -0.6153392
C -1.3383696 -0.2230039 -0.8627953
C 1.3296296 -0.3397294 -0.5376428
H 1.8192641 2.6351189 -1.3794083
H 2.0093543 2.4152947 0.3730958
H -2.0852259 2.6063652 -0.6946401
H -1.0219245 2.7259580 -2.1007460
Co -0.0043990 -1.7340966 -0.8453471
C 1.3121993 -2.9328568 -1.9127511
H 2.3587279 -3.0487798 -1.6719810
C 0.2519394 -3.7559448 -1.4479098
H 0.3532897 -4.5804248 -0.7571243
C -0.9762515 -3.2711150 -1.9766911
H -1.9562547 -3.6805307 -1.7788044
C 0.7390755 -1.9209689 -2.7585671
H 1.2705385 -1.1265933 -3.2623973
C -0.6690909 -2.1397201 -2.7924924
H -1.3809927 -1.5290145 -3.3289879
C -2.8008942 -0.3497573 -1.1990272
H -3.4208047 0.2788255 -0.5425269
H -2.9938765 -0.0293912 -2.2299767
C -1.0858575 -1.1310982 0.8749752
H -0.7101678 -0.2380442 1.3651982
C -0.2774581 -2.3016903 1.1057220
C 0.8418878 -2.3984953 2.0419850
O -0.9565374 -3.5439379 1.1324756
C 0.8894790 -3.6793452 2.4924933
C -0.2171165 -4.4370524 1.9281102
H 1.5832671 -4.1062994 3.2046868
C 1.6509853 -1.2384900 2.5367252
H 1.4606251 -0.3307942 1.9624282
H 1.3870753 -1.0431650 3.5829398
H 2.7223733 -1.4578761 2.5065584
C 2.8068764 -0.5722511 -0.4081742
H 3.2682079 -0.6772514 -1.4012767
H 3.3062384 0.2693814 0.0920196
H 3.0370592 -1.4874629 0.1454885
O -0.5586672 -5.5949428 2.0421110
C 0.0215175 3.1407503 -0.2433497
C 0.2117022 4.5794822 -0.7075801
O -0.2230661 5.0586905 -1.7327102
O 1.0014166 5.2547791 0.1653446
C -0.3663159 3.0933836 1.2382900
O 0.1402553 2.3889378 2.0866477
O -1.4155749 3.9176039 1.4781080
C 1.2791323 6.6306716 -0.2010617
H 1.9121535 7.0148738 0.5982368
H 1.7960406 6.6652917 -1.1633504
H 0.3450923 7.1939900 -0.2693462
C -1.8883276 3.9224169 2.8491277
H -1.0835446 4.2325502 3.5202389
H -2.7099358 4.6378488 2.8634430
H -2.2319745 2.9235629 3.1302866
H -3.1500939 -1.3812798 -1.0991379
H -2.1535281 -1.3046461 0.9892493

III$_{exo2}$
58
Energy = -2765.825935290
C 0.4563840 1.9483653 1.4483755
C -1.5381885 1.4843601 0.0130059
C -0.9141992 0.1887693 0.5082929
C 0.4210846 0.5012744 1.0309107
C -1.5665739 -1.0297251 0.6519953

C	1.3137707	-0.4184367	0.6212715
H	1.4463078	2.4068253	1.4401814
H	0.0042811	2.1143955	2.4334802
H	-2.4825688	1.6595997	0.5426875
H	-1.7443493	1.5109521	-1.0583514
Co	0.1582793	-1.4674736	-0.5635114
C	1.5851586	-1.9305323	-1.9642861
H	2.6022896	-2.2036992	-1.7196950
C	0.4842445	-2.8300278	-2.0972938
H	0.5203020	-3.8960576	-1.9233342
C	-0.6794377	-2.0764168	-2.4061636
H	-1.6760348	-2.4768223	-2.5232708
C	1.0977531	-0.6056761	-2.2476502
H	1.6645235	0.3132001	-2.2197481
C	-0.2885924	-0.7002614	-2.5063058
H	-0.9365484	0.1417083	-2.7042757
C	-2.9537330	-1.2458925	0.1044812
H	-3.6973551	-1.0358088	0.8881405
H	-3.1634378	-0.5960706	-0.7495163
C	-1.0319722	-2.0753368	1.6234230
H	-0.3665707	-1.6037673	2.3509037
C	-0.2453786	-3.0077872	0.7286550
C	0.8514040	-3.8465812	1.2204513
O	-1.1565235	-3.9139050	0.0757013
C	0.6509270	-5.1204177	0.7971915
C	-0.6049420	-5.1960390	0.0632383
H	1.2808371	-5.9845055	0.9656745
C	1.9737650	-3.3508249	2.0773365
H	1.7691501	-2.3503376	2.4649111
H	2.1412862	-4.0325213	2.9172272
H	2.9065300	-3.3030939	1.5044839
C	2.8040002	-0.2932327	0.6853327
H	3.1865025	0.0806349	-0.2748839
H	3.1200913	0.4101112	1.4672242
H	3.3007309	-1.2508079	0.8638699
O	-1.1633561	-6.1169573	-0.4993772
C	-0.4905052	2.5915186	0.3781643
C	0.3151869	2.9797328	-0.8664089
O	0.1712163	2.5294553	-1.9841163
O	1.2517611	3.9052045	-0.5508208
C	-1.2170750	3.8212858	0.9256667
O	-1.3932939	4.0727627	2.0975476
O	-1.7040694	4.5749780	-0.0901784
C	2.0608467	4.3608632	-1.6650173
H	2.7300368	5.1092366	-1.2419310
H	2.6242086	3.5240155	-2.0857074
H	1.4207919	4.7940802	-2.4374871
C	-2.4577792	5.7459081	0.3215713
H	-1.8226199	6.4065967	0.9165485
H	-2.7644782	6.2256116	-0.6071945
H	-3.3247514	5.4426310	0.9135482
H	-3.0848931	-2.2867954	-0.2020645
H	-1.8444243	-2.5982652	2.1470964

$TS_{III\text{-}P2exo2}$

58

Energy = -2765.790757850

C	-1.4728290	1.7052356	0.6266861
C	-0.1892180	1.8424475	-1.4841007
C	-0.4315855	0.3827358	-1.1359135
C	-1.0277461	0.3332076	0.2064027
C	-0.3263592	-0.7285518	-2.0155468
C	-0.5886881	-0.7637645	0.8804127
H	-1.4486556	1.8877828	1.7010094
H	-2.4832786	1.9241907	0.2516975
H	-0.9166614	2.1742677	-2.2352107
H	0.8110592	2.0645256	-1.8611976
Co	0.8306958	-1.0677598	-0.4276234
C	2.3157783	-2.1187133	0.5995617
H	2.0944966	-2.9070766	1.3059485
C	2.5176513	-2.2879757	-0.7956418
H	2.4655949	-3.2185690	-1.3420272
C	2.6996219	-0.9825127	-1.3421138
H	2.8413825	-0.7500540	-2.3896771
C	2.4960353	-0.7186632	0.9228626
H	2.4061385	-0.2913867	1.9122729
C	2.7484497	-0.0202862	-0.2658502
H	2.8907381	1.0457703	-0.3766172
C	0.1491964	-0.5409802	-3.4337057
H	-0.7039714	-0.3387871	-4.0989718
H	0.8472927	0.2953224	-3.5238111
C	-1.1595449	-1.9573577	-1.7325972
H	-2.2210980	-1.8135488	-1.9947190
C	-0.9860222	-2.3508278	-0.2525205
C	-2.2687391	-2.6486725	0.4741738
O	-0.2069751	-3.5481929	-0.0838905
C	-2.1689687	-3.8590504	1.0595021
C	-0.8634388	-4.4424068	0.7661109
H	-2.9241143	-4.3789513	1.6348034
C	-3.4663392	-1.7573277	0.4653514
H	-3.3006148	-0.8615458	1.0733831
H	-3.6874227	-1.4058873	-0.5494385
H	-4.3408363	-2.2875882	0.8507229
C	-0.6447771	-1.0740403	2.3393796
H	-0.0131857	-0.3566538	2.8772675
H	-1.6605786	-0.9991390	2.7478323
H	-0.2688846	-2.0797231	2.5470041
O	-0.3398065	-5.4753276	1.1201879
C	-0.4582693	2.6127766	-0.1576812
C	0.8705868	2.8326317	0.5753476
O	1.8543471	3.2991561	0.0359088
O	0.8378588	2.4696679	1.8761329
C	-1.1045365	3.9759868	-0.4189361
O	-1.8128408	4.2400349	-1.3666599
O	-0.8463627	4.8380714	0.5920381
C	2.0670435	2.7270679	2.6035149
H	1.8870879	2.3446669	3.6079461
H	2.9023826	2.2095150	2.1269862
H	2.2669018	3.8012017	2.6209672
C	-1.4578731	6.1478120	0.4527149
H	-2.5457366	6.0502328	0.4193227
H	-1.1393637	6.7034338	1.3339577
H	-1.1048981	6.6262737	-0.4638128
H	0.6450796	-1.4458628	-3.8006425
H	-0.7882902	-2.7993390	-2.3240763

II_{endo}

58

Energy = -2765.8059269

C	1.5495803	1.6832893	-0.7754259
C	-0.8547834	2.2788984	-0.8063111
C	-0.7007729	0.7718039	-0.7659656
C	0.7064375	0.4244100	-0.7566897
C	-1.5915927	-0.2335153	-0.7407025
C	1.0188308	-0.8804247	-0.7209389
H	1.8994706	1.9192833	-1.7878341
H	2.4210348	1.6581044	-0.1163293
H	-1.6606583	2.6716979	-0.1849329
H	-1.0241136	2.6176741	-1.8382487
Co	-0.6643555	-1.9911765	-0.7364242
C	0.2490102	-3.5365767	-1.8914061
H	1.2189068	-3.9734113	-1.7026038
C	-0.9962604	-4.0010159	-1.4127843
H	-1.1472905	-4.8550791	-0.7669070
C	-2.0240856	-3.1220083	-1.8824597
H	-3.0804011	-3.2001205	-1.6669655
C	0.0032785	-2.3534046	-2.6684005
H	0.7430724	-1.7585502	-3.1827016
C	-1.4022615	-2.1158921	-2.6775783
H	-1.8950486	-1.2979022	-3.1810077

C	-3.0812491	-0.0721945	-0.7995067
H	-3.3663725	0.9701712	-0.6053197
H	-3.4837973	-0.3413879	-1.7873626
C	-1.6215485	-2.3188441	1.0133465
H	-2.3685246	-1.5802276	1.2782401
C	-0.2933912	-2.0483910	1.3925506
C	0.7593897	-2.9799510	1.8044965
O	-0.0270953	-0.8093982	1.9740590
C	1.6506412	-2.2765238	2.5414402
C	1.1968426	-0.8925180	2.6521188
H	2.5583302	-2.6323579	3.0100236
C	0.7913453	-4.4415357	1.4950418
H	-0.2081801	-4.8826251	1.5723895
H	1.1514822	-4.6210895	0.4775383
H	1.4560749	-4.9633271	2.1879235
C	2.4001365	-1.4565617	-0.7559699
H	2.6546125	-1.8493050	-1.7520834
H	3.1413479	-0.6845938	-0.5108677
H	2.5305185	-2.2797363	-0.0457260
O	1.6689052	0.0666899	3.2185676
C	0.5462158	2.7931492	-0.3339182
C	0.8457194	4.1316753	-1.0092757
O	1.5307574	4.2936919	-1.9966389
O	0.1703023	5.1335816	-0.3933974
C	0.6759589	2.9897101	1.1833932
O	1.7067176	3.3623000	1.7061941
O	-0.4519391	2.6967481	1.8580502
C	0.3636898	6.4474660	-0.9736180
H	-0.2346805	7.1198456	-0.3592892
H	1.4216630	6.7185929	-0.9362827
H	0.0221837	6.4544689	-2.0121081
C	-0.3368149	2.8088625	3.3029048
H	-0.0755342	3.8352258	3.5734196
H	-1.3231095	2.5409797	3.6820735
H	0.4274293	2.1154924	3.6578027
H	-3.6082369	-0.7026216	-0.0731858
H	-1.9577878	-3.3515450	1.0255936

$TS_{II\text{-}IIIendo1}$

58

Energy = -2765.787986300

C	0.6249615	1.4804531	0.8778853
C	-1.2772161	1.8421156	-0.6738116
C	-0.7477238	0.4300226	-0.7829110
C	0.2817591	0.2147196	0.1398971
C	-1.0644872	-0.6670773	-1.5729211
C	0.7593144	-1.1021843	0.2395252
H	1.6971332	1.6719421	0.9777113
H	0.2034965	1.4793518	1.8918599
H	-2.1656201	1.8710303	-0.0294257
H	-1.5190024	2.3150654	-1.6271333
Co	-0.0811048	-2.2032855	-1.1567502
C	1.2622506	-3.8572024	-1.3283765
H	1.8239174	-4.3320569	-0.5361846
C	-0.0171684	-4.2476241	-1.8055748
H	-0.6258915	-5.0428869	-1.3945660
C	-0.3973093	-3.3922039	-2.8766385
H	-1.3171746	-3.4452556	-3.4414922
C	1.6826471	-2.7280254	-2.1037110
H	2.6080046	-2.1814829	-1.9865753
C	0.6641464	-2.4465514	-3.0627527
H	0.6882903	-1.6455555	-3.7891096
C	-2.1289156	-0.6039755	-2.6278875
H	-2.6238995	0.3744335	-2.6712456
H	-1.7129944	-0.8187631	-3.6199663
C	-1.4748197	-2.5565137	0.2882802
H	-2.4733591	-2.2334618	-0.0006937
C	-0.9381570	-1.8183636	1.4149385
C	-0.2083710	-2.3837866	2.5442899
O	-1.6475463	-0.7196904	1.8660926
C	-0.4101063	-1.5740521	3.6165437
C	-1.3149294	-0.4984132	3.2366484
H	-0.0084016	-1.6716023	4.6159757
C	0.5131088	-3.6895682	2.4767151
H	-0.1547811	-4.4942926	2.8100302
H	0.8116609	-3.9133763	1.4500610
H	1.3953106	-3.6968301	3.1230906
C	2.0835476	-1.3461886	0.9228214
H	2.8771850	-0.9088547	0.2998316
H	2.1430902	-0.8673980	1.9099971
H	2.3197586	-2.4052635	1.0360592
O	-1.7816138	0.4393488	3.8361492
C	-0.0958407	2.5791350	0.0342912
C	0.8667894	3.1295876	-1.0279591
O	0.7783819	2.9753585	-2.2262541
O	1.8751783	3.8166728	-0.4319986
C	-0.5766200	3.7391616	0.9044060
O	-0.4751572	3.8204661	2.1075231
O	-1.1718921	4.6826337	0.1289445
C	2.8481798	4.3837835	-1.3445552
H	3.5647052	4.9030395	-0.7086950
H	3.3336868	3.5890235	-1.9167941
H	2.3561849	5.0768763	-2.0317337
C	-1.6855751	5.8277097	0.8564403
H	-0.8706457	6.3324433	1.3816528
H	-2.1231628	6.4740533	0.0960430
H	-2.4383695	5.5043055	1.5795933
H	-2.8918613	-1.3713134	-2.4414017
H	-1.4318178	-3.6361255	0.4414341

III_{endo1}

58

Energy = -2765.8062047

C	1.3939264	1.5666874	-0.2886926
C	-0.9749495	2.2693993	-0.6427340
C	-0.7948121	0.7710639	-0.7333021
C	0.4896151	0.3903668	-0.4859500
C	-1.6741062	-0.2925880	-1.0676661
C	0.7828358	-1.0564684	-0.4294829
H	1.9840394	1.7662931	-1.1947752
H	2.1005133	1.4500236	0.5374426
H	-1.8067137	2.5773583	-0.0056061
H	-1.1411795	2.7087433	-1.6357338
Co	-0.9279743	-1.9526286	-1.0551202
C	-0.1618146	-3.7810880	-1.8698521
H	0.7870684	-4.2369191	-1.6324218
C	-1.4032385	-4.0494294	-1.2369402
H	-1.5555978	-4.7221773	-0.4033487
C	-2.4162351	-3.2629728	-1.8554673
H	-3.4656089	-3.2553287	-1.5964382
C	-0.3876254	-2.7967617	-2.8811708
H	0.3560482	-2.3748141	-3.5427540
C	-1.7837344	-2.4880240	-2.8749165
H	-2.2707555	-1.7751393	-3.5266988
C	-3.1010629	0.0519426	-1.3760282
H	-3.5496136	0.5202989	-0.4865071
H	-3.1560697	0.8051097	-2.1763806
C	-0.9546388	-1.9230760	0.9534611
H	-1.6025376	-1.1513095	1.3676531
C	0.5058598	-1.5368957	1.0492476
C	1.4028164	-2.6232510	1.6129329
O	0.7220668	-0.4160214	1.9939902
C	2.0309599	-2.1539053	2.7028337
C	1.6241729	-0.7697904	2.9674781
H	2.7057526	-2.6946358	3.3547652
C	1.4759344	-4.0256209	1.1042385
H	0.4754592	-4.4141182	0.8914090
H	2.0481035	-4.0857087	0.1731064
H	1.9595410	-4.6733010	1.8403109
C	2.1508743	-1.3979387	-1.0139351

