

Electronic Supporting Information

S-functionalization of 3,5-*bis*(2-pyridyl)-1,2,4,6-thiatriazine: Probing the effect of alkyl chain length in the development of tethered materials

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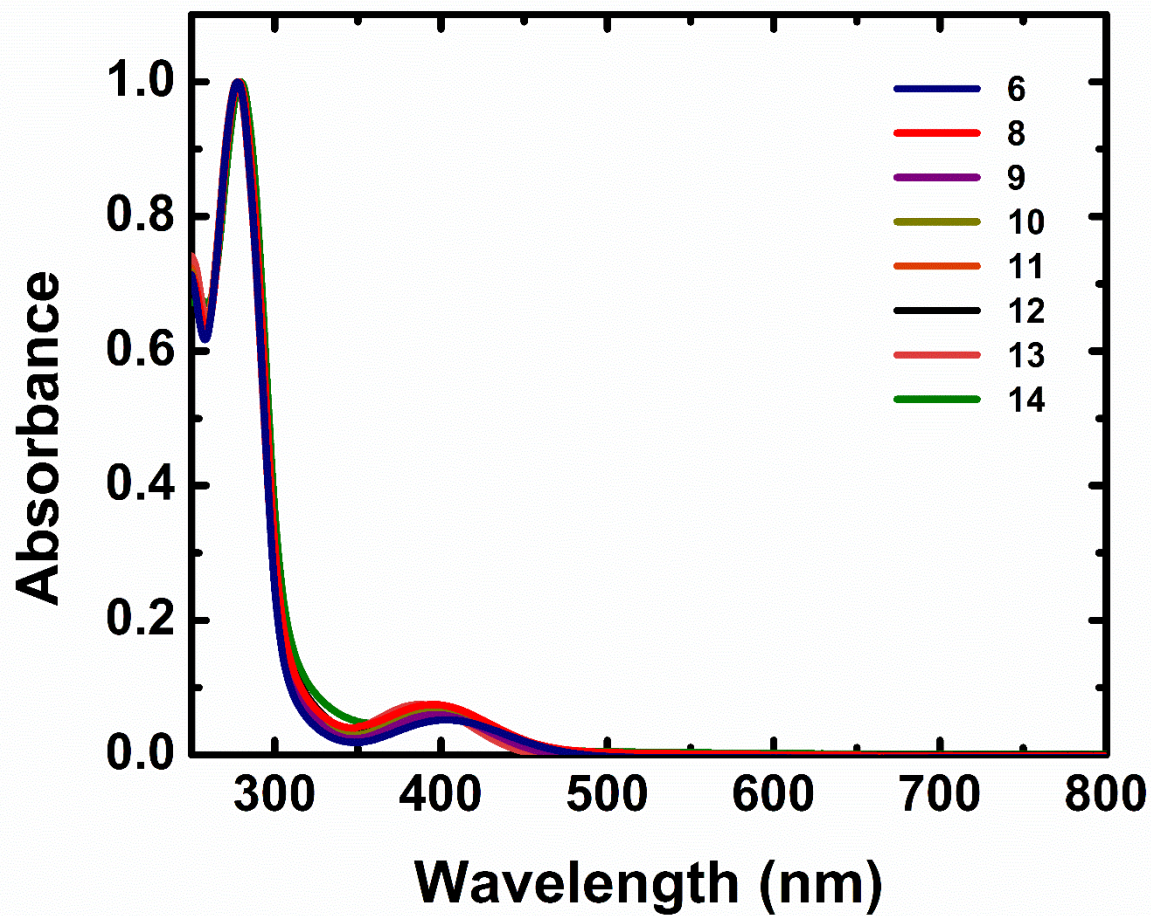


Figure S1. Experimental absorption spectra of **6** (blue line), **8** (red line), **9** (purple line), **10** (yellow line), **11** (orange line), **12** (black line), **13** (coral line) and **14** (green line) in CH₂Cl₂.