H	2.2262323	-1.0183132	-2.0380683
H	2.9625531	-0.9444562	-0.4259059
H	2.3263087	-2.4742790	-1.0508612
O	1.9438969	-0.0080581	3.8570553
C	0.3979286	2.7515328	-0.0535450
C	0.8564496	4.0238732	-0.7645681
O	1.7439242	4.0960947	-1.5878621
O	0.0786457	5.0688509	-0.3992940
C	0.3859321	3.0144333	1.4576238
O	1.2861132	3.5961324	2.0274302
O	-0.6742804	2.4608244	2.0740369
C	0.4247196	6.3347181	-1.0174063
H	-0.2858133	7.0528201	-0.6092444
H	1.4505514	6.6051401	-0.7562915
H	0.3307073	6.2607750	-2.1039192
C	-0.6054917	2.4823202	3.5294592
H	-0.5335294	3.5140550	3.8813234
H	-1.5345717	2.0169280	3.8577809
H	0.2631771	1.9053815	3.8551453
H	-3.7091009	-0.8093169	-1.6523833
H	-1.2016720	-2.8968314	1.3825478

$Ts_{III\text{-}P2endo1}$

58

Energy = -2765.7976644

C	-1.3876504	-1.5997334	-0.3113288
C	0.8456065	-1.8236984	-1.4042681
C	0.5182302	-0.3944827	-1.0479382
C	-0.6812562	-0.2800635	-0.4115370
C	1.2209069	0.8405984	-1.2047566
C	-0.9919681	1.0277723	0.1759523
H	-2.1789764	-1.6891987	-1.0679827
H	-1.8443461	-1.7893421	0.6636856
H	1.8496206	-2.1399057	-1.1134616
H	0.7470129	-1.9955480	-2.4852706
Co	0.1588909	2.3208405	-0.8897153
C	-1.1738608	3.9310861	-1.1375861
H	-2.0391770	4.1404802	-0.5239595
C	0.1251087	4.4765455	-0.9733501
H	0.4283117	5.1696812	-0.2006344
C	0.9708323	3.9336111	-1.9835709
H	2.0208236	4.1515612	-2.1246671
C	-1.1558725	3.0487376	-2.2726843
H	-1.9935780	2.4875335	-2.6629058
C	0.1744288	3.0564741	-2.7917656
H	0.5227802	2.4853142	-3.6419697
C	2.5682584	0.8573611	-1.8755289
H	3.2308038	0.0695774	-1.4915416
H	2.4274412	0.6610020	-2.9464175
C	1.3513205	1.5689028	0.6426822
H	2.1024026	0.7882653	0.7545580
C	0.0546064	1.2179185	1.3462644
C	-0.3284765	2.1822415	2.4517587
O	0.2036504	-0.0707148	2.0795235
C	-0.4218197	1.5117820	3.6115171
C	-0.0842485	0.0990518	3.4127675
H	-0.6691147	1.9185458	4.5839225
C	-0.5013988	3.6523706	2.2742230
H	0.4143092	4.0987740	1.8710568
H	-1.2950507	3.8784724	1.5579996
H	-0.7339330	4.1286455	3.2304787
C	-2.4464678	1.2566181	0.5462931
H	-3.0803367	1.1704077	-0.3421020
H	-2.7957263	0.5149659	1.2797968
H	-2.6111646	2.2468709	0.9778912
O	-0.0205652	-0.8160656	4.2077413
C	-0.2504538	-2.6288376	-0.6205007
C	-0.7511000	-3.7911931	-1.4782623
O	-1.7878345	-3.8153034	-2.1061463
O	0.1688839	-4.7848568	-1.5034887
C	0.2180385	-3.1930363	0.7301034
O	-0.5087988	-3.8618541	1.4362688
O	1.4721541	-2.8339893	1.0593017
C	-0.1955599	-5.9357715	-2.3078050
H	0.6396768	-6.6280868	-2.2066722
H	-1.1198996	-6.3764469	-1.9266995
H	-0.3356423	-5.6365485	-3.3497445
C	1.8737620	-3.2192755	2.4058361
H	1.7933147	-4.3027623	2.5197274
H	2.9092556	-2.8898788	2.4914646
H	1.2346902	-2.7102091	3.1311367
H	3.0652035	1.8240780	-1.7718350
H	1.8026313	2.5292593	0.9060378

$Ts_{II\text{-}IIIendo2}$

58

Energy = -2765.8007335

C	1.3738456	2.2439878	-0.1107801
C	-0.9021634	2.3951453	-1.0803492
C	-0.5395758	0.9533184	-0.8364841
C	0.8183067	0.8555780	-0.3754777
C	-1.2585949	-0.2030728	-0.8970644
C	1.3351900	-0.3895592	-0.2342944
H	2.0580969	2.5614794	-0.9089232
H	1.8934141	2.3373660	0.8452576
H	-1.9436472	2.6499388	-0.8649893
H	-0.6931423	2.7109586	-2.1106370
Co	0.0338494	-1.7339116	-0.8445767
C	1.4022607	-3.0562796	-1.6673317
H	2.2926532	-3.3901739	-1.1539601
C	0.1289037	-3.7036387	-1.6559245
H	-0.1008961	-4.6073083	-1.1094512
C	-0.7805180	-2.9406601	-2.4319367
H	-1.8222051	-3.1667758	-2.6115053
C	1.2797755	-1.8884690	-2.4919393
H	2.0610892	-1.1761940	-2.7135453
C	-0.0655525	-1.8109236	-2.9448336
H	-0.4763395	-1.0161786	-3.5513652
C	-2.6593591	-0.3169690	-1.4299407
H	-3.2622526	0.5612348	-1.1595472
H	-2.6634601	-0.3900086	-2.5250217
C	-1.1261550	-1.1585211	0.8086355
H	-0.7406453	-0.3228922	1.3871340
C	-0.3834236	-2.3878849	1.0166104
C	-1.0095746	-3.7035018	1.1654479
O	0.7441936	-2.3696876	1.8598779
C	-0.2334060	-4.4480498	1.9900320
C	0.9008220	-3.6448442	2.4324433
H	-0.3958885	-5.4644731	2.3233095
C	-2.3381184	-4.0583615	0.5759827
H	-2.4722502	-3.5953077	-0.4050322
H	-2.4562665	-5.1409666	0.4801606
H	-3.1426388	-3.6909498	1.2262897
C	2.7300950	-0.6991825	0.2065407
H	3.3522638	-1.0252218	-0.6398226
H	3.2108667	0.1855325	0.6453386
H	2.7425481	-1.5033326	0.9473565
O	1.8459154	-3.8954227	3.1470832
C	0.0943655	3.1417335	-0.1355027
C	0.4242918	4.5445130	-0.6328896
O	0.1833577	4.9829791	-1.7375157
O	1.0952188	5.2353314	0.3222894
C	-0.5225180	3.1996550	1.2655298
O	-0.1873671	2.5361139	2.2222224
O	-1.5604274	4.0756793	1.2858812
C	1.4974806	6.5751797	-0.0603419
H	2.0132068	6.9762289	0.8116513
H	2.1629990	6.5339014	-0.9262899
H	0.6163424	7.1730153	-0.3066000
C	-2.2344828	4.1887085	2.5644641

H	-1.5283914	4.5176970	3.3309945
H	-3.0182794	4.9294188	2.4081178
H	-2.6576730	3.2227787	2.8522122
H	-3.1709199	-1.2072388	-1.0480813
H	-2.2074964	-1.2854265	0.8468206

III$_{endo2}$

58

Energy = -2765.826293

C	0.5480202	2.2481879	1.1712960
C	-1.4663355	1.4396438	-0.0792651
C	-0.7139526	0.2779754	0.5533590
C	0.6124682	0.7608299	0.9496977
C	-1.2617977	-0.9413065	0.9609167
C	1.5336737	-0.1657237	0.6497760
H	1.4956584	2.7748377	1.0511219
H	0.1234421	2.5117477	2.1473080
H	-2.3944875	1.6213840	0.4768541
H	-1.7263275	1.3040471	-1.1306076
Co	0.3776274	-1.4353275	-0.2823077
C	1.7307344	-2.1684396	-1.6338315
H	2.7347516	-2.4664422	-1.3650887
C	0.5787545	-3.0189581	-1.6555834
H	0.5753391	-4.0632175	-1.3798426
C	-0.5427055	-2.2425564	-2.0369374
H	-1.5635569	-2.5903556	-2.1211931
C	1.3091888	-0.8673021	-2.0781883
H	1.9289911	0.0131978	-2.1686839
C	-0.0839929	-0.9092747	-2.3084025
H	-0.6856671	-0.0643120	-2.6092994
C	-2.6908665	-1.2713025	0.6054884
H	-3.3636552	-0.8939627	1.3909062
H	-2.9897855	-0.8166185	-0.3429029
C	-0.5888844	-1.7296530	2.0838614
H	-0.0566310	-1.0504861	2.7556807
C	0.4421700	-2.6083520	1.3885684
C	0.1388577	-4.0351399	1.1598269
O	1.7232605	-2.6032942	2.0261753
C	1.2195505	-4.7742701	1.5049709
C	2.2536721	-3.8915278	2.0331082
H	1.3383398	-5.8482903	1.4411993
C	-1.1880995	-4.5567154	0.7078911
H	-1.5485560	-4.0279505	-0.1789768
H	-1.1354598	-5.6259166	0.4864611
H	-1.9371275	-4.4121791	1.4976635
C	3.0179242	-0.1130717	0.7432131
H	3.4755055	-0.1491044	-0.2540068
H	3.3562620	0.8045139	1.2434130
H	3.3939389	-0.9771225	1.3006596
O	3.3804795	-4.1086810	2.4303477
C	-0.4926065	2.6610387	0.0727041
C	0.2290495	2.9254887	-1.2535565
O	0.0720271	2.3160032	-2.2914833
O	1.1059805	3.9471097	-1.1158107
C	-1.2922508	3.8993450	0.4804455
O	-1.4501072	4.2951329	1.6144547
O	-1.8679561	4.4719284	-0.6056090
C	1.8361504	4.2933052	-2.3203012
H	2.4706181	5.1319214	-2.0356560
H	2.4361170	3.4420297	-2.6517170
H	1.1370556	4.5767562	-3.1109613
C	-2.6915737	5.6333680	-0.3214657
H	-2.0874223	6.4109722	0.1521549
H	-3.0638123	5.9603175	-1.2917464
H	-3.5135886	5.3551457	0.3426768
H	-2.8539782	-2.3489011	0.5336649
H	-1.3244241	-2.3004723	2.6675598

Ts$_{III\text{-}P2endo2}$

58

Energy = -2765.7875758

C	1.5392473	-1.6457846	0.3124482
C	-0.1704143	-1.7867634	-1.4877863
C	0.1283666	-0.3310120	-1.1714874
C	0.9801953	-0.2835509	0.0141059
C	-0.1089301	0.8076471	-1.9917604
C	0.7501034	0.8341406	0.7435528
H	1.7253001	-1.8497192	1.3662080
H	2.4760359	-1.7931182	-0.2434021
H	0.3467802	-2.0802182	-2.4093875
H	-1.2288952	-2.0260577	-1.6089235
Co	-0.9753524	1.0869833	-0.2020774
C	-2.3123408	2.0384187	1.0956490
H	-2.0816832	2.9248179	1.6715258
C	-2.8562577	1.9901112	-0.2174409
H	-3.1549498	2.8248408	-0.8332581
C	-2.9582880	0.6072005	-0.5750464
H	-3.3153571	0.2294491	-1.5244097
C	-2.1796021	0.6784928	1.5701760
H	-1.7761928	0.3936920	2.5326140
C	-2.6142256	-0.1964013	0.5648022
H	-2.6255200	-1.2756574	0.5942481
C	-0.8509447	0.6666988	-3.2963643
H	-0.1492935	0.4573218	-4.1182001
H	-1.5795494	-0.1474411	-3.2638866
C	0.8967372	1.9399580	-1.8928941
H	1.9035672	1.6268978	-2.2011663
C	0.9425903	2.4349162	-0.4558294
C	0.3171431	3.7318001	-0.1052458
O	2.2918020	2.5408332	0.0324501
C	1.1325524	4.3782964	0.7700510
C	2.3948899	3.6644887	0.8705692
H	0.9711580	5.3408567	1.2376187
C	-0.8684878	4.3417498	-0.7894592
H	-1.2460433	3.6910821	-1.5800189
H	-1.6920472	4.5410658	-0.0971482
H	-0.5681600	5.3027253	-1.2244718
C	1.1517563	1.1561378	2.1425556
H	0.7112817	0.4153849	2.8219428
H	2.2392547	1.1400482	2.2676860
H	0.7891940	2.1440793	2.4435749
O	3.4222139	3.8996644	1.4670836
C	0.4425807	-2.5879808	-0.2966005
C	-0.6649332	-2.9671376	0.6927193
O	-1.6897691	-3.5281340	0.3563310
O	-0.3926112	-2.6197545	1.9689966
C	1.1094362	-3.8818731	-0.7778556
O	1.5275361	-4.0811258	-1.8974127
O	1.2401560	-4.7591853	0.2443090
C	-1.4036466	-3.0107439	2.9338457
H	-1.0168794	-2.6799104	3.8972432
H	-2.3530121	-2.5215547	2.7029142
H	-1.5373305	-4.0947742	2.9120259
C	1.9072839	-6.0035119	-0.0966496
H	2.9233585	-5.7989940	-0.4426175
H	1.9149874	-6.5819068	0.8264585
H	1.3496336	-6.5201006	-0.8812982
H	-1.3818473	1.5919360	-3.5463574
H	0.5991264	2.7663071	-2.5476151

P2$_{endo}$

58

Energy = -2765.8937449

C	0.9256702	1.1578759	1.1288098
C	-1.3807684	1.6768643	0.3056233
C	-1.1003964	0.1979588	0.2398468
C	0.2130873	-0.0927900	0.6959541
C	-1.8513940	-0.9216143	-0.2332953
C	0.6107071	-1.4698132	0.6332659
H	1.9503170	1.2432909	0.7653267

H	0.9518031	1.2046292	2.2242908
H	-2.0708721	1.8766847	1.1359226
H	-1.8093387	2.1046085	-0.6025765
Co	-0.0395547	-0.7475985	-1.1485495
C	1.5034516	-1.3339036	-2.3517670
H	2.3896321	-1.8413459	-1.9942711
C	0.2841956	-1.9666364	-2.7662142
H	0.0946904	-3.0285150	-2.8243470
C	-0.6303125	-0.9220184	-3.1047127
H	-1.6556362	-1.0595362	-3.4204467
C	1.3460116	0.0834926	-2.4705882
H	2.0916920	0.8245504	-2.2171734
C	0.0234782	0.3394786	-2.9328730
H	-0.4178699	1.3139071	-3.0831168
C	-3.1478040	-0.6887258	-0.9745986
H	-3.9818041	-0.5611332	-0.2680374
H	-3.0979246	0.2050489	-1.6031602
C	-1.8088283	-2.2095677	0.5725864
H	-2.5569801	-2.2029231	1.3790948
C	-0.4197007	-2.4620031	1.1923345
C	0.0111055	-3.9105896	1.0938858
O	-0.4931534	-2.2314369	2.6491835
C	0.1539333	-4.4166403	2.3262771
C	-0.1487839	-3.3820183	3.3294708
H	0.4516553	-5.4201513	2.6035200
C	0.2269673	-4.5864362	-0.2175383
H	-0.6982822	-4.6020493	-0.8066128
H	0.9611588	-4.0314062	-0.8122294
H	0.5729153	-5.6142023	-0.0830125
C	2.0608113	-1.8032800	0.9152001
H	2.7192237	-1.0204392	0.5288134
H	2.2331906	-1.8899011	1.9967883
H	2.3618545	-2.7518335	0.4600004
O	-0.1233283	-3.4342474	4.5388308
C	0.0221294	2.3158137	0.5982849
C	0.5761750	2.9747380	-0.6708429
O	-0.0483059	3.2361403	-1.6768986
O	1.8877772	3.2846903	-0.5114661
C	-0.1402817	3.4090278	1.6654568
O	0.0219822	3.2567751	2.8559464
O	-0.5537737	4.5699948	1.1045737
C	2.4800302	4.0027109	-1.6236966
H	3.5164214	4.1714693	-1.3329588
H	2.4196788	3.4027290	-2.5353288
H	1.9537177	4.9479999	-1.7775997
C	-0.7984146	5.6500187	2.0436859
H	0.1174622	5.8810608	2.5929963
H	-1.1129573	6.4924341	1.4287011
H	-1.5825612	5.3611969	2.7477489
H	-3.3931153	-1.5448381	-1.6129231
H	-2.0707837	-3.0375959	-0.0955848

I^N

63

Energy = -2823.3612133

C	-0.2942191	-1.2156818	4.5513761
N	-1.4367301	-1.1869698	3.7450393
C	-1.7878250	0.1196637	3.3930281
C	-0.8217468	0.9927694	4.0789261
C	0.0521863	0.2086631	4.7538173
C	-2.7734325	0.5125552	2.5596106
C	-3.6737459	-0.3681982	1.7485127
C	-3.1449644	-0.4918163	0.2952530
C	-1.9113847	-1.4137206	0.2181191
C	-1.0905065	-1.1979584	-0.9873212
Co	0.3503900	-2.1445815	-1.9465243
C	-0.2183209	-2.8167331	-3.8671208
C	-0.9307751	-3.5119801	-2.8364756
C	0.0114728	-4.1946791	-2.0084614
C	1.3105360	-3.8905500	-2.5205913
C	1.1670263	-3.0519975	-3.6729933
C	-0.8507381	2.4848221	3.9795098
O	0.2606205	-2.2293783	4.9579350
C	-0.6448087	-0.4358545	-1.8957099
C	-0.3514379	0.8756628	-2.4969920
C	0.9983648	1.4282477	-1.9289080
C	2.1478625	0.3927348	-2.1627042
C	1.8035291	-0.8790053	-1.5069218
C	1.6977354	-1.6990329	-0.5499070
C	2.0704919	-2.2597276	0.7616776
H	2.2582802	0.2700497	-3.2450047
H	3.0829262	0.7998251	-1.7631777
H	-1.1466504	1.5920725	-2.2593813
H	-0.2447368	0.8129752	-3.5850163
H	2.2510354	-4.2116253	-2.0923669
H	-0.2135513	-4.8180585	-1.1544417
H	-2.0029336	-3.4905146	-2.6919548
H	1.9760780	-2.6453802	-4.2644306
H	-0.6620427	-2.1949183	-4.6327154
H	-2.2188224	-2.4644930	0.3027739
H	-1.2556308	-1.2133179	1.0773575
H	-3.9351783	-0.8766391	-0.3600777
H	-2.8699707	0.5033715	-0.0699799
H	-4.6818805	0.0640013	1.7273327
H	-3.7688612	-1.3681995	2.1924967
H	-2.8558787	1.5813738	2.3799227
H	0.8946626	0.5208290	5.3574867
H	-0.8077270	2.8020022	2.9311724
H	-1.7760865	2.8881212	4.4076663
H	-0.0052468	2.9246490	4.5147615
H	2.3661921	-3.3115929	0.6714122
H	2.9030745	-1.7019139	1.2094841
H	1.2201512	-2.2260151	1.4525685
C	1.3437260	2.6945575	-2.7156801
C	0.8240951	1.7358719	-0.4327855
O	1.5836763	2.7015390	-3.9054878
O	-0.2333432	1.9679917	0.1169153
O	2.0140766	1.7252179	0.2095005
O	1.3375326	3.8048131	-1.9426677
C	1.6420187	5.0395081	-2.6441428
H	1.5876573	5.8169254	-1.8829289
H	2.6421125	4.9830402	-3.0806931
H	0.9076486	5.2093953	-3.4351386
C	1.9460853	1.9776009	1.6328027
H	1.3165183	1.2266025	2.1158872
H	2.9753010	1.9061247	1.9838611
H	1.5385813	2.9749272	1.8172466
H	-1.8724690	-2.0279715	3.3952486

$Ts^N_{I\text{-}II}$

63

Energy = -2823.3439105

C	0.0207724	0.1898027	6.2146846
C	-0.5206336	1.6756344	4.5250191
C	0.6961734	2.1616019	5.1986065
C	1.0085760	1.2917496	6.1871377
C	-1.1524948	2.2422352	3.4745576
C	-2.3654669	1.7079779	2.7759704
C	-2.0235699	1.0803987	1.4023230
C	-1.1610736	-0.1890642	1.5345511
C	-0.6824072	-0.6950092	0.2338467
Co	0.1340279	-2.2370383	-0.5722927
C	-1.3368455	-3.7042637	-1.0578816
C	-1.1556639	-3.5926599	0.3495458
C	0.2132685	-3.8820660	0.6578908
C	0.8654887	-4.1881469	-0.5813046
C	-0.0849251	-4.0738973	-1.6347552
C	1.4155524	3.4130228	4.8053703
O	-0.0434760	-0.7957248	6.9382874
C	-0.6363889	-0.4485089	-1.0375178

C	-1.2608411	0.2794159	-2.1785137
C	-0.1043440	0.8501360	-3.0464130
C	0.9178326	-0.3167748	-3.1438070
C	1.0440458	-0.9189182	-1.7866494
C	1.8483117	-1.4351176	-0.9126603
C	3.2572763	-1.5627788	-0.4912986
H	0.5193740	-1.0455266	-3.8601725
H	1.8885656	0.0325886	-3.5034856
H	-1.9038315	1.0844973	-1.8147705
H	-1.8505605	-0.4051078	-2.8002216
H	1.9125591	-4.4323882	-0.6987644
H	0.6616243	-3.8945621	1.6412540
H	-1.9138218	-3.3002709	1.0633751
H	0.1170501	-4.2058727	-2.6890914
H	-2.2529057	-3.5049414	-1.5972962
H	-1.7190249	-0.9768607	2.0625060
H	-0.2883730	0.0272804	2.1698863
H	-2.9544933	0.8366475	0.8758823
H	-1.4881127	1.8125931	0.7867272
H	-3.0777190	2.5279736	2.6144525
H	-2.8822285	0.9649375	3.3976250
H	-0.7117934	3.1485581	3.0657846
H	1.8400740	1.3433137	6.8780228
H	1.7453030	3.3652637	3.7606508
H	0.7628202	4.2889287	4.8997490
H	2.2935397	3.5681639	5.4371091
H	3.5757087	-2.6124596	-0.4957390
H	3.9291486	-0.9942032	-1.1484923
H	3.3906577	-1.1983456	0.5359229
C	-0.6299947	1.2172333	-4.4293293
C	0.4909289	2.0701226	-2.3302955
O	-1.0030116	0.4035797	-5.2503876
O	-0.0679392	2.7233266	-1.4739232
O	1.7391784	2.3436609	-2.7800335
O	-0.6713406	2.5564865	-4.6268114
C	-1.2003129	2.9687952	-5.9139590
H	-1.1643984	4.0575618	-5.8984113
H	-0.5810641	2.5647280	-6.7185740
H	-2.2260382	2.6097888	-6.0283750
C	2.3562911	3.5076197	-2.1775529
H	2.4426929	3.3672688	-1.0970494
H	3.3387326	3.5822907	-2.6432053
H	1.7544067	4.3967560	-2.3823501
N	-0.8801095	0.5024770	5.1914662
H	-1.6444229	-0.1068095	4.9393580

IIa^{N}

63

Energy = -2823.369750775

C	-1.4026247	-1.8067627	-0.2512995
C	0.5530776	-1.3676781	1.1581997
C	0.7290708	-0.6418404	-0.1662758
C	-0.3894357	-1.0384736	-1.0704215
C	1.6091889	0.2216952	-0.7063185
C	-0.3172442	-0.8060122	-2.4098096
H	-1.9750075	-2.5341148	-0.8279735
H	-2.0988159	-1.1371422	0.2671251
H	0.1287946	-0.7178893	1.9337052
H	1.4804887	-1.8056296	1.5343577
Co	0.3700655	0.8569197	-2.0292993
C	-0.4322648	2.8475902	-2.1185455
H	-1.1374708	3.2755134	-1.4186948
C	0.9742370	2.8755320	-1.9771289
H	1.5142628	3.3386839	-1.1649896
C	1.5399696	2.1160846	-3.0580393
H	2.5902971	1.9286745	-3.2332012
C	-0.7646397	2.1143628	-3.2996143
H	-1.7628848	1.9096879	-3.6610623
C	0.4538730	1.6616984	-3.8848839
H	0.5522219	1.0543350	-4.7743028
C	2.9603861	0.6803579	-0.2497643
H	3.6777417	-0.1121358	-0.5135247
H	3.2732575	1.5595237	-0.8264662
C	3.1337891	0.9987102	1.2533037
H	4.2071751	1.0967582	1.4615165
H	2.7751209	0.1571284	1.8572058
C	2.4322381	2.2891156	1.7181445
H	2.7472537	2.4911189	2.7547007
H	2.7960870	3.1382641	1.1210324
C	0.9376458	2.2122677	1.6623758
H	0.4894003	1.2437469	1.8509976
C	0.0862228	3.2311350	1.4235732
C	-1.3758130	3.1396739	1.3164699
N	0.4077818	4.5712209	1.1847561
C	-1.8616426	4.3829450	1.0772012
C	-0.7473529	5.3526242	1.0233273
H	-2.8933372	4.6746512	0.9289484
C	-2.1156496	1.8419593	1.3733586
H	-1.8014635	1.2023863	0.5387736
H	-1.9072162	1.2892140	2.2959459
H	-3.1941779	2.0023611	1.3025284
C	-1.0723215	-1.4119402	-3.5370826
H	-0.3753655	-1.8313807	-4.2748749
H	-1.7265208	-2.2270060	-3.1985023
H	-1.6832571	-0.6702542	-4.0667371
O	-0.7607299	6.5676106	0.8713815
C	-0.4960244	-2.4736509	0.8348667
C	0.2239043	-3.7204239	0.3036424
O	1.3685030	-4.0251988	0.5638253
O	-0.5814917	-4.4605909	-0.4960872
C	-1.3181361	-2.7952806	2.0788937
O	-1.9812188	-1.9704543	2.6763806
O	-1.2220595	-4.0919628	2.4489090
C	0.0225744	-5.6798891	-0.9950313
H	0.2981131	-6.3278475	-0.1590440
H	-0.7438586	-6.1436983	-1.6156694
H	0.9141645	-5.4429656	-1.5808518
C	-1.9745808	-4.4476169	3.6384527
H	-1.7766265	-5.5079834	3.7907490
H	-1.6285069	-3.8555713	4.4890543
H	-3.0392377	-4.2639026	3.4747299
H	1.3100699	4.9917462	1.3570640

^{3}IIa^{N}

63

Energy = -2823.378197925

C	-1.4570262	-2.0626655	0.1624821
C	0.7584333	-1.9884892	1.2883939
C	0.6194709	-0.8434130	0.3122757
C	-0.6507651	-0.8842993	-0.3339217
C	1.4342304	0.2023706	-0.0614624
C	-0.8777747	0.1225897	-1.2478195
H	-2.0070284	-2.6005562	-0.6135681
H	-2.1829879	-1.7631706	0.9294207
H	0.5688174	-1.6532306	2.3178484
H	1.7319705	-2.4840289	1.2652820
Co	0.6129785	1.3086889	-1.3869426
C	0.9069140	3.1463555	-2.4826219
H	0.5405489	4.1068929	-2.1500393
C	2.1753672	2.5757444	-2.1780550
H	2.9559800	3.0329466	-1.5847804
C	2.2541758	1.3008115	-2.8214781
H	3.0795722	0.6051523	-2.7547407
C	0.1891492	2.2118088	-3.2793307
H	-0.8126203	2.3449147	-3.6633235
C	1.0335264	1.0751200	-3.5027104
H	0.7676625	0.1806325	-4.0488724
C	2.7559964	0.4758597	0.5937131
H	3.2522460	-0.4612661	0.8887932
H	3.4298115	0.9999836	-0.0941915

C	2.5691524	1.3495643	1.8590867
H	3.5522624	1.5601506	2.2981098
H	2.0008654	0.7803214	2.6065519
C	1.8435847	2.6766179	1.5905115
H	1.9090441	3.2968392	2.4988556
H	2.3746216	3.2319676	0.8047913
C	0.3904011	2.5243055	1.2242435
H	-0.1174758	1.6178155	1.5368629
C	-0.3870331	3.5191705	0.7184173
C	-1.8340162	3.4821867	0.4682508
N	0.0419307	4.7798922	0.3158067
C	-2.1938173	4.6624883	-0.0953290
C	-1.0104741	5.5355521	-0.2245138
H	-3.1822914	4.9741224	-0.4063458
C	-2.7050149	2.3268058	0.8444402
H	-2.2634640	1.3806594	0.5145986
H	-2.8201840	2.2739113	1.9343128
H	-3.6989172	2.4277459	0.4016085
C	-2.1261888	0.1971985	-2.0819171
H	-1.8957959	0.0004077	-3.1382961
H	-2.8868536	-0.5292465	-1.7638720
H	-2.5734865	1.1978764	-2.0461288
O	-0.8988605	6.6649849	-0.6857444
C	-0.3782322	-2.9675799	0.8399827
C	0.1833198	-3.9718205	-0.1747637
O	1.3257206	-4.0261686	-0.5738602
O	-0.7999002	-4.8083729	-0.5952065
C	-0.9361845	-3.7172982	2.0484488
O	-1.9538551	-3.4403507	2.6466139
O	-0.0938161	-4.7134128	2.4180267
C	-0.3752992	-5.8112362	-1.5522819
H	0.4029148	-6.4402665	-1.1125590
H	-1.2712549	-6.3909475	-1.7727331
H	0.0130244	-5.3291079	-2.4529534
C	-0.5035599	-5.4576444	3.5941071
H	0.2737691	-6.2070317	3.7399435
H	-0.5717672	-4.7885648	4.4555736
H	-1.4752527	-5.9260674	3.4190753
H	0.9937357	5.1157804	0.3439342

Ts^{N}_{II}

63

Energy = -2823.367271875

C	-1.3094926	-2.2038761	0.2748254
C	1.0848300	-1.9796221	0.7564797
C	0.6833043	-0.9120848	-0.2416689
C	-0.7517094	-1.0767353	-0.5644066
C	1.3420111	0.0830885	-0.8671727
C	-1.2859707	-0.2896538	-1.5247445
H	-2.0924084	-2.7837340	-0.2171116
H	-1.6990859	-1.8396269	1.2342324
H	1.0429663	-1.6069121	1.7895125
H	2.0755761	-2.4020993	0.5726178
Co	-0.1184104	1.2102595	-1.4694724
C	-0.5429813	3.3257485	-1.5268414
H	-0.9258105	3.9141096	-0.7040233
C	0.8318751	3.0773003	-1.7877681
H	1.6665482	3.4789561	-1.2325944
C	0.9024864	2.1712550	-2.8917718
H	1.7986742	1.7546221	-3.3302360
C	-1.3363759	2.6151344	-2.4641697
H	-2.4159871	2.6012085	-2.5053844
C	-0.4449705	1.8794772	-3.3133556
H	-0.7223396	1.2192388	-4.1232965
C	2.8049052	0.4017662	-0.7205425
H	3.3904740	-0.4559881	-1.0856435
H	3.0827407	1.2512851	-1.3553945
C	3.2561410	0.7026336	0.7271923
H	4.3420954	0.8639898	0.7299238
H	3.0694268	-0.1755216	1.3570009
C	2.5820698	1.9259320	1.3748055
H	3.0922787	2.1252895	2.3313334
H	2.7551004	2.8147709	0.7516001
C	1.1145099	1.7568744	1.6393354
H	0.7519244	0.7507022	1.8174791
C	0.2112755	2.7581275	1.7475887
C	-1.2291611	2.6281124	2.0115100
N	0.4575026	4.1266423	1.6194767
C	-1.7622581	3.8734391	2.0656065
C	-0.7033135	4.8812293	1.8498577
H	-2.7963864	4.1444992	2.2335771
C	-1.9261434	1.3111347	2.1379482
H	-1.8467594	0.7464984	1.2004919
H	-1.4767185	0.6955243	2.9257013
H	-2.9841000	1.4529976	2.3713601
C	-2.6473940	-0.4176621	-2.1330197
H	-2.6047231	-0.3412974	-3.2268562
H	-3.1109363	-1.3823541	-1.8845621
H	-3.3223915	0.3776220	-1.7883069
O	-0.7598367	6.1045463	1.8486242
C	-0.0372161	-3.0543596	0.5869269
C	0.3249834	-3.9901400	-0.5728812
O	1.4338222	-4.1344238	-1.0410764
O	-0.7674933	-4.6587772	-1.0186898
C	-0.2097206	-3.8315350	1.8888508
O	-0.6755132	-3.3554303	2.9045786
O	0.2570388	-5.0979489	1.7997869
C	-0.5016183	-5.6021704	-2.0859055
H	0.2034647	-6.3636769	-1.7425848
H	-1.4696359	-6.0423460	-2.3244946
H	-0.0818643	-5.0813746	-2.9501287
C	0.1619243	-5.8737733	3.0228383
H	0.5816772	-6.8474796	2.7727104
H	0.7350304	-5.3895992	3.8172919
H	-0.8835259	-5.9610527	3.3285832
H	1.3710377	4.5540018	1.5653749

II^{N}

63

Energy = -2823.402672616

C	1.2933245	2.0544810	-1.1009581
C	-1.1651560	2.1849199	-1.1987612
C	-0.7385962	0.7347807	-1.0980282
C	0.7084889	0.6553461	-1.0658190
C	-1.4115467	-0.4216809	-0.9591250
C	1.2572688	-0.5709245	-0.9420395
H	1.5679593	2.3548937	-2.1214339
H	2.1598994	2.1949883	-0.4510852
H	-2.0752212	2.4396002	-0.6511123
H	-1.2972934	2.5061357	-2.2393329
Co	-0.1336193	-1.9587630	-0.8574151
C	0.9807174	-3.3156375	-2.0315920
H	2.0387504	-3.4950428	-1.9085178
C	-0.0648990	-4.0636844	-1.4299345
H	0.0879405	-4.9029675	-0.7671648
C	-1.3137269	-3.5087518	-1.8116607
H	-2.2932312	-3.8607439	-1.5182221
C	0.3766430	-2.2897913	-2.8291238
H	0.8880001	-1.5494269	-3.4264083
C	-1.0389052	-2.4091890	-2.6833854
H	-1.7690887	-1.7723393	-3.1607267
C	-2.8847910	-0.5853565	-0.7515596
H	-3.4197074	0.3010072	-1.1198896
H	-3.2728211	-1.4481312	-1.3102488
C	-3.1857126	-0.7880372	0.7477941
H	-4.2403755	-1.0451186	0.9049594
H	-2.9951101	0.1567335	1.2739692
C	-2.2745706	-1.8719929	1.3334333
H	-2.4304366	-1.9458599	2.4203101
H	-2.5366441	-2.8483852	0.9077507