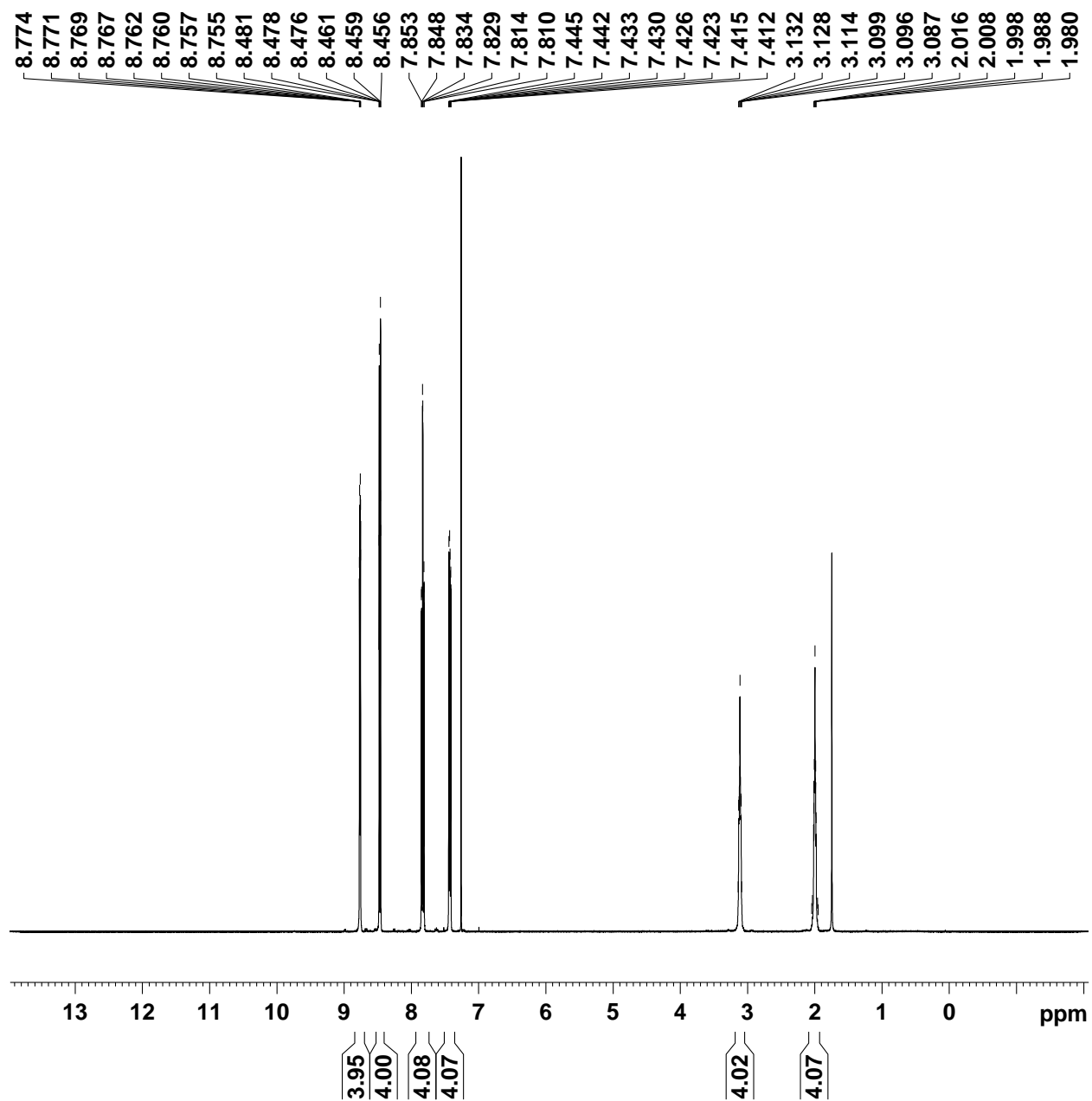


Figure S2. ^1H NMR spectrum of *S,S'*-butyl-bis(Py₂TTA) (8) in CDCl₃.