C	-0.8182596	-1.5582326	1.0706806
H	-0.5211307	-0.5344995	1.2926599
C	0.2089479	-2.5026087	1.2752019
C	1.5598335	-2.2341815	1.8151324
N	-0.0136325	-3.8678293	1.5268865
C	2.1149739	-3.4200142	2.1721877
C	1.1503926	-4.5121151	1.9575530
H	3.0881525	-3.5808245	2.6176543
C	2.0839063	-0.8652929	2.1117856
H	1.7839456	-0.1283106	1.3651749
H	1.6730878	-0.5273228	3.0721195
H	3.1735236	-0.8753387	2.1996983
C	2.7281269	-0.8613688	-1.0096175
H	3.0182936	-1.1754438	-2.0228157
H	3.3220551	0.0302238	-0.7648778
H	3.0237637	-1.6691698	-0.3321642
O	1.2600139	-5.7234663	2.1215078
C	0.0837327	2.9243689	-0.6267763
C	0.2053806	4.3533376	-1.1438224
O	-0.3408082	4.7981153	-2.1305888
O	1.0739690	5.0636892	-0.3801377
C	0.0184587	2.9118607	0.9040251
O	0.7710967	2.3238532	1.6515131
O	-1.0464851	3.6349589	1.3357236
C	1.2993439	6.4276586	-0.8189559
H	2.0069169	6.8430159	-0.1019688
H	1.7150971	6.4323096	-1.8296975
H	0.3579284	6.9827951	-0.8104774
C	-1.2085240	3.6778030	2.7749768
H	-0.3182702	4.1093372	3.2393992
H	-2.0834679	4.3048660	2.9443548
H	-1.3677976	2.6686101	3.1642614
H	-0.8201047	-4.3818461	1.2047309

$Ts^{N}_{II\text{-}III}$

63

Energy = -2823.395070937

C	1.3690908	2.2901308	-0.7706631
C	-1.0846938	2.3979833	-0.9688149
C	-0.6455523	0.9597779	-0.8331105
C	0.7848640	0.8893841	-0.8282581
C	-1.3354816	-0.2033264	-0.6185955
C	1.3373714	-0.3529608	-0.8440848
H	1.7141349	2.6288193	-1.7568912
H	2.1917817	2.4006176	-0.0601294
H	-2.0227582	2.6469866	-0.4672333
H	-1.1682239	2.7171248	-2.0157379
Co	-0.0384114	-1.7218478	-0.9182835
C	1.0473589	-2.9024145	-2.2407120
H	2.1197414	-3.0264544	-2.2035524
C	0.0931269	-3.7413015	-1.6104161
H	0.3337726	-4.5881272	-0.9820517
C	-1.2109871	-3.2399364	-1.8829695
H	-2.1491449	-3.6667733	-1.5534016
C	0.3285255	-1.8714065	-2.9442556
H	0.7600053	-1.0663327	-3.5215509
C	-1.0578893	-2.0834730	-2.7124381
H	-1.8561910	-1.4544088	-3.0801729
C	-2.8404760	-0.2616925	-0.5498470
H	-3.2849883	0.5725012	-1.1043815
H	-3.2243088	-1.1902833	-0.9914336
C	-3.1925618	-0.2242202	0.9456869
H	-4.2451351	-0.4534273	1.1465299
H	-2.9822361	0.7778161	1.3417325
C	-2.2508802	-1.2499077	1.5758487
H	-2.2090965	-1.1752435	2.6693236
H	-2.6014686	-2.2598380	1.3387463
C	-0.8366600	-1.0568039	1.0315920
H	-0.3317612	-0.1696122	1.4082826
C	0.0602543	-2.2086035	1.0813467
C	1.3620528	-2.1884350	1.7825300
N	-0.4303508	-3.5298370	1.3106643
C	1.6679698	-3.4547094	2.1679914
C	0.5726078	-4.3646923	1.8106781
H	2.5490389	-3.7796496	2.7068212
C	2.0942893	-0.9455265	2.1900222
H	1.9032703	-0.1025688	1.5255427
H	1.7602564	-0.6468076	3.1923442
H	3.1716713	-1.1269804	2.2430096
C	2.8122545	-0.6108150	-0.9387229
H	3.1084354	-0.7735170	-1.9851501
H	3.3983439	0.2408402	-0.5661192
H	3.1055811	-1.5058707	-0.3807747
O	0.4826334	-5.5883759	1.9031380
C	0.1338584	3.1398231	-0.3340811
C	0.2561768	4.5823542	-0.8087963
O	-0.2862730	5.0542914	-1.7848629
O	1.1177538	5.2693613	-0.0175826
C	-0.0097710	3.0739587	1.1909250
O	0.6721339	2.4139015	1.9465434
O	-1.0639100	3.8240764	1.5979806
C	1.3413362	6.6483304	-0.4096637
H	2.0442314	7.0412798	0.3242460
H	1.7617753	6.6875437	-1.4176412
H	0.3980597	7.1997688	-0.3868318
C	-1.3143460	3.7991126	3.0259205
H	-0.4361175	4.1608834	3.5661900
H	-2.1683551	4.4588285	3.1761910
H	-1.5443527	2.7797119	3.3471380
H	-1.1829950	-3.9301164	0.7683730

III^{N}

63

Energy = -2823.405709902

C	1.5571293	2.0714278	-0.0016355
C	-0.6322467	1.7046555	-1.1354369
C	-0.2475000	0.4618859	-0.3689481
C	1.1827374	0.6028117	-0.0639620
C	-1.0753223	-0.5051138	0.1866060
C	1.8139630	-0.5654199	-0.2645371
H	2.3365805	2.3234944	-0.7305653
H	1.8849847	2.4044536	0.9869157
H	-1.6967908	1.9428225	-1.1416780
H	-0.2723973	1.6852037	-2.1687777
Co	0.3206789	-1.5795050	-0.9965618
C	1.4438986	-2.5788948	-2.4098351
H	2.4438253	-2.9475637	-2.2300073
C	0.2365334	-3.3055093	-2.1936455
H	0.1721539	-4.3044054	-1.7850705
C	-0.8574042	-2.4687120	-2.5384711
H	-1.9065204	-2.7274441	-2.4864224
C	1.0899520	-1.2926783	-2.9515512
H	1.7750388	-0.4961403	-3.2072896
C	-0.3202899	-1.2250419	-3.0108995
H	-0.9001713	-0.3675127	-3.3249297
C	-2.5854123	-0.5206217	0.1132093
H	-3.0025003	0.3178002	-0.4521262
H	-2.9505865	-1.4437212	-0.3546785
C	-2.9609524	-0.5139198	1.6128534
H	-3.9971007	-0.8181212	1.7909919
H	-2.8354600	0.5023500	2.0063359
C	-1.9352211	-1.4675665	2.2680309
H	-1.7423272	-1.2112976	3.3134309
H	-2.2970537	-2.4997297	2.2360623
C	-0.6514937	-1.3370348	1.3983009
H	0.1534368	-0.8150344	1.9230458
C	-0.0794829	-2.6106673	0.7874363
C	1.0332147	-3.3302264	1.4431381
N	-1.0174140	-3.6645954	0.5032250
C	0.8379279	-4.6699150	1.3300508

C	-0.4427369	-4.9264997	0.6593658
H	1.4837369	-5.4624838	1.6873459
C	2.0961511	-2.6543254	2.2530246
H	2.2933394	-1.6391179	1.9052865
H	1.7647996	-2.5813747	3.2976704
H	3.0289523	-3.2263474	2.2446538
C	3.2856904	-0.8176293	-0.3427567
H	3.6296505	-0.6891599	-1.3793753
H	3.8522669	-0.1149005	0.2828035
H	3.5488069	-1.8375853	-0.0462610
O	-0.9479602	-5.9832179	0.2757661
C	0.2082167	2.7810856	-0.3716507
C	0.4778840	4.0002162	-1.2473355
O	0.4217421	4.0216249	-2.4585653
O	0.8570318	5.0558557	-0.4889713
C	-0.5409322	3.1816930	0.9061365
O	-0.1805147	2.9720023	2.0436989
O	-1.7174505	3.7788129	0.5896450
C	1.1892844	6.2574421	-1.2328876
H	1.4639429	6.9914005	-0.4761528
H	2.0235620	6.0587813	-1.9101437
H	0.3224603	6.5898716	-1.8092045
C	-2.5189185	4.1854036	1.7282158
H	-1.9587493	4.8922435	2.3451921
H	-3.4046902	4.6529704	1.2994037
H	-2.7869706	3.3117880	2.3279588
H	-1.7670029	-3.5490627	-0.1654669

$Ts^{N}_{III\text{-}IV}$

63

Energy = -2823.373443038

C	1.8471159	1.2616301	0.7672359
C	1.8651538	-1.0523244	-0.0268997
C	0.5139002	-0.4386605	-0.3705449
C	0.4732881	0.8832664	0.2468709
C	-0.4552331	-1.1471135	-1.1127029
C	-0.7361011	1.4178887	0.6011855
H	1.8649953	1.2198080	1.8643588
H	2.1462446	2.2656188	0.4555245
H	2.2475183	-1.7181091	-0.8022804
H	1.8360685	-1.6153579	0.9108020
Co	-1.3106726	-0.4975863	0.6881917
C	-1.4602552	-0.4291509	2.8633666
H	-1.1456266	0.4104397	3.4670794
C	-2.7286618	-0.5270026	2.1779873
H	-3.5373240	0.1899816	2.2311345
C	-2.7489548	-1.7790853	1.4907374
H	-3.5749055	-2.1990090	0.9335338
C	-0.6927782	-1.5612542	2.5600233
H	0.3245993	-1.7513352	2.8737388
C	-1.4685180	-2.3744327	1.6625942
H	-1.1483247	-3.3129693	1.2299636
C	-0.1821900	-2.5804060	-1.5742774
H	0.8152422	-2.6595915	-2.0242508
H	-0.1957156	-3.2831272	-0.7349502
C	-1.2934829	-2.8913561	-2.6014400
H	-1.6092850	-3.9385379	-2.5781826
H	-0.9336887	-2.6793921	-3.6152580
C	-2.4234992	-1.9166899	-2.2399879
H	-3.1516836	-1.7642288	-3.0406625
H	-2.9566500	-2.2884866	-1.3561082
C	-1.6763356	-0.6243930	-1.8714035
H	-1.3933103	-0.1010438	-2.8018548
C	-2.3828615	0.2899323	-0.8957077
C	-2.0244662	1.7556921	-0.8975702
C	-3.1718971	2.4562501	-0.5024503
C	-4.2711334	1.5497045	-0.3092060
H	-3.2646247	3.5294386	-0.4029532
C	-1.0678106	2.3582585	-1.9101272
H	-0.1625598	1.7617906	-2.0464366
H	-1.5811161	2.4580891	-2.8754107
H	-0.7667839	3.3606371	-1.5895893
C	-0.9263648	2.5324769	1.5735852
H	-0.3359802	2.3803085	2.4875209
H	-0.6151948	3.4890142	1.1314799
H	-1.9848942	2.6292595	1.8378754
O	-5.4262087	1.7044315	0.0900545
C	2.7869858	0.1801163	0.1745401
C	3.9245109	-0.1201196	1.1479758
O	3.9153115	-0.9981103	1.9850583
C	3.3377149	0.6497435	-1.1775285
O	3.0978442	1.7084223	-1.7158743
O	4.1229169	-0.3119198	-1.7229908
O	4.9265272	0.7777031	1.0056960
C	4.7053416	0.0337514	-3.0061809
H	5.3314747	0.9233262	-2.9023067
H	5.2992972	-0.8340280	-3.2912538
H	3.9152480	0.2278800	-3.7358640
C	6.0334690	0.6150992	1.9314956
H	6.4869327	-0.3701578	1.7991714
H	6.7343192	1.4088461	1.6757279
H	5.6783011	0.7189647	2.9596324
N	-3.7762963	0.2769836	-0.7444181
H	-4.2903296	-0.5529389	-0.4794409

IV^{N}

63

Energy = -2823.4172912

C	1.6760923	-1.3450420	0.2454401
C	1.6085004	0.8804488	1.3043148
C	0.2154793	0.4203912	0.9508729
C	0.2420623	-0.8596502	0.3246793
C	-1.0146010	1.1237785	1.0940453
C	-0.9268909	-1.4561538	-0.2689589
H	1.9437799	-1.8306794	-0.6907977
H	1.8387060	-2.0631733	1.0601101
H	1.7767683	0.7362333	2.3789789
H	1.8089936	1.9246133	1.0572625
Co	-0.6656864	0.4948866	-0.8309134
C	0.2189980	1.7633163	-2.2642448
H	1.1724524	2.2629121	-2.1662596
C	-0.0128278	0.4691618	-2.8118145
H	0.7354071	-0.1982004	-3.2159714
C	-1.4188861	0.1895523	-2.7120691
H	-1.9141269	-0.7230952	-3.0114739
C	-1.0353046	2.2696286	-1.8124133
H	-1.1906914	3.2247428	-1.3300628
C	-2.0590869	1.3049870	-2.1027783
H	-3.1166930	1.3980529	-1.9013490
C	-1.0242764	2.6094330	1.4323441
H	-0.5854065	2.7662615	2.4320781
H	-0.4454661	3.2096986	0.7270057
C	-2.5172030	2.9499642	1.4793851
H	-2.9197696	2.9799195	0.4596130
H	-2.7355085	3.9077058	1.9609815
C	-3.1018410	1.7531704	2.2503532
H	-2.9626209	1.9066053	3.3255444
H	-4.1777920	1.6195858	2.0955730
C	-2.2568084	0.5261155	1.8144572
H	-1.9242605	-0.0381633	2.6966367
C	-2.9104966	-0.4423832	0.9002335
C	-2.2781611	-1.7478767	0.4735657
N	-4.0664275	-0.3258963	0.3487172
C	-3.3323921	-2.3478216	-0.4154461
C	-4.4503392	-1.5600363	-0.5715217
H	-3.2563625	-3.3384103	-0.8390616
C	-1.9906891	-2.6257440	1.7257318
H	-1.2407488	-2.1600116	2.3772007
H	-2.9116049	-2.8029819	2.2897269
H	-1.6040071	-3.5939102	1.3951381

C	-0.6178468	-2.5350741	-1.2984532
H	0.2765156	-2.2881286	-1.8745513
H	-0.4505138	-3.5068682	-0.8105642
H	-1.4551660	-2.6572154	-1.9868174
O	-5.5397115	-1.5215089	-1.1336907
C	2.5439671	-0.0722143	0.5059944
C	3.0250820	0.6224253	-0.7737453
O	3.2565482	1.8121812	-0.8568597
C	3.7592566	-0.4633985	1.3571901
O	3.6836898	-0.8200156	2.5143526
O	3.2169085	-0.2435648	-1.7950019
O	4.9178749	-0.3985392	0.6653425
C	3.8009670	0.3434600	-2.9854702
H	3.1450074	1.1202327	-3.3850615
H	4.7743480	0.7770385	-2.7436362
H	3.9015033	-0.4828428	-3.6887022
C	6.1023931	-0.7802463	1.4149234
H	6.0124801	-1.8162393	1.7502043
H	6.9286762	-0.6626597	0.7149086
H	6.2215137	-0.1242700	2.2802955
H	-4.6937562	0.4655128	0.4744888