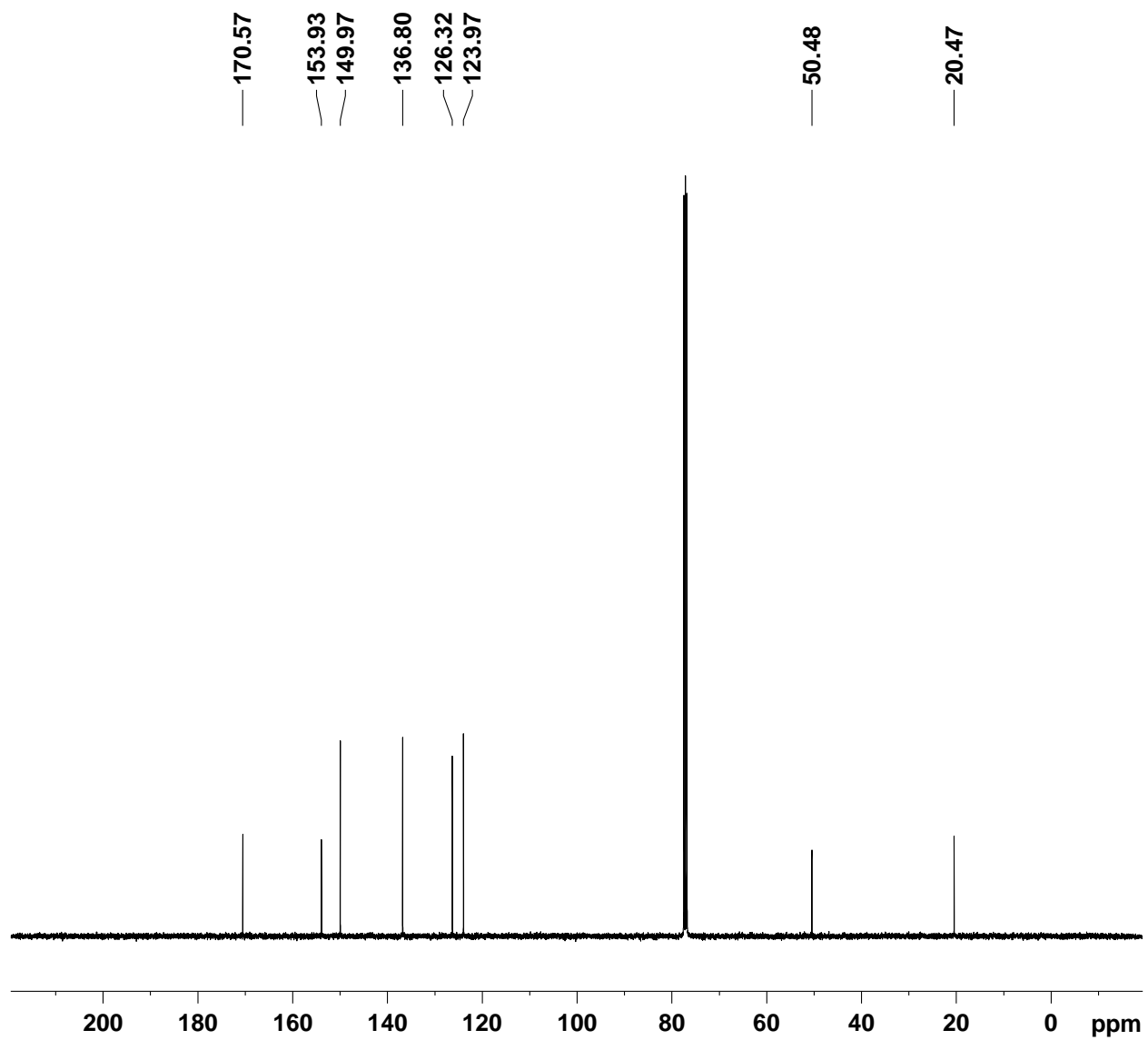


Figure S3. ^{13}C NMR spectrum of *S,S'*-butyl-*bis*(Py₂TTA) (**8**) in CDCl₃.