$Ts^{N}_{IV\text{-}V}$

63

Energy = -2823.397252372

C	-1.0748384	-1.5092886	1.1696374
C	1.3110817	-1.7268021	0.5320648
C	0.8649477	-0.2868867	0.4595726
C	-0.5064918	-0.1537307	0.8087102
C	1.5829287	0.8425157	-0.0306773
C	-1.1930341	1.1105121	0.6484208
H	-2.0587336	-1.7148708	0.7496348
H	-1.1557736	-1.5857703	2.2613412
H	1.9408675	-1.8634498	1.4215107
H	1.8744730	-2.0630493	-0.3403357
Co	-0.1713022	0.5595369	-1.0167326
C	0.1466524	-0.3885650	-2.8600536
H	0.7782437	-1.2518306	-3.0139923
C	-1.2403487	-0.4169561	-2.5380489
H	-1.8533072	-1.2993593	-2.4188187
C	-1.6786050	0.9316886	-2.3712731
H	-2.6780951	1.2420315	-2.1042122
C	0.5541651	0.9829994	-2.8963676
H	1.5556823	1.3359939	-3.0959355
C	-0.5713426	1.8104708	-2.5997265
H	-0.5896205	2.8898779	-2.5510348
C	2.9039426	0.6389112	-0.7727879
H	3.6275045	0.1552959	-0.0989102
H	2.8018478	-0.0155048	-1.6419502
C	3.3938254	2.0714487	-1.1296345
H	3.4115750	2.2430524	-2.2101908
H	4.4147565	2.2301602	-0.7680689
C	2.4094191	3.0338833	-0.4238865
H	2.8952441	3.9334119	-0.0350001
H	1.6086128	3.3448422	-1.1020202
C	1.7810052	2.1586710	0.6907715
H	2.5696829	1.9915894	1.4499210
C	0.6607146	2.8443188	1.4320692
C	-0.8100127	2.3885339	1.4436763
N	0.8763010	3.9110422	2.1064349
C	-1.5965794	3.5904219	0.9153962
C	-1.1883686	4.8470461	0.9389508
H	-2.6232996	3.4755898	0.5856522
C	-1.1736847	2.1311979	2.9431137
H	-0.6026623	1.2774031	3.3276561
H	-0.9304038	3.0206085	3.5269353
H	-2.2399314	1.9161985	3.0489014
C	-2.7110667	0.9308218	0.5457596
H	-2.9495885	0.0188791	-0.0047985
H	-3.1851465	0.8586394	1.5335936
H	-3.1883104	1.7563900	0.0134292
O	-0.9583805	5.9946512	0.8636496
C	-0.0156604	-2.5383047	0.6760269
C	-0.3852040	-3.1826628	-0.6656764
O	0.3520985	-3.3289494	-1.6170367
C	0.1878705	-3.6489577	1.7147766
O	0.0560232	-3.5100785	2.9120693
O	-1.6673491	-3.6282880	-0.6447828
O	0.6000499	-4.7992737	1.1336671
C	-2.0710670	-4.3657710	-1.8261225
H	-1.9729421	-3.7397240	-2.7165363
H	-1.4447922	-5.2543353	-1.9390136
H	-3.1115407	-4.6371598	-1.6500609
C	0.8801413	-5.8862316	2.0546397
H	-0.0200641	-6.1355329	2.6215789
H	1.1915890	-6.7174721	1.4231236
H	1.6763909	-5.5947745	2.7438286
H	1.8567734	4.2092229	2.0542711

V^{N}

63

Energy = -2823.402959546

C	-1.3859813	-1.3362120	0.6898372
C	0.9504586	-1.3094046	1.5312450
C	0.5924109	0.0155445	0.9101217
C	-0.7455797	0.0068594	0.4167251
C	1.3953937	1.1677573	0.6612797
C	-1.2660395	1.1111699	-0.3628775
H	-1.9465987	-1.7484892	-0.1478774
H	-2.0777007	-1.2222779	1.5351426
H	0.9516040	-1.2031286	2.6227700
H	1.9218055	-1.7004807	1.2220465
Co	0.5388966	0.4333730	-1.0317581
C	1.6101386	-1.0105588	-2.1337742
H	2.0414255	-1.9150665	-1.7287584
C	0.2958319	-0.8595025	-2.6641706
H	-0.4563208	-1.6323968	-2.7365362
C	0.1331274	0.5070210	-3.0518697
H	-0.7599400	0.9428583	-3.4747550
C	2.2486340	0.2621789	-2.1963987
H	3.2519427	0.4775636	-1.8591012
C	1.3446802	1.2094880	-2.7705663
H	1.5428843	2.2502004	-2.9769467
C	2.9135768	1.1905845	0.7599802
H	3.2089881	1.1181605	1.8185491
H	3.4050484	0.3674585	0.2379817
C	3.2860675	2.5971747	0.2053766
H	3.6567625	2.5272460	-0.8216119
H	4.0773439	3.0596803	0.8030620
C	1.9715772	3.4356678	0.2520127
H	2.1166688	4.4371594	0.6680174
H	1.5365600	3.5348199	-0.7448629
C	1.0400345	2.5672347	1.1278578
H	1.4445697	2.6395285	2.1560150
C	-0.4100121	2.9428818	1.2830976
C	-1.4525637	2.5311482	0.2329907
N	-0.8186571	3.6468552	2.2732538
C	-1.3801425	3.6360435	-0.8264820
C	-0.9792522	3.5545750	-2.0736410
H	-1.6896300	4.6315482	-0.5144456
C	-2.8655869	2.6138555	0.8760606
H	-2.9873954	1.8129816	1.6132982
H	-2.9831291	3.5670548	1.3923654
H	-3.6360454	2.5228179	0.1083323
C	-2.4463598	0.7162185	-1.2573411
H	-2.2166448	-0.1874609	-1.8246269
H	-3.3493976	0.5142942	-0.6671420
H	-2.6908670	1.5115818	-1.9673864
O	-0.6592901	3.5530938	-3.2046268
C	-0.2008207	-2.2731625	1.1093550

C	0.2802087	-3.2134723	-0.0010173
O	1.4120481	-3.6485698	-0.0802208
C	-0.6490837	-3.1185734	2.3109656
O	-0.8123196	-2.6734963	3.4270568
O	-0.7030518	-3.5526730	-0.8663265
O	-0.8795774	-4.4081335	1.9766723
C	-0.3192852	-4.5398166	-1.8573067
H	0.5000979	-4.1589726	-2.4716711
H	-0.0039800	-5.4596135	-1.3588615
H	-1.2150648	-4.7032788	-2.4559375
C	-1.3333403	-5.2516340	3.0686662
H	-2.2784924	-4.8720245	3.4641471
H	-1.4589490	-6.2399495	2.6280095
H	-0.5837143	-5.2659037	3.8632411
H	-0.0279720	3.8905737	2.8833657

$Ts^{N}_{V\text{-}P1}$

63

Energy = -2823.378837122

C	-1.3995140	-1.4628399	0.2991860
C	1.0323948	-1.3033792	0.8753601
C	0.4562132	0.0614278	0.5746255
C	-0.9331232	-0.0272004	0.2641430
C	1.0395204	1.3439839	0.9288311
C	-1.6545890	1.1238519	-0.1934040
H	-1.9383631	-1.7878532	-0.5909687
H	-2.0723537	-1.5914797	1.1551545
H	1.2878653	-1.3592878	1.9424141
H	1.9330061	-1.5502736	0.3102197
Co	0.1030638	0.7994844	-1.2236625
C	1.2190633	-0.4044639	-2.5180056
H	1.8384019	-1.2297949	-2.1987539
C	-0.1816857	-0.4770324	-2.8161282
H	-0.7927859	-1.3698442	-2.7843126
C	-0.6313859	0.8379873	-3.1771126
H	-1.6435802	1.1117289	-3.4392022
C	1.6100841	0.9505438	-2.6357833
H	2.5757413	1.3680979	-2.3885478
C	0.4663928	1.7210885	-3.0601103
H	0.4519758	2.7915125	-3.2016617
C	2.5419348	1.4567937	1.1548281
H	2.9799304	0.4768974	1.3778455
H	3.0210068	1.8391113	0.2482986
C	2.7180298	2.4458848	2.3414620
H	3.5050353	3.1797844	2.1476693
H	2.9953761	1.8961146	3.2489407
C	1.3416902	3.1156637	2.5424169
H	1.1777592	3.4565414	3.5693606
H	1.2207179	3.9724791	1.8739261
C	0.3560377	2.0009535	2.1391138
H	0.3696720	1.2421900	2.9417513
C	-1.0940854	2.3885528	1.9423453
C	-1.5437949	2.5402250	0.4809078
N	-1.9181153	2.6187137	2.8932988
C	-0.4890594	3.3587834	-0.2160365
C	0.7756820	2.8770353	-0.4264665
H	-0.6799350	4.4130403	-0.4154764
C	-2.8800461	3.3055465	0.4389816
H	-3.6775803	2.7614097	0.9471372
H	-2.7524143	4.2570596	0.9612143
H	-3.1730458	3.5160799	-0.5931221
C	-2.9571044	0.8336678	-0.9146941
H	-2.8841025	-0.0912584	-1.4925966
H	-3.7852138	0.7226572	-0.2019159
H	-3.2216465	1.6391099	-1.6027222
O	1.8423005	3.3130405	-0.8433933
C	-0.1147130	-2.3138638	0.5343547
C	0.2565189	-3.1803029	-0.6732387
O	1.3516939	-3.2702616	-1.1864390
C	-0.3027849	-3.2456420	1.7428431
O	-1.0965310	-3.0744551	2.6420685
O	-0.8227970	-3.8818773	-1.1001859
O	0.5917670	-4.2595731	1.7095469
C	-0.5605291	-4.7878442	-2.2035801
H	-0.2055261	-4.2276353	-3.0723215
H	0.1950470	-5.5206249	-1.9102532
H	-1.5167328	-5.2676433	-2.4093335
C	0.5439193	-5.1587965	2.8493993
H	-0.4441364	-5.6200502	2.9182224
H	1.3145485	-5.9032465	2.6532038
H	0.7541198	-4.6061362	3.7682512
H	-1.4648644	2.4891947	3.8070196

$P1^{N}$

63

Energy = -2823.444015064

C	1.4710222	-0.9961969	-0.8059445
C	1.1661315	1.3539793	-0.0750634
C	-0.1426007	0.5916863	0.1012641
C	0.0273798	-0.7324635	-0.4166479
C	-1.1221683	0.9183654	1.2172924
C	-1.0717802	-1.5981434	-0.6736894
H	1.6106475	-1.0835120	-1.8876580
H	1.8388617	-1.9135176	-0.3378630
H	1.4027931	2.0006658	0.7716297
H	1.1757524	1.9810362	-0.9681579
Co	-1.2169765	0.1879780	-1.6661898
C	-0.0404994	0.9019731	-3.2493331
H	1.0385232	0.9859812	-3.2492404
C	-0.8031711	-0.2342039	-3.6529836
H	-0.4015183	-1.1742936	-4.0081479
C	-2.1896253	0.0612689	-3.4623346
H	-3.0215016	-0.5971239	-3.6704614
C	-0.9531047	1.9111132	-2.8073058
H	-0.6918308	2.8806550	-2.4057459
C	-2.2732783	1.3978702	-2.9380149
H	-3.1747871	1.9079339	-2.6260765
C	-0.7739298	2.0652715	2.1690266
H	0.2629495	1.9639473	2.5158301
H	-0.8942506	3.0427759	1.6935885
C	-1.7447175	1.8498125	3.3409158
H	-2.7255598	2.2431177	3.0589162
H	-1.4254636	2.3639764	4.2527813
C	-1.8186015	0.3130683	3.5244890
H	-1.1759351	-0.0182359	4.3460956
H	-2.8371476	-0.0140265	3.7577073
C	-1.3239560	-0.2954946	2.1768337
H	-0.3294260	-0.7394005	2.3286876
C	-2.1914786	-1.4041323	1.6016871
C	-2.4013397	-1.3697706	0.0877443
N	-2.7281402	-2.3431874	2.2834471
C	-2.7710906	0.0462245	-0.3992015
C	-2.4285582	1.1982936	0.4280641
H	-3.7467903	0.1151396	-0.8803395
C	-3.4903767	-2.3531590	-0.3480384
H	-3.2366484	-3.3829864	-0.0884991
H	-4.4253238	-2.1045564	0.1603483
H	-3.6457574	-2.2750859	-1.4300048
C	-0.8123681	-2.9363063	-1.3200719
H	0.1039301	-2.9182411	-1.9161054
H	-0.7030666	-3.7139593	-0.5509803
H	-1.6348275	-3.2353792	-1.9740644
O	-3.0038625	2.2856766	0.4252416
C	2.2386389	0.2344427	-0.2390562
C	3.3566139	0.6265821	-1.1985619
O	3.2926523	1.5005296	-2.0384784
C	2.7809117	-0.0910701	1.1552311
O	2.4910976	-1.0655196	1.8175602
O	4.4201520	-0.1978142	-1.0515183
O	3.5779844	0.9097949	1.5990549

C	5.5212820	0.0504641	-1.9647516
H	5.1862100	-0.0741293	-2.9974568
H	5.8991807	1.0658865	-1.8236311
H	6.2766144	-0.6902622	-1.7048479
C	4.0916204	0.7318432	2.9441569
H	4.6800676	-0.1871743	3.0003634
H	4.7117850	1.6083104	3.1287247
H	3.2638004	0.6790171	3.6559485
H	-2.5151433	-2.2353353	3.2838357

$Ts^{N}_{III\text{-}P2}$

63

Energy = -2823.375639444

C	1.5184602	1.8368824	0.0720828
C	-0.7623529	1.9079035	-0.8697539
C	-0.5253206	0.5339981	-0.2743733
C	0.8886133	0.4613572	0.1000310
C	-1.4967841	-0.4296459	0.0843488
C	1.3814628	-0.8008406	0.0067843
H	2.1999935	1.9467058	-0.7819760
H	2.0680565	2.0785625	0.9861924
H	-1.7791045	2.2834927	-0.7363905
H	-0.5190292	1.9552678	-1.9349576
Co	-0.1435688	-1.2941997	-1.1211212
C	1.0491809	-1.5796186	-2.9467418
H	2.0912740	-1.3113054	-3.0564208
C	0.5641021	-2.8168976	-2.3699286
H	1.1917850	-3.6347301	-2.0393894
C	-0.8580614	-2.7963758	-2.4012927
H	-1.5330417	-3.5993228	-2.1336791
C	-0.0508624	-0.7880623	-3.2905670
H	-0.0232875	0.2105817	-3.7054407
C	-1.2335159	-1.4995909	-2.8817260
H	-2.2483462	-1.1438624	-3.0053058
C	-2.9949626	-0.2862198	-0.1507040
H	-3.3373191	0.7265958	0.1005971
H	-3.2631658	-0.4533621	-1.1975803
C	-3.6335596	-1.3501149	0.7810266
H	-4.5083383	-1.8309305	0.3334143
H	-3.9618829	-0.8791233	1.7151687
C	-2.4983304	-2.3474086	1.0772518
H	-2.6675386	-2.9575493	1.9683080
H	-2.3614153	-3.0168914	0.2207787
C	-1.2709004	-1.4284277	1.2037058
H	-1.3178380	-0.9300847	2.1862340
C	0.1084450	-2.0892161	1.0212954
C	1.0124083	-1.9755621	2.2301273
N	0.1780991	-3.4787284	0.7269343
C	1.5751350	-3.1767323	2.4826126
C	1.1091913	-4.1695187	1.4975633
H	2.2535556	-3.4275135	3.2884936
C	1.1965734	-0.7195887	3.0257354
H	0.3911905	0.0014792	2.8660396
H	1.2620657	-0.9521393	4.0931576
H	2.1245832	-0.2103017	2.7400870
C	2.7872466	-1.2932157	0.0145687
H	3.3030999	-0.9425152	-0.8891036
H	3.3509389	-0.9320147	0.8837453
H	2.8242262	-2.3870311	0.0175346
O	1.4263274	-5.3447815	1.3422424
C	0.2860939	2.7756809	-0.1032528
C	0.6710546	4.0280543	-0.8844704
O	0.4994912	4.1988896	-2.0722980
O	1.3003877	4.9157978	-0.0765764
C	-0.2789007	3.1451066	1.2724408
O	0.1174769	2.7335239	2.3422154
O	-1.3397956	3.9781141	1.1355514
C	1.7506590	6.1293201	-0.7336223
H	2.2234367	6.7177186	0.0519862
H	2.4632727	5.8838471	-1.5249056
H	0.8966077	6.6585442	-1.1633394
C	-1.9639816	4.3802601	2.3814297
H	-1.2377117	4.8996867	3.0114782
H	-2.7775017	5.0438698	2.0900401
H	-2.3428042	3.5021913	2.9107197
H	-0.2255946	-3.8824257	-0.1048623