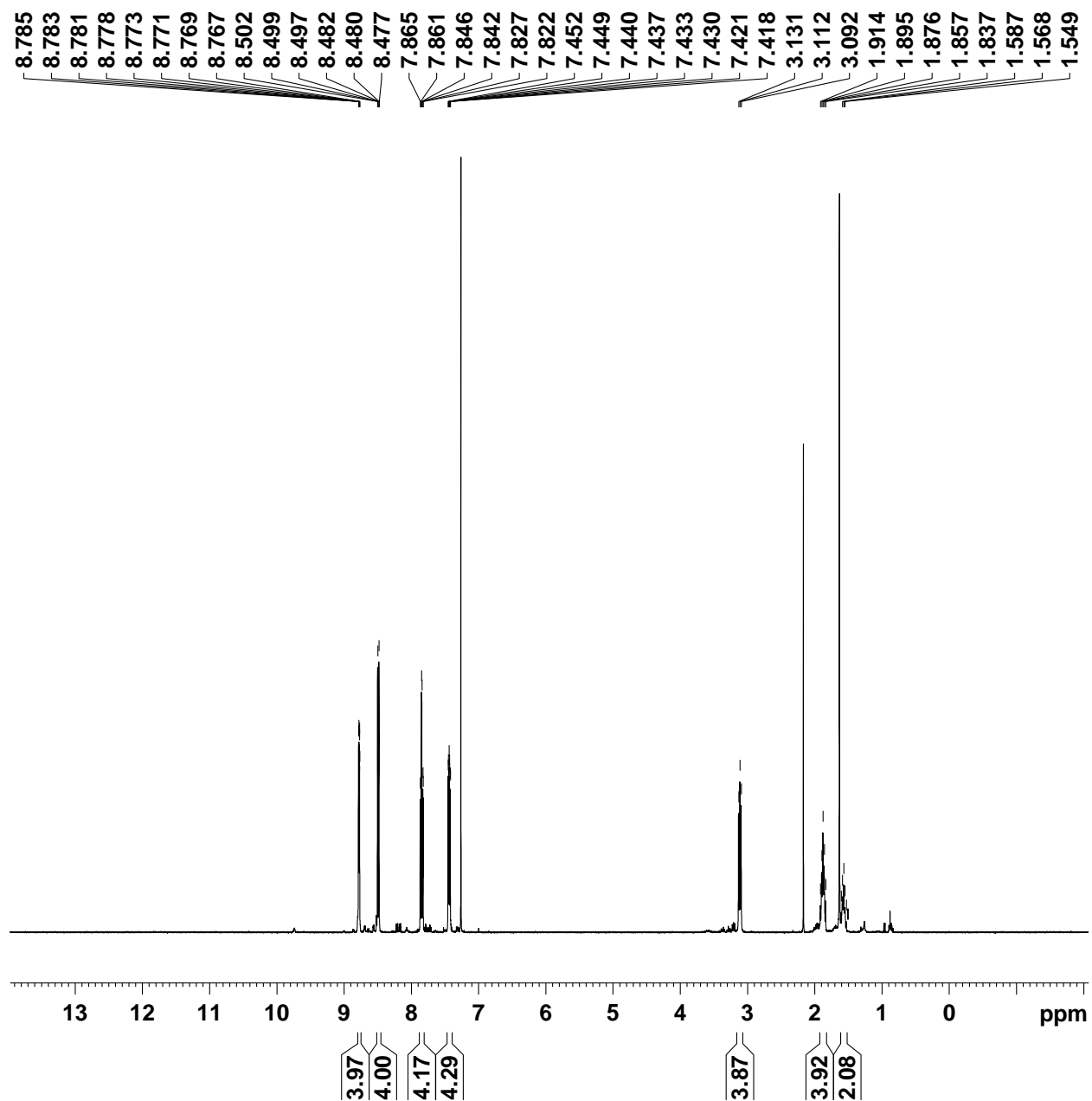


Figure S4. ^1H NMR spectrum of *S,S'*-pentyl-*bis*(Py_2TTA) (**9**) in CDCl_3 .