$P2^{N}$

63

Energy = -2823.475735995

C	1.8033291	0.1796567	0.6578368
C	-0.0558572	1.5173586	1.6583201
C	-0.5945766	0.4021469	0.8043942
C	0.4644051	-0.3618381	0.2300181
C	-1.8875929	-0.0807995	0.4594613
C	0.1054156	-1.4051807	-0.6850543
H	2.5385286	0.2642943	-0.1418880
H	2.2198174	-0.4733888	1.4359564
H	-0.1563086	1.2493361	2.7172030
H	-0.5315782	2.4863820	1.4972154
Co	-0.7276958	0.3803113	-1.1663690
C	-0.4968615	2.2601385	-2.0682891
H	-0.1512352	3.1603660	-1.5805863
C	0.3031420	1.2868400	-2.7325093
H	1.3789234	1.3085565	-2.8408751
C	-0.5672192	0.2477923	-3.2063437
H	-0.2529674	-0.6429481	-3.7343832
C	-1.8506484	1.8130083	-2.1104661
H	-2.6939327	2.3251748	-1.6672059
C	-1.9061983	0.5746083	-2.8370350
H	-2.8002374	0.0122590	-3.0712904
C	-3.2166117	0.5841120	0.8119682
H	-3.1229448	1.2606736	1.6700818
H	-3.5922064	1.1846303	-0.0215619
C	-4.1801072	-0.5976554	1.0941009
H	-5.2151936	-0.3702150	0.8212256
H	-4.1679707	-0.8427968	2.1634085
C	-3.5902854	-1.7717843	0.2905649
H	-3.9726586	-2.7489779	0.5996994
H	-3.8081086	-1.6484906	-0.7759968
C	-2.0875518	-1.6012369	0.5364404
H	-1.8872783	-1.9039765	1.5763682
C	-1.0896945	-2.3458873	-0.3817582
C	-0.6245630	-3.6814955	0.1995878
C	-0.9022701	-4.6779297	-0.6562105
C	-1.5537337	-4.1369806	-1.8780832
H	-0.6769708	-5.7313694	-0.5390865
C	0.0725970	-3.7572549	1.5183906
H	0.9028809	-3.0405620	1.5596061
H	-0.6029215	-3.5003977	2.3440990
H	0.4652701	-4.7612471	1.6985471
C	1.2026641	-2.0152876	-1.5327604
H	1.8686189	-1.2405243	-1.9225176
H	1.8093935	-2.7215478	-0.9488119
H	0.7856424	-2.5684763	-2.3787162
O	-1.8887051	-4.7264348	-2.9004660
C	1.4642761	1.5791111	1.2869944
C	1.7240192	2.7626153	0.3483588
O	1.1374628	3.8245602	0.4136104
C	2.3077917	1.7545432	2.5579187
O	2.1434037	1.1065880	3.5702022
O	2.7159655	2.5187393	-0.5389741
O	3.2775261	2.6837296	2.4106568
C	3.0818361	3.6531229	-1.3648316
H	2.2315898	3.9658662	-1.9755739
H	3.4007512	4.4842113	-0.7312238
H	3.9005312	3.2964706	-1.9892928
C	4.1253506	2.8755956	3.5745596
H	4.6423560	1.9437483	3.8158375
H	4.8301346	3.6538783	3.2845045

H	3.5193705	3.1895338	4.4275711
N	-1.6927028	-2.7863338	-1.6331420
H	-1.9283306	-2.1241212	-2.3590417

I^{O}

62

Energy = -2843.236304688

C	-0.3801614	-1.1272799	4.5837507
O	-1.5237694	-1.1515823	3.7518077
C	-1.8275724	0.1587802	3.4055281
C	-0.8734567	1.0527654	4.0472104
C	-0.0112423	0.2790739	4.7497018
C	-2.8344462	0.4626030	2.5688779
C	-3.7049649	-0.5082252	1.8368017
C	-3.2045846	-0.6644767	0.3758985
C	-1.9412717	-1.5489232	0.2990550
C	-1.1079544	-1.2675223	-0.8845273
Co	0.3304146	-2.1741109	-1.8867537
C	-0.2563681	-2.8140181	-3.8145137
C	-0.9591275	-3.5242968	-2.7875365
C	-0.0096801	-4.2221267	-1.9797917
C	1.2842538	-3.9113958	-2.4995753
C	1.1302755	-3.0537697	-3.6368205
C	-0.8882082	2.5374852	3.8812638
O	0.1082664	-2.1494108	5.0008187
C	-0.6758406	-0.4732899	-1.7715076
C	-0.4059683	0.8520437	-2.3523359
C	0.9592593	1.4042921	-1.8214801
C	2.1048338	0.3756452	-2.1013180
C	1.7811909	-0.9060705	-1.4544724
C	1.6986714	-1.7416160	-0.5083610
C	2.0943977	-2.3223754	0.7873375
H	2.1839455	0.2676029	-3.1878936
H	3.0498802	0.7806700	-1.7238279
H	-1.1962739	1.5599303	-2.0754759
H	-0.3348767	0.8113898	-3.4444355
H	2.2286066	-4.2405208	-2.0862601
H	-0.2278367	-4.8570977	-1.1326261
H	-2.0296651	-3.5040622	-2.6314701
H	1.9343281	-2.6387718	-4.2294840
H	-0.7066447	-2.1807939	-4.5668934
H	-2.2202877	-2.6088160	0.3420200
H	-1.3141776	-1.3710208	1.1831503
H	-3.9975335	-1.0977536	-0.2444998
H	-2.9765801	0.3258951	-0.0332107
H	-4.7359340	-0.1333258	1.8256304
H	-3.7060930	-1.4819563	2.3377639
H	-2.9579251	1.5171567	2.3339554
H	0.8348648	0.5896707	5.3480139
H	-0.8038199	2.7962750	2.8194658
H	-1.8291549	2.9600572	4.2520222
H	-0.0624491	3.0004334	4.4269500
H	2.4112997	-3.3655786	0.6706151
H	2.9195066	-1.7577768	1.2409908
H	1.2476293	-2.3235981	1.4833906
C	1.2755522	2.6794321	-2.6067703
C	0.8342356	1.7007005	-0.3188798
O	1.4675777	2.7001662	-3.8049342
O	-0.2034363	1.9336188	0.2674785
O	2.0450527	1.6843687	0.2840999
O	1.3049727	3.7810672	-1.8211449
C	1.5857977	5.0226500	-2.5204038
H	1.5664014	5.7914660	-1.7487858
H	2.5667232	4.9673476	-2.9985989
H	0.8201574	5.2047034	-3.2783581
C	2.0276885	1.9372772	1.7075352
H	1.4090851	1.1910259	2.2119910
H	3.0675975	1.8579827	2.0238439
H	1.6348393	2.9379865	1.9059774

$Ts^{O}_{I\text{-}II}$

62

Energy = -2843.224288651

C	1.3318301	2.5811401	-0.1245989
C	-1.1031020	2.7583631	-0.2895808
C	-0.9032929	1.3326727	-0.6756612
C	0.9920970	1.1964189	-0.5576016
C	-1.4653793	0.1758091	-0.8237398
C	1.4257753	-0.0182973	-0.6784935
H	1.5194548	3.2293953	-0.9894859
H	2.2193086	2.5758037	0.5124721
H	-2.0517049	2.8778698	0.2396113
H	-1.0885646	3.4150295	-1.1675648
Co	0.0484341	0.1735113	-2.0132241
C	0.8869667	0.7570517	-3.8869883
H	1.5922407	1.5655535	-4.0230303
C	1.2132156	-0.5891136	-3.5608219
H	2.2114590	-0.9817502	-3.4219296
C	-0.0056867	-1.3302777	-3.4104639
H	-0.0936715	-2.3850483	-3.1924488
C	-0.5349131	0.8620324	-3.9453812
H	-1.0999551	1.7648890	-4.1331692
C	-1.0833045	-0.4202019	-3.6599985
H	-2.1367252	-0.6579204	-3.5972166
C	-2.5918372	-0.6878827	-0.3995775
H	-3.5526336	-0.1727116	-0.5481454
H	-2.6193038	-1.5972428	-1.0109555
C	-2.4535557	-1.0688784	1.0955070
H	-3.1926595	-1.8429920	1.3351033
H	-2.6718353	-0.1888813	1.7095474
C	-1.0346886	-1.5614978	1.4663228
H	-0.3555688	-0.7018601	1.3633501
H	-1.0205445	-1.8883003	2.5099443
C	-0.5277485	-2.6441468	0.5715396
H	-0.3553004	-2.3717419	-0.4688513
C	-0.2263104	-3.9023395	0.9371254
C	0.3130440	-4.9870992	0.1276952
O	-0.3818110	-4.3499555	2.2424290
C	0.4750151	-6.0553288	0.9436226
C	0.0453987	-5.6955859	2.2965069
H	0.8564476	-7.0372270	0.6976498
C	0.6133816	-4.8678672	-1.3322892
H	-0.3046101	-4.6733891	-1.8994349
H	1.2951729	-4.0306441	-1.5212724
H	1.0686895	-5.7838588	-1.7155811
C	2.5043860	-0.9427197	-0.2695918
H	3.0698961	-1.2948513	-1.1412728
H	3.2045364	-0.4589551	0.4242090
H	2.0937993	-1.8325463	0.2250471
O	0.0131110	-6.3201141	3.3289963
C	0.0912856	3.1425879	0.6246661
C	0.1944036	4.6576611	0.7525619
O	0.3470472	5.4027886	-0.1946182
O	0.0906222	5.0788962	2.0337132
C	-0.1124154	2.4638636	1.9878703
O	-1.1927446	2.1781002	2.4613397
O	1.0632042	2.2123280	2.6072468
C	0.1689133	6.5175845	2.2140996
H	-0.6369973	7.0065811	1.6616628
H	0.0615179	6.6734469	3.2868682
H	1.1331679	6.8861205	1.8556842
C	0.9371007	1.5735901	3.9036229
H	1.9593843	1.4498542	4.2597171
H	0.3575424	2.2090640	4.5776104
H	0.4391411	0.6068753	3.7943594

IIa^{O}

62

Energy = -2843.258287721

C	1.7016935	-0.6881601	-1.6088397

C	-0.6060953	-1.4986155	-1.7027368
C	-0.3154444	-1.0556740	-0.2827645
C	1.1197263	-0.7022884	-0.2047495
C	-1.1420467	-0.8779210	0.7955377
C	1.6055607	-0.5454885	1.0408445
H	2.2646775	-1.6059282	-1.8197569
H	2.3480749	0.1731986	-1.7949774
H	-1.6333158	-1.3205601	-2.0241379
H	-0.3687138	-2.5572476	-1.8598853
Co	0.2083922	-1.6151011	1.8020236
C	1.3965150	-2.8134067	3.0575777
H	2.4389822	-3.0496651	2.8975620
C	0.8806123	-1.6384186	3.7021090
H	1.4553611	-0.8361965	4.1417638
C	-0.5525828	-1.7112113	3.6742208
H	-1.2186681	-0.9561682	4.0678817
C	0.2869649	-3.5812698	2.6156639
H	0.3448740	-4.4906624	2.0308864
C	-0.9162476	-2.9222904	3.0051789
H	-1.9219699	-3.2576207	2.7928963
C	-2.6336379	-0.8790956	0.8347376
H	-3.0126729	-1.7739895	0.3150835
H	-2.9840337	-0.9446299	1.8708972
C	-3.2400404	0.3755284	0.1770085
H	-4.3345509	0.2936053	0.1718523
H	-2.9125467	0.4337834	-0.8687750
C	-2.8315229	1.6628772	0.9215097
H	-3.3763499	2.5076101	0.4744475
H	-3.1430244	1.5932026	1.9687789
C	-1.3655104	1.9551568	0.8495633
H	-0.9339364	2.1971345	-0.1184269
C	-0.5310397	2.0165145	1.9083442
C	0.8599184	2.4250550	1.9689368
O	-0.9567225	1.6639536	3.1781475
C	1.2525202	2.3074353	3.2660453
C	0.1460540	1.7895202	4.0557585
H	2.2188529	2.5350721	3.6951410
C	1.6383363	2.9453026	0.8037912
H	1.4845688	2.3286500	-0.0853836
H	1.3132791	3.9636553	0.5562900
H	2.7055385	2.9775620	1.0368834
C	2.9904897	-0.2126212	1.4740258
H	3.5580914	-1.1238941	1.7087613
H	3.5381971	0.3261423	0.6885122
H	2.9937808	0.4061915	2.3793449
O	0.0441262	1.4679253	5.2197396
C	0.4299147	-0.6582532	-2.5115170
C	0.7272472	-1.2840382	-3.8691567
O	0.7390785	-2.4766309	-4.0912361
C	-0.0644739	0.7833666	-2.6642412
O	0.5291201	1.7840205	-2.3181295
O	1.0391730	-0.3426829	-4.7925415
O	-1.2954124	0.8106880	-3.2327726
C	1.3880656	-0.8620910	-6.1023247
H	1.6065244	0.0179234	-6.7062845
H	2.2617871	-1.5137669	-6.0248542
H	0.5481012	-1.4259151	-6.5154741
C	-1.8390622	2.1374186	-3.4459146
H	-1.9627404	2.6511207	-2.4890085
H	-1.1691680	2.7167206	-4.0859491
H	-2.8026698	1.9751677	-3.9279085

Ts^{O}$_{II}$

62

Energy = -2843.242970061

C	1.4572070	2.2889285	-0.7107025
C	-0.9944277	2.2741924	-0.9468948
C	-0.4915324	0.8457551	-0.9397678
C	0.9688752	0.8654569	-0.8999444
C	-1.0623073	-0.3782679	-0.9152275
C	1.5991508	-0.3279274	-0.9610418
H	1.7996147	2.7186170	-1.6619916
H	2.2594432	2.3961619	0.0234768
H	-1.9519233	2.4553727	-0.4579179
H	-1.0726680	2.6536504	-1.9745228
Co	0.3266870	-1.7834762	-1.1019921
C	1.5330661	-2.9672239	-2.3782335
H	2.6118202	-2.9335297	-2.4256776
C	0.7610463	-3.8549041	-1.6058026
H	1.1450837	-4.6106768	-0.9339902
C	-0.6326081	-3.5647142	-1.7927498
H	-1.4517243	-4.0782077	-1.3094152
C	0.6233665	-2.0674132	-3.0422778
H	0.8865753	-1.2588519	-3.7101141
C	-0.7179549	-2.4803743	-2.6991833
H	-1.6227134	-2.0061015	-3.0517026
C	-2.5474869	-0.6516659	-0.8209254
H	-3.0464921	-0.2585395	-1.7216651
H	-2.7330730	-1.7322142	-0.8143978
C	-3.2337331	-0.0394459	0.4192312
H	-4.3239468	-0.1305138	0.3235267
H	-3.0068539	1.0293672	0.4825800
C	-2.8012306	-0.7297336	1.7353447
H	-3.2683643	-0.1964749	2.5752948
H	-3.1718880	-1.7590461	1.7477663
C	-1.3186321	-0.7293571	1.9022296
H	-0.8007958	0.2147442	2.0414327
C	-0.5469362	-1.8338531	1.8290997
C	0.9028677	-1.9506195	1.8620967
O	-1.1012606	-3.0932855	1.6238626
C	1.1955838	-3.2577195	1.5964855
C	-0.0444460	-4.0137739	1.4627758
H	2.1714419	-3.7203952	1.5423578
C	1.8305015	-0.8535610	2.2706784
H	1.5593774	0.1007577	1.8162945
H	1.7779835	-0.7293804	3.3599985
H	2.8613121	-1.0962341	2.0048060
C	3.0896013	-0.5092755	-0.9397205
H	3.4835720	-0.6798160	-1.9522252
H	3.6024990	0.3746294	-0.5338728
H	3.3849348	-1.3799252	-0.3412969
O	-0.2655583	-5.1851455	1.2485528
C	0.1671878	3.0446492	-0.2508836
C	0.2267604	4.5110210	-0.6663862
O	-0.2597172	4.9794964	-1.6729866
O	0.9649325	5.2290662	0.2175599
C	0.0051096	2.9295346	1.2658549
O	0.7588007	2.3635996	2.0314301
O	-1.1484222	3.5216778	1.6651809
C	1.1273250	6.6312016	-0.1178331
H	1.7331797	7.0468238	0.6867739
H	1.6326369	6.7294068	-1.0818518
H	0.1503298	7.1183692	-0.1678521
C	-1.4068752	3.4586417	3.0899059
H	-0.5866248	3.9254838	3.6406199
H	-2.3389541	4.0042513	3.2336604
H	-1.5109250	2.4173669	3.4068458

II^{O}

62

Energy = -2843.281710616

C	1.2681150	1.9852163	-1.0771725
C	-1.1939249	2.1093176	-1.1361185
C	-0.7616388	0.6608424	-1.0402284
C	0.6868338	0.5846676	-1.0328037
C	-1.4295252	-0.4981644	-0.8986838
C	1.2420508	-0.6402041	-0.9247545
H	1.5328505	2.2804991	-2.1016579
H	2.1414104	2.1298807	-0.4371939
H	-2.0932393	2.3623920	-0.5701979

H	-1.3505242	2.4259647	-2.1746710
Co	-0.1407870	-2.0333051	-0.8301453
C	0.9035567	-3.5024420	-1.9152025
H	1.9256102	-3.7913647	-1.7149960
C	-0.2660360	-4.1337832	-1.3940491
H	-0.2743978	-4.9554772	-0.6948461
C	-1.4043229	-3.4493015	-1.8699961
H	-2.4328798	-3.6800341	-1.6317714
C	0.4758302	-2.4333495	-2.7644738
H	1.1066238	-1.7651237	-3.3315758
C	-0.9495510	-2.3849418	-2.7167183
H	-1.5687124	-1.6731598	-3.2427924
C	-2.9004443	-0.6873316	-0.7013982
H	-3.4391458	0.2233628	-0.9983672
H	-3.2803408	-1.4996293	-1.3352849
C	-3.2154508	-1.0122679	0.7758621
H	-4.2595586	-1.3273113	0.8896522
H	-3.0848449	-0.0956207	1.3665711
C	-2.2652189	-2.0855953	1.3240652
H	-2.4232299	-2.1993149	2.4070038
H	-2.4588835	-3.0631818	0.8727682
C	-0.8315317	-1.6818176	1.0815577
H	-0.5898604	-0.6534414	1.3478613
C	0.2685680	-2.5565236	1.2123159
C	1.5632625	-2.2444022	1.8291720
O	0.0433850	-3.9343636	1.3832206
C	2.1248421	-3.4186829	2.2104161
C	1.2081322	-4.5134595	1.9241312
H	3.0730604	-3.5687057	2.7091596
C	2.0452826	-0.8653211	2.1428733
H	1.7551988	-0.1380694	1.3835574
H	1.5872456	-0.5378825	3.0851416
H	3.1301970	-0.8496351	2.2750646
C	2.7127611	-0.9315010	-0.9885424
H	3.0074299	-1.2669069	-1.9932172
H	3.3074874	-0.0367895	-0.7578485
H	3.0075189	-1.7276984	-0.2965622
O	1.2837589	-5.7110591	2.0830187
C	0.0637732	2.8574870	-0.5948001
C	0.1739255	4.2799148	-1.1332477
O	-0.4013015	4.7154857	-2.1073799
O	1.0687950	4.9950744	-0.4052494
C	0.0231858	2.8691843	0.9365049
O	0.7824257	2.2850971	1.6807657
O	-1.0265425	3.6100146	1.3735619
C	1.2847868	6.3535159	-0.8655996
H	2.0161437	6.7738388	-0.1758885
H	1.6682477	6.3459089	-1.8890054
H	0.3459860	6.9121710	-0.8331756
C	-1.1648469	3.6795795	2.8143585
H	-0.2626622	4.1096305	3.2566149
H	-2.0302453	4.3189306	2.9865736
H	-1.3286339	2.6791875	3.2238229