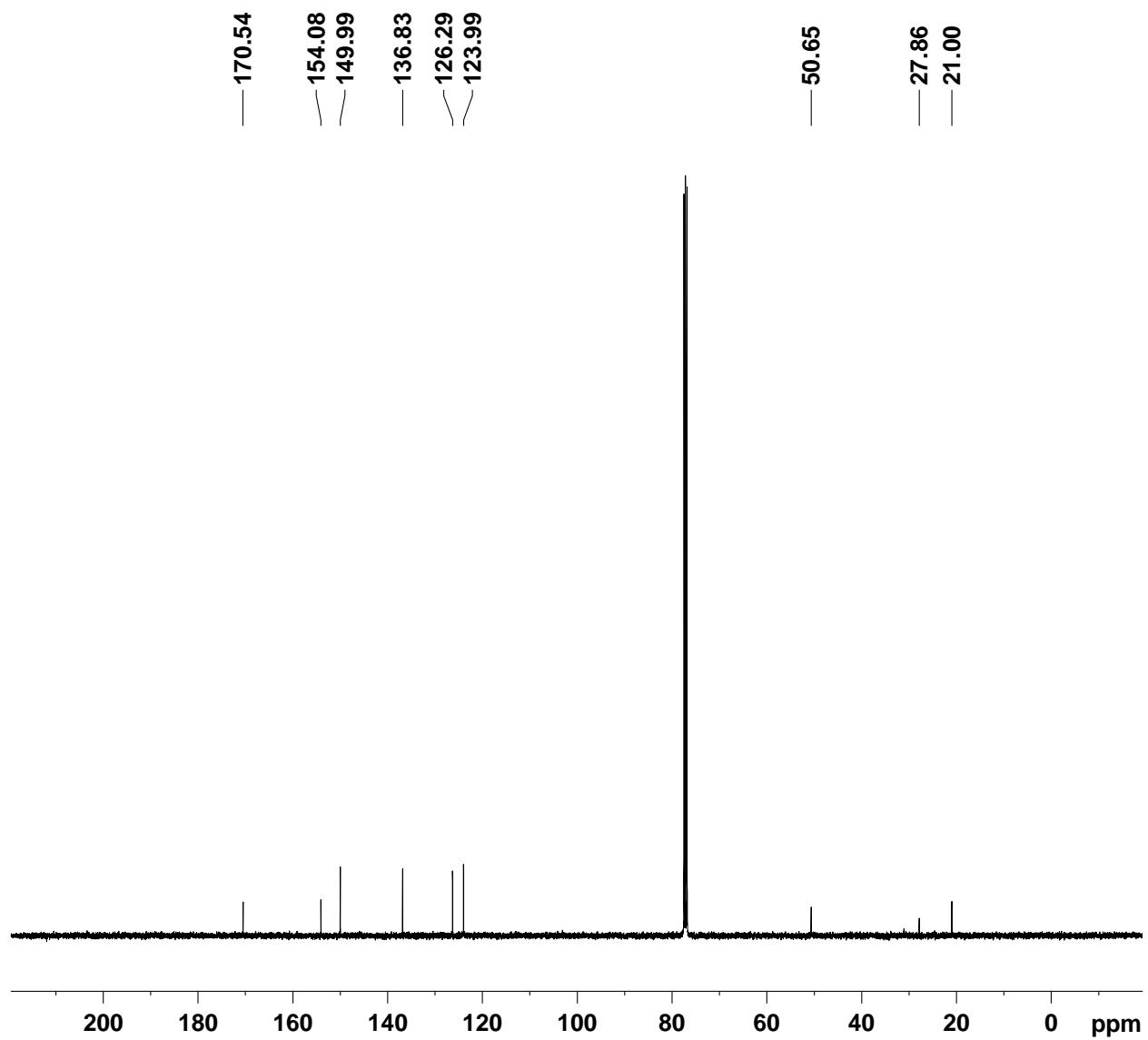


Figure S5. ^{13}C NMR spectrum of *S,S'*-pentyl-*bis*(Py₂TTA) (**9**) in CDCl₃.

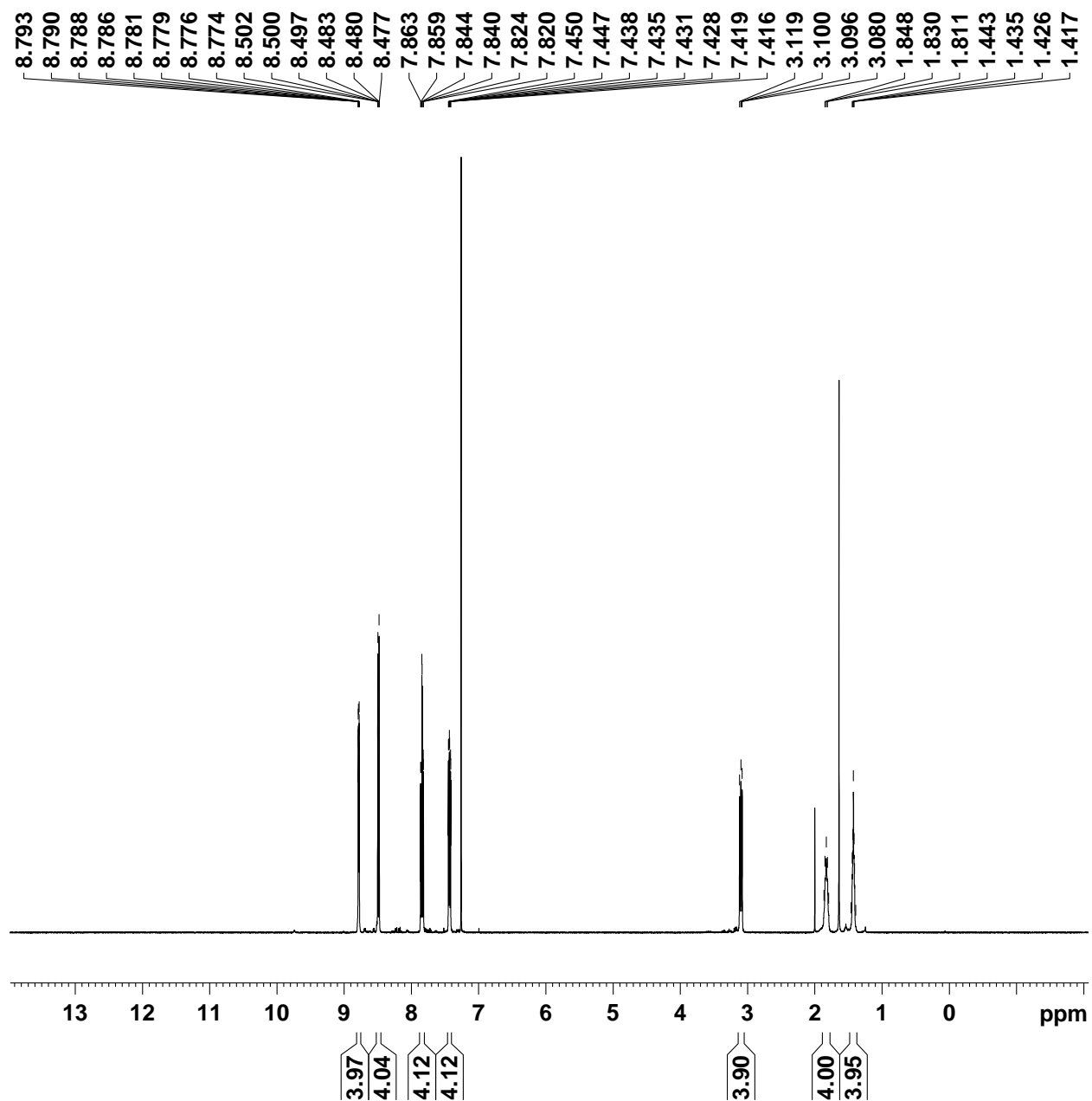


Figure S6. ^1H NMR spectrum of *S,S'*-hexyl-*bis*(Py_2TTA) (**10**) in CDCl_3 .