$Ts^{O}_{II\text{-}III}$

62

Energy = -2843.274674052

C	1.3470478	2.3236083	-0.7922884
C	-1.1094041	2.4042144	-0.9543301
C	-0.6529196	0.9694893	-0.8378271
C	0.7796269	0.9160394	-0.8521249
C	-1.3294144	-0.2010241	-0.6296875
C	1.3474604	-0.3181696	-0.8903656
H	1.6704004	2.6756916	-1.7811593
H	2.1807360	2.4382016	-0.0953461
H	-2.0438814	2.6370973	-0.4386078
H	-1.2094576	2.7327645	-1.9968189
Co	-0.0085998	-1.7079393	-0.9365912
C	1.0489651	-2.9332583	-2.2310989
H	2.1186097	-3.0810865	-2.1942792
C	0.0711371	-3.7337243	-1.5801408
H	0.2762929	-4.5644216	-0.9209420
C	-1.2172661	-3.2065176	-1.8603791
H	-2.1549287	-3.5883561	-1.4822779
C	0.3542108	-1.9006683	-2.9554236
H	0.8036903	-1.1189035	-3.5508808
C	-1.0379297	-2.0738439	-2.7176424
H	-1.8194525	-1.4306146	-3.0969443
C	-2.8322908	-0.2873192	-0.5547827
H	-3.2913329	0.5655437	-1.0677444
H	-3.2026919	-1.1988621	-1.0401452
C	-3.1853832	-0.3282805	0.9406276
H	-4.2305708	-0.5998533	1.1256931
H	-3.0096279	0.6620117	1.3810612
C	-2.2146991	-1.3505930	1.5309772
H	-2.1813824	-1.3180596	2.6270580
H	-2.5096573	-2.3639328	1.2447013
C	-0.8094360	-1.0779929	1.0016965
H	-0.3384644	-0.1811160	1.3997607
C	0.1332089	-2.1922667	1.0283025
C	1.4008346	-2.1741270	1.7654137
O	-0.4180183	-3.4912208	1.2053136
C	1.6413031	-3.4341447	2.2119160
C	0.5261355	-4.2972944	1.8593874
H	2.4860606	-3.7806561	2.7926810
C	2.1868039	-0.9456081	2.1104356
H	1.8837125	-0.0776942	1.5244141
H	2.0238130	-0.7078319	3.1688077
H	3.2596152	-1.1112760	1.9744490
C	2.8227874	-0.5561574	-1.0222835
H	3.0937387	-0.7020599	-2.0780748
H	3.4095325	0.2962677	-0.6523335
H	3.1412680	-1.4565748	-0.4874849
O	0.3155845	-5.4792923	2.0357332
C	0.1088565	3.1530945	-0.3273568
C	0.2067906	4.6033514	-0.7836457
O	-0.3624545	5.0844442	-1.7396838
O	1.0802809	5.2865021	-0.0020906
C	-0.0136357	3.0642955	1.1982531
O	0.6793562	2.3929644	1.9341098
O	-1.0629704	3.8056734	1.6308342
C	1.2814161	6.6735555	-0.3775214
H	1.9975621	7.0620540	0.3458868
H	1.6777028	6.7326313	-1.3942789
H	0.3337247	7.2151743	-0.3239795
C	-1.2976316	3.7552734	3.0609559
H	-0.4134082	4.1074029	3.5977728
H	-2.1497892	4.4121922	3.2322244
H	-1.5244941	2.7302692	3.3660971

III^{O}

62

Energy = -2843.286613301

C	1.5292076	2.0679541	0.0204000
C	-0.6459708	1.6510390	-1.1253410
C	-0.2467405	0.4263871	-0.3384664
C	1.1785707	0.5925798	-0.0230265
C	-1.0629098	-0.5483857	0.2149198
C	1.8355032	-0.5648951	-0.2043841
H	2.3134830	2.3194373	-0.7036200
H	1.8410109	2.4217166	1.0069222
H	-1.7143180	1.8709780	-1.1388230
H	-0.2821547	1.6189400	-2.1571541
Co	0.3651701	-1.6126541	-0.9576588
C	1.5240753	-2.5494329	-2.3804806
H	2.5535032	-2.8389573	-2.2226997
C	0.3772076	-3.3493857	-2.0964380
H	0.3929244	-4.3328188	-1.6477620
C	-0.7866505	-2.6044284	-2.4337120
H	-1.8064506	-2.9300670	-2.2909824

C	1.0635996	-1.3042372	-2.9329219
H	1.6817563	-0.4674189	-3.2276551
C	-0.3534029	-1.3427919	-2.9489050
H	-1.0015995	-0.5315430	-3.2534094
C	-2.5667160	-0.6275668	0.1157016
H	-3.0112842	0.1880735	-0.4620492
H	-2.8653677	-1.5772302	-0.3420279
C	-2.9684008	-0.6299192	1.6091316
H	-3.9911585	-0.9847154	1.7679119
H	-2.9008222	0.3923095	2.0017715
C	-1.9124633	-1.5324931	2.2930062
H	-1.7213406	-1.2299274	3.3263478
H	-2.2487979	-2.5720778	2.2986377
C	-0.6351931	-1.3915186	1.4148506
H	0.1882967	-0.8969075	1.9373610
C	-0.0963559	-2.6522808	0.7583541
C	0.9235686	-3.4919123	1.3942351
O	-1.1627164	-3.5490811	0.4037185
C	0.5394052	-4.7909764	1.3023420
C	-0.7722151	-4.8631048	0.6746052
H	1.0698088	-5.6691147	1.6477142
C	2.1317744	-2.9549800	2.0973918
H	2.2229729	-1.8758753	1.9642983
H	2.0577294	-3.1656225	3.1707097
H	3.0489761	-3.4312554	1.7354324
C	3.3168265	-0.7636607	-0.2700647
H	3.6682182	-0.5929097	-1.2984574
H	3.8489171	-0.0571546	0.3810410
H	3.6177705	-1.7792196	0.0024437
O	-1.4843325	-5.8026056	0.3797529
C	0.1747466	2.7527423	-0.3761757
C	0.4389899	3.9565085	-1.2746921
O	0.4008685	3.9499674	-2.4868221
O	0.7912543	5.0345691	-0.5351129
C	-0.5900375	3.1717634	0.8866629
O	-0.2340664	2.9945366	2.0311846
O	-1.7726635	3.7433952	0.5482474
C	1.1164660	6.2239282	-1.3015653
H	1.3696830	6.9787240	-0.5579525
H	1.9629833	6.0224368	-1.9625994
H	0.2530664	6.5303008	-1.8971221
C	-2.5899368	4.1608920	1.6717336
H	-2.0467313	4.8907247	2.2770220
H	-3.4801913	4.6034554	1.2260494
H	-2.8473461	3.2957661	2.2881805

Ts$^{O}_{III\text{-}IV}$

62

Energy = -2843.254315736

C	1.6431520	1.5059049	0.5477363
C	1.6349340	-0.3581374	-1.0800773
C	0.2053786	0.1036366	-0.8251227
C	0.2246160	1.0653782	0.2735776
C	-0.8560197	-0.4149194	-1.5984731
C	-0.8920442	1.1905317	1.0544764
H	1.8462832	1.7012623	1.6017611
H	1.8641442	2.4231910	-0.0136589
H	1.9282930	-0.0607810	-2.0949230
H	1.7646110	-1.4397962	-1.0022099
Co	-1.3072117	-0.6705163	0.4292290
C	-0.7369097	-1.6313387	2.2778254
H	-0.0921122	-1.1843932	3.0221034
C	-2.1580271	-1.3937364	2.1394666
H	-2.7758005	-0.7895554	2.7898452
C	-2.6241787	-2.1732324	1.0348534
H	-3.6420342	-2.2026000	0.6759774
C	-0.3286550	-2.4641928	1.2263541
H	0.6872349	-2.7632074	1.0115019
C	-1.4946101	-2.7827923	0.4380979
H	-1.5066848	-3.4026768	-0.4483936
C	-0.5811766	-1.5056303	-2.6334097
H	0.2630680	-1.2216244	-3.2755549
H	-0.2964313	-2.4480978	-2.1536936
C	-1.8931463	-1.6324484	-3.4419070
H	-2.1076427	-2.6640980	-3.7363121
H	-1.8205854	-1.0393749	-4.3612395
C	-2.9737596	-1.0401950	-2.5227905
H	-3.8781731	-0.7276674	-3.0500817
H	-3.2655476	-1.7668872	-1.7578029
C	-2.2618649	0.1390480	-1.8386534
H	-2.2632882	1.0110360	-2.5167329
C	-2.7495921	0.4702389	-0.4494766
C	-2.5369960	1.8527630	0.0908294
O	-4.0428896	0.0790765	-0.1103822
C	-3.6321446	2.1037028	0.9231359
C	-4.5684533	1.0290941	0.8583966
H	-3.8284728	3.0093807	1.4805699
C	-1.9005813	2.9706215	-0.7146995
H	-1.0319350	2.6307516	-1.2838712
H	-2.6439704	3.3794793	-1.4111634
H	-1.5815014	3.7819381	-0.0526189
C	-0.9319943	1.7724195	2.4268100
H	-0.1891878	1.3036584	3.0866609
H	-0.7269442	2.8515071	2.4039508
H	-1.9283641	1.6412649	2.8630883
O	-5.6409505	0.7949154	1.3753543
C	2.5251377	0.3637402	-0.0217942
C	2.9704483	-0.6176689	1.0710013
O	2.8308783	-1.8222998	1.0536422
C	3.7756822	0.9233384	-0.7144431
O	3.8833236	2.0428866	-1.1652458
O	4.7324922	-0.0271776	-0.8160599
O	3.5760219	0.0474446	2.0823742
C	5.9408600	0.3875649	-1.5080779
H	6.3963623	1.2322902	-0.9859868
H	6.5910558	-0.4861245	-1.4879266
H	5.7012625	0.6776003	-2.5338705
C	4.0834474	-0.7961367	3.1492246
H	4.8220641	-1.4952382	2.7497084
H	4.5362181	-0.1085229	3.8625998
H	3.2629121	-1.3545980	3.6065007

IV^{O}

62

Energy = -2843.306681077

C	1.5641692	-1.3672516	0.2093884
C	1.5320284	0.8348107	1.3211651
C	0.1299643	0.4033877	0.9650377
C	0.1405566	-0.8594608	0.3046831
C	-1.0843652	1.1321135	1.1179947
C	-1.0505322	-1.4257870	-0.2758328
H	1.8201324	-1.8328727	-0.7406769
H	1.7202981	-2.1075830	1.0052817
H	1.7008164	0.6658653	2.3920347
H	1.7475737	1.8806747	1.0955829
Co	-0.7454478	0.5207792	-0.8206588
C	0.1558773	1.8096985	-2.2274615
H	1.1183214	2.2901603	-2.1228117
C	-0.1019330	0.5351773	-2.8082021
H	0.6314159	-0.1332135	-3.2376030
C	-1.5115628	0.2798788	-2.7046837
H	-2.0204365	-0.6156151	-3.0320076
C	-1.0868519	2.3274488	-1.7561974
H	-1.2200382	3.2709725	-1.2460790
C	-2.1300668	1.3903292	-2.0607804
H	-3.1802346	1.4892569	-1.8252514
C	-1.0512031	2.6142617	1.4709183
H	-0.6457543	2.7367268	2.4895096
H	-0.4181551	3.1983672	0.7980854
C	-2.5306853	3.0129024	1.4640618

H	-2.8881458	3.0904276	0.4309749
H	-2.7266234	3.9662598	1.9642957
C	-3.2107713	1.8224309	2.1642942
H	-3.1763351	1.9593530	3.2505024
H	-4.2551414	1.6969372	1.8699784
C	-2.3657606	0.5803467	1.7864686
H	-2.0917868	0.0121774	2.6845464
C	-3.0460206	-0.3694813	0.8322033
C	-2.3659959	-1.7075753	0.5376979
O	-4.1139817	-0.1030660	0.2949163
C	-3.3624484	-2.5189860	-0.2508488
C	-4.5067305	-2.0710541	-0.7556162
H	-3.1710191	-3.5724415	-0.4302152
C	-2.0007263	-2.4638323	1.8426931
H	-1.2340369	-1.9265339	2.4092523
H	-2.8853658	-2.6106182	2.4707923
H	-1.5987282	-3.4489131	1.5845314
C	-0.7811550	-2.4863677	-1.3347758
H	0.0979472	-2.2281230	-1.9292535
H	-0.6030814	-3.4697317	-0.8731974
H	-1.6340051	-2.5949072	-2.0071237
O	-5.5352359	-1.9413474	-1.3095575
C	2.4521293	-0.1146501	0.4987931
C	2.9431965	0.6022150	-0.7645382
O	3.1850231	1.7910504	-0.8245347
C	3.6609296	-0.5430201	1.3409692
O	3.5741430	-0.9641424	2.4755095
O	3.1323332	-0.2460816	-1.8018701
O	4.8284737	-0.4254558	0.6711632
C	3.7230071	0.3602870	-2.9790496
H	3.0721405	1.1477450	-3.3658942
H	4.6977833	0.7845320	-2.7264028
H	3.8217046	-0.4529996	-3.6976337
C	6.0070968	-0.8318584	1.4166493
H	5.9276719	-1.8861225	1.6924419
H	6.8419094	-0.6637587	0.7373518
H	6.1037192	-0.2237219	2.3189891

Ts$^{O}_{IV\text{-}V}$

62

Energy = -2843.292859497

C	-1.2766472	-1.4870248	0.5324357
C	1.2017643	-1.6431178	0.4585965
C	0.7542604	-0.2070562	0.5703486
C	-0.6619644	-0.1057650	0.6060533
C	1.5363403	0.9873346	0.5643546
C	-1.3331183	1.1754194	0.5261648
H	-2.1114269	-1.5749592	-0.1615585
H	-1.6405189	-1.7699977	1.5282633
H	1.6194423	-1.9649595	1.4222295
H	1.9547888	-1.8173353	-0.3123196
Co	0.1005702	0.9500076	-0.8980373
C	0.8356572	0.2660938	-2.7379459
H	1.4570674	-0.6076574	-2.8719395
C	-0.5892782	0.2901030	-2.7616537
H	-1.2416351	-0.5560000	-2.9286675
C	-1.0101603	1.6284457	-2.4922862
H	-2.0325711	1.9697634	-2.4221980
C	1.2855511	1.5926609	-2.4567948
H	2.3174634	1.8967736	-2.3544220
C	0.1500342	2.4476508	-2.3093037
H	0.1586591	3.5096888	-2.1138870
C	3.0088766	0.9261980	0.1735029
H	3.5578545	0.3170811	0.9121322
H	3.1801736	0.4743059	-0.8072915
C	3.4631515	2.3868339	0.2884367
H	3.1088553	2.9501141	-0.5823716
H	4.5507343	2.4974191	0.3394447
C	2.7541595	2.8944527	1.5608026
H	3.4028326	2.7910913	2.4353694
H	2.4671362	3.9464482	1.5010628
C	1.4949183	1.9843535	1.7208837
H	1.6164088	1.3964176	2.6491602
C	0.2365117	2.7682470	2.0165546
C	-1.1833763	2.3078890	1.5685396
O	0.3191532	3.7695539	2.7107677
C	-1.8241041	3.6136253	1.0889006
C	-2.0382562	3.9793787	-0.1524889
H	-1.9246264	4.4059864	1.8262372
C	-1.8867905	1.8724872	2.8904744
H	-1.4168331	0.9616197	3.2776399
H	-1.7977305	2.6651347	3.6384187
H	-2.9457831	1.6740242	2.7093427
C	-2.7878653	1.0104577	0.0615617
H	-2.8409196	0.3187231	-0.7817943
H	-3.4159099	0.6010877	0.8649743
H	-3.2436764	1.9500258	-0.2511491
O	-2.3026963	4.3316101	-1.2426128
C	-0.1063894	-2.4371308	0.1393993
C	-0.1313707	-2.8401319	-1.3400109
O	0.8181095	-2.8506185	-2.0942917
C	-0.1346710	-3.7104779	0.9957262
O	-0.5431570	-3.7676337	2.1360823
O	-1.3750853	-3.2387590	-1.7078842
O	0.4161233	-4.7588475	0.3424347
C	-1.4729096	-3.7401628	-3.0653727
H	-1.1719668	-2.9667347	-3.7765412
H	-0.8260573	-4.6128690	-3.1849957
H	-2.5215627	-4.0060495	-3.1949203
C	0.4897451	-5.9901570	1.1086950
H	-0.5139390	-6.3061460	1.4030393
H	0.9499011	-6.7132199	0.4362956
H	1.1009548	-5.8371904	2.0013772

V^{O}

62

Energy = -2843.297224314

C	-1.4792631	-1.2424285	0.6365249
C	0.8359192	-1.2810648	1.5372997
C	0.5207508	0.0626227	0.9291634
C	-0.8037836	0.0897018	0.4056396
C	1.3653210	1.1931346	0.7165536
C	-1.2823619	1.2190964	-0.3629099
H	-2.0212723	-1.6260881	-0.2270284
H	-2.1919520	-1.1348964	1.4639952
H	0.8281207	-1.1847740	2.6302423
H	1.8001755	-1.6942708	1.2350824
Co	0.5213605	0.5171552	-1.0073594
C	1.6342970	-0.8977749	-2.0999900
H	2.0755829	-1.7952207	-1.6911403
C	0.3230404	-0.7739142	-2.6452586
H	-0.4112826	-1.5631236	-2.7327817
C	0.1350388	0.5907734	-3.0285587
H	-0.7622147	1.0107672	-3.4589403
C	2.2457329	0.3894368	-2.1505142
H	3.2387406	0.6264817	-1.7975962
C	1.3291634	1.3187335	-2.7315762
H	1.5078789	2.3639990	-2.9323582
C	2.8804517	1.1357788	0.8688396
H	3.1298377	1.0022715	1.9330251
H	3.3453301	0.3078335	0.3292928
C	3.3545775	2.5398500	0.3935342
H	3.7926377	2.4920167	-0.6079675
H	4.1222495	2.9412190	1.0618184
C	2.0834682	3.4397024	0.3892539
H	2.2465066	4.4231138	0.8370602
H	1.7074950	3.5762824	-0.6283879
C	1.0618618	2.5990770	1.1918397
H	1.3796338	2.6557103	2.2479746
C	-0.3534989	3.1116023	1.2404732

C	-1.4456114	2.6257721	0.2537124
O	-0.6320642	3.9775262	2.0585930
C	-1.4120900	3.7432992	-0.7931109
C	-0.9936332	3.6726924	-2.0366591
H	-1.7176852	4.7345707	-0.4650653
C	-2.8078577	2.7018984	0.9946637
H	-2.8807605	1.8827540	1.7186260
H	-2.8820493	3.6480340	1.5339984
H	-3.6348134	2.6290952	0.2858389
C	-2.4663698	0.8669103	-1.2713959
H	-2.2584472	-0.0379258	-1.8459387
H	-3.3782206	0.6842169	-0.6879646
H	-2.6864531	1.6738868	-1.9757149
O	-0.6727933	3.6732868	-3.1662591
C	-0.3348975	-2.2116796	1.0768327
C	0.1442744	-3.1475006	-0.0380980
O	1.2933277	-3.5000809	-0.2089474
C	-0.8065031	-3.0536022	2.2713838
O	-1.3403770	-2.5849177	3.2545164
O	-0.8851920	-3.5874648	-0.8013622
O	-0.5372790	-4.3687958	2.1183984
C	-0.5160795	-4.5686074	-1.8038427
H	0.2170870	-4.1444461	-2.4943080
H	-0.0905031	-5.4504227	-1.3187337
H	-1.4453191	-4.8117665	-2.3183873
C	-0.9310867	-5.2096609	3.2355338
H	-2.0103168	-5.1399344	3.3910969
H	-0.6381129	-6.2180380	2.9458632
H	-0.4097165	-4.8919034	4.1414852

$Ts^{O}_{V\text{-}P1}$

62

Energy = -2843.273323036

C	-1.4379893	-1.2355955	0.5672197
C	1.0422681	-1.2063058	0.9104590
C	0.5537947	0.1219560	0.3790807
C	-0.8614144	0.1130123	0.2068337
C	1.2744812	1.3865608	0.4248848
C	-1.5309507	1.2140674	-0.4210097
H	-2.0781952	-1.6748854	-0.1982086
H	-2.0411481	-1.1303957	1.4766282
H	1.3963270	-1.0739010	1.9419267
H	1.8599092	-1.6497100	0.3393783
Co	0.0907834	0.5226869	-1.5000977
C	0.9756303	-1.0161210	-2.6028972
H	1.5515214	-1.8211385	-2.1705417
C	-0.4475153	-1.0050988	-2.7735575
H	-1.1246400	-1.8091317	-2.5156751
C	-0.8189943	0.2541170	-3.3568618
H	-1.8254464	0.5710277	-3.5913536
C	1.4646522	0.2447364	-3.0208411
H	2.4803479	0.6040526	-2.9351809
C	0.3541067	1.0289925	-3.5050171
H	0.4153497	2.0476196	-3.8583299
C	2.7971838	1.3755800	0.5236065
H	3.1631301	0.3971083	0.8537621
H	3.2265607	1.5789029	-0.4625154
C	3.1609800	2.4971289	1.5352451
H	4.0234956	3.0831747	1.2053702
H	3.4125531	2.0570072	2.5078671
C	1.8909282	3.3601434	1.6745475
H	1.8267150	3.8947095	2.6254610
H	1.8264889	4.0903595	0.8620150
C	0.7595148	2.3231992	1.5252348
H	0.7089808	1.7413379	2.4605505
C	-0.6371690	2.8863132	1.3288036
C	-1.2443138	2.7172543	-0.0881363
O	-1.1995542	3.4997323	2.2200007
C	-0.1815207	3.2681041	-0.9963209
C	1.0203766	2.6226082	-1.1651848
H	-0.2916023	4.2756926	-1.3960990
C	-2.5067411	3.5921817	-0.1660639
H	-3.2807868	3.2455542	0.5219476
H	-2.2446513	4.6118892	0.1267804
H	-2.9049965	3.6182064	-1.1834967
C	-2.9171462	0.9137214	-0.9608288
H	-2.9731585	-0.1108971	-1.3371863
H	-3.6803352	1.0283546	-0.1794403
H	-3.1816846	1.5858359	-1.7797169
O	2.0736833	2.8693472	-1.7430592
C	-0.2108173	-2.1441113	0.8781972
C	-0.0310068	-3.2691592	-0.1461120
O	0.9932684	-3.5591238	-0.7271486
C	-0.3609488	-2.7932142	2.2644195
O	-1.0840986	-2.3961031	3.1513278
O	-1.1958392	-3.9432506	-0.3131930
O	0.4825121	-3.8428134	2.3905659
C	-1.1193120	-5.0747065	-1.2196280
H	-0.8265898	-4.7368006	-2.2169677
H	-0.3866822	-5.7965333	-0.8508475
H	-2.1225127	-5.4993646	-1.2273330
C	0.4729828	-4.4858002	3.6933690
H	-0.5273658	-4.8662233	3.9130870
H	1.1951170	-5.2972167	3.6119262
H	0.7692358	-3.7696632	4.4635488

$P1^{O}$

62

Energy = -2843.336703031

C	1.4251608	-1.0303342	-0.7696841
C	1.1279838	1.3239078	-0.0536041
C	-0.1798669	0.5647897	0.1382138
C	-0.0154667	-0.7632764	-0.3704269
C	-1.1495630	0.8942192	1.2613615
C	-1.1161255	-1.6331513	-0.6105654
H	1.5577531	-1.1155054	-1.8524657
H	1.7949270	-1.9485895	-0.3051975
H	1.3675054	1.9815305	0.7837466
H	1.1353965	1.9380200	-0.9556724
Co	-1.2710724	0.1443224	-1.6193595
C	-0.1019303	0.8460055	-3.2149093
H	0.9772463	0.9282844	-3.2211749
C	-0.8682297	-0.2923540	-3.6055571
H	-0.4694246	-1.2352115	-3.9565387
C	-2.2533351	0.0060715	-3.4097689
H	-3.0872445	-0.6520995	-3.6103308
C	-1.0106749	1.8591327	-2.7749978
H	-0.7462158	2.8310854	-2.3815369
C	-2.3322095	1.3463589	-2.8941464
H	-3.2311947	1.8601196	-2.5809840
C	-0.8083844	2.0479610	2.2089384
H	0.2342285	1.9650216	2.5434168
H	-0.9522075	3.0223056	1.7336010
C	-1.7604333	1.8109115	3.3932814
H	-2.7596194	2.1588707	3.1139226
H	-1.4558711	2.3536141	4.2936464
C	-1.7616478	0.2777699	3.5989825
H	-1.0396898	-0.0167092	4.3663140
H	-2.7351769	-0.1095551	3.9111488
C	-1.3417929	-0.3166305	2.2259941
H	-0.3644598	-0.8130270	2.3235983
C	-2.2619471	-1.3942673	1.6782575
C	-2.4438534	-1.4021822	0.1468144
O	-2.8324883	-2.1903282	2.4035074
C	-2.8170138	0.0124294	-0.3432407
C	-2.4637192	1.1688566	0.4766620
H	-3.7987375	0.0786337	-0.8127074
C	-3.5333816	-2.3990894	-0.2483336
H	-3.2685914	-3.4210183	0.0340631
H	-4.4622856	-2.1428439	0.2676197

H	-3.7081994	-2.3547523	-1.3286228
C	-0.8576299	-2.9762560	-1.2485277
H	0.0452588	-2.9536221	-1.8642267
H	-0.7218751	-3.7469948	-0.4764572
H	-1.6900864	-3.2899856	-1.8826971
O	-3.0347692	2.2574711	0.4648340
C	2.1965340	0.1991603	-0.2055338
C	3.3200677	0.5807349	-1.1628436
O	3.2544175	1.4379133	-2.0198673
C	2.7267725	-0.1245971	1.1941216
O	2.4326068	-1.1008830	1.8520023
O	4.3884041	-0.2319571	-0.9924199
O	3.5153688	0.8780196	1.6467817
C	5.4947105	0.0071068	-1.9021644
H	5.1682744	-0.1396389	-2.9346957
H	5.8639644	1.0278048	-1.7775287
H	6.2533960	-0.7228356	-1.6224711
C	4.0141850	0.7009960	2.9980758
H	4.6064496	-0.2151369	3.0599206
H	4.6276774	1.5803403	3.1907705
H	3.1781252	0.6430638	3.6996618

$Ts^{O}_{III\text{-}P2}$

62

Energy = -2843.251196445

C	1.5127441	1.8780360	0.2449732
C	-0.6268423	1.9051200	-0.9899588
C	-0.4599409	0.5457637	-0.3436758
C	0.9037917	0.4965469	0.1965893
C	-1.4607917	-0.4047932	-0.0413004
C	1.4062659	-0.7658314	0.1196972
H	2.2984124	2.0004480	-0.5129953
H	1.9340090	2.1380207	1.2208414
H	-1.6550767	2.2722584	-1.0114140
H	-0.2298388	1.9354219	-2.0092728
Co	-0.0194190	-1.2924162	-1.1125354
C	1.1174091	-2.4399989	-2.4484904
H	2.0985496	-2.8352685	-2.2193558
C	-0.1170566	-3.1493260	-2.2675869
H	-0.2191580	-4.1278212	-1.8222791
C	-1.1562419	-2.2763864	-2.6273189
H	-2.2169628	-2.4816489	-2.5664393
C	0.8465604	-1.1714073	-3.0597714
H	1.5750889	-0.4307677	-3.3597005
C	-0.5635512	-1.0396863	-3.1047664
H	-1.1145891	-0.1801512	-3.4653860
C	-2.9256873	-0.3116874	-0.4316217
H	-3.3408035	0.6673129	-0.1538947
H	-3.0683035	-0.4143144	-1.5114306
C	-3.6067059	-1.4584756	0.3666736
H	-4.3564685	-1.9922781	-0.2247421
H	-4.1195219	-1.0455747	1.2430876
C	-2.4594411	-2.3848982	0.8214845
H	-2.7116746	-2.9889712	1.6971984
H	-2.1645345	-3.0593617	0.0130242
C	-1.3059282	-1.4000241	1.0891755
H	-1.4672643	-0.9239457	2.0713999
C	0.1220010	-1.9896683	1.0149911
C	0.8665131	-1.8988765	2.3200186
O	0.1844852	-3.3778603	0.6703241
C	1.3348728	-3.1224217	2.6394156
C	0.9536958	-4.0801547	1.6073870
H	1.8860932	-3.4106437	3.5251649
C	1.0011071	-0.6438048	3.1216978
H	1.9575669	-0.1524518	2.9080342
H	0.2217345	0.0855667	2.8859163
H	0.9759502	-0.8707427	4.1917910
C	2.8168705	-1.2382343	0.2379025
H	3.3690692	-0.9406242	-0.6627934
H	3.3316739	-0.8060179	1.1054609
H	2.8709573	-2.3280952	0.3156372
O	1.1862247	-5.2595339	1.4671379
C	0.2970754	2.7952106	-0.0962298
C	0.7565789	4.0532546	-0.8255311
O	0.7105654	4.2318851	-2.0234778
O	1.2920725	4.9385152	0.0504579
C	-0.4534952	3.1528069	1.1901930
O	-0.2141581	2.7251312	2.3000972
O	-1.4828273	3.9909871	0.9158489
C	1.8012601	6.1589190	-0.5481777
H	2.1841561	6.7452920	0.2863999
H	2.5953838	5.9229184	-1.2608543
H	0.9940996	6.6856700	-1.0631190
C	-2.2794748	4.3760522	2.0650140
H	-1.6510929	4.8834164	2.8011677
H	-3.0418417	5.0466338	1.6698411
H	-2.7314851	3.4911165	2.5202840

$P2^{O}$

62

Energy = -2843.354145503

C	1.0267698	1.5678026	-0.7078269
C	0.1754322	1.5352672	-2.0291383
C	-1.1796833	0.8455885	-1.6518707
C	-0.8651410	0.1061244	-0.3813731
C	0.3878849	0.5145473	0.1610678
C	-1.5157732	-0.9183858	0.3551789
C	0.8333563	-0.1815371	1.3368891
H	2.0839516	1.3987787	-0.9140565
H	0.9303750	2.5515368	-0.2334815
H	-1.9475628	1.6041243	-1.4559773
H	-1.5226578	0.2102801	-2.4707232
Co	0.3829776	-1.4234780	-0.1877554
C	1.7540607	-2.0916773	-1.6204188
H	2.3390624	-1.4727040	-2.2848271
C	2.1302325	-2.4830269	-0.2998536
H	3.0437283	-2.2038178	0.2070103
C	1.0839679	-3.2951053	0.2562604
H	1.0732646	-3.7335282	1.2440491
C	0.4603130	-2.6260834	-1.8836940
H	-0.1161401	-2.4709650	-2.7850413
C	0.0523330	-3.3706376	-0.7253614
H	-0.8951073	-3.8781710	-0.6036788
C	-2.7540243	-1.6765367	-0.0843871
H	-3.5653328	-0.9713369	-0.3168875
H	-2.5826152	-2.2598798	-0.9932598
C	-3.1341291	-2.5563242	1.1463296
H	-3.1899974	-3.6187575	0.8904531
H	-4.1209600	-2.2682601	1.5237620
C	-2.0481663	-2.2910587	2.2183133
H	-2.4258727	-2.3780531	3.2406861
H	-1.2164737	-2.9902337	2.1065588
C	-1.5470130	-0.8771179	1.8776390
H	-2.3223433	-0.1593388	2.1980775
C	-0.1851244	-0.4457531	2.4651098
C	-0.2989571	0.7347407	3.4138217
O	0.3525693	-1.5074875	3.3096906
C	0.1142411	0.3639521	4.6340968
C	0.5283310	-1.0476060	4.6032287
H	0.1700669	0.9628744	5.5345244
C	-0.7553485	2.0742242	2.9410874
H	-0.0215043	2.4944012	2.2416524
H	-1.7012037	2.0007656	2.3915221
H	-0.8819526	2.7701987	3.7738352
C	2.2566540	0.0265445	1.8109454
H	2.9289610	0.1720749	0.9615795
H	2.3349959	0.9108327	2.4601763
H	2.6054943	-0.8337164	2.3873164
O	0.9634304	-1.7599763	5.4792827
C	-0.0725394	2.9380853	-2.5908205

O	-0.6135398	3.7504010	-1.6468624
C	-0.9191501	5.0929510	-2.1073480
H	-1.6410042	5.0514936	-2.9266351
H	-1.3382951	5.6007742	-1.2391539
H	-0.0071635	5.5870156	-2.4509674
O	0.1500744	3.2929144	-3.7291259
C	0.8589275	0.7569079	-3.1654487
O	0.3001143	-0.0004711	-3.9292939
O	2.1720782	1.0707074	-3.2504330
C	2.8467158	0.5397735	-4.4203295
H	2.3866615	0.9508911	-5.3219604
H	3.8819412	0.8650522	-4.3228510
H	2.7758094	-0.5506008	-4.4393024