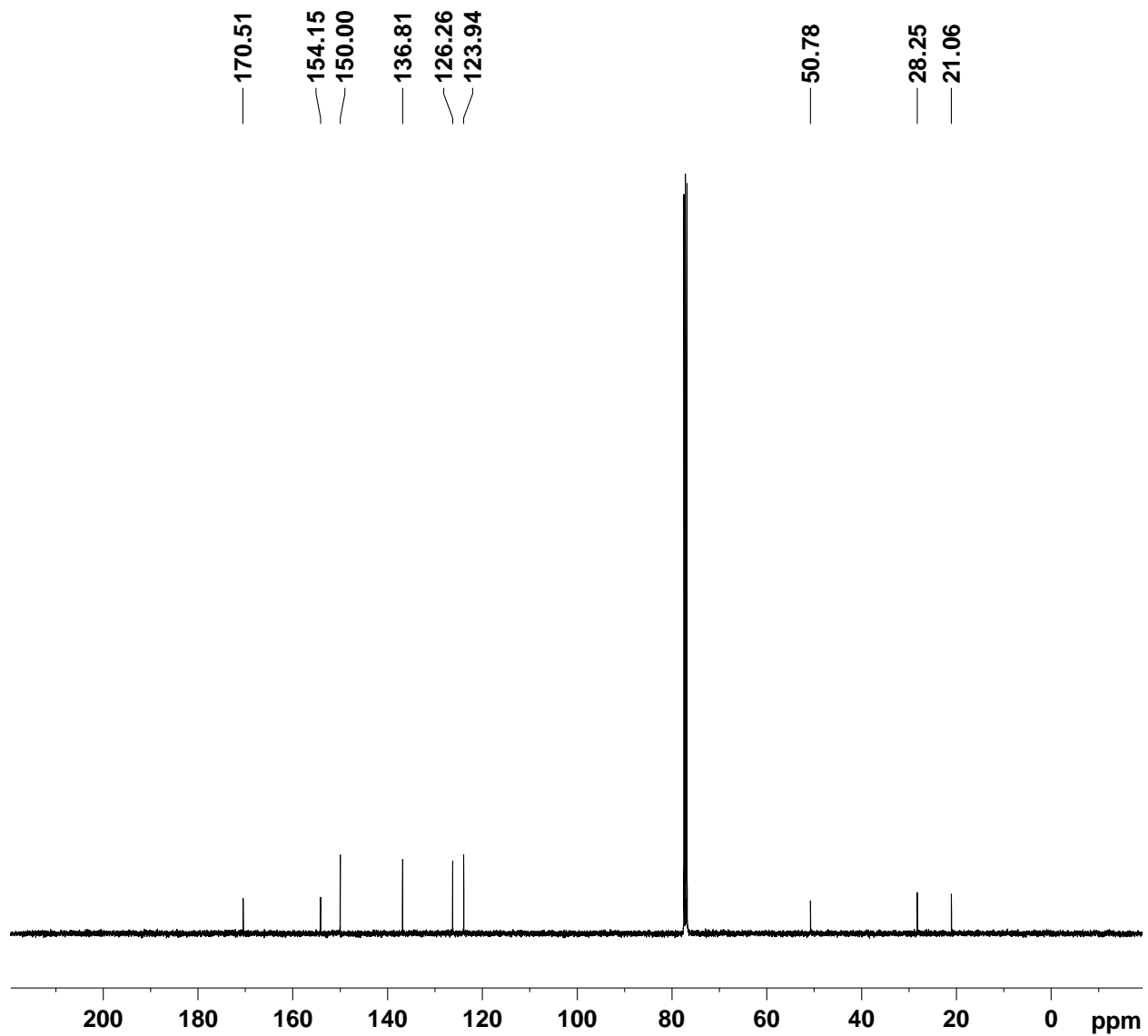


Figure S7. ^{13}C NMR spectrum of *S,S'*-hexyl-*bis*(Py₂TTA) (**10**) in CDCl₃.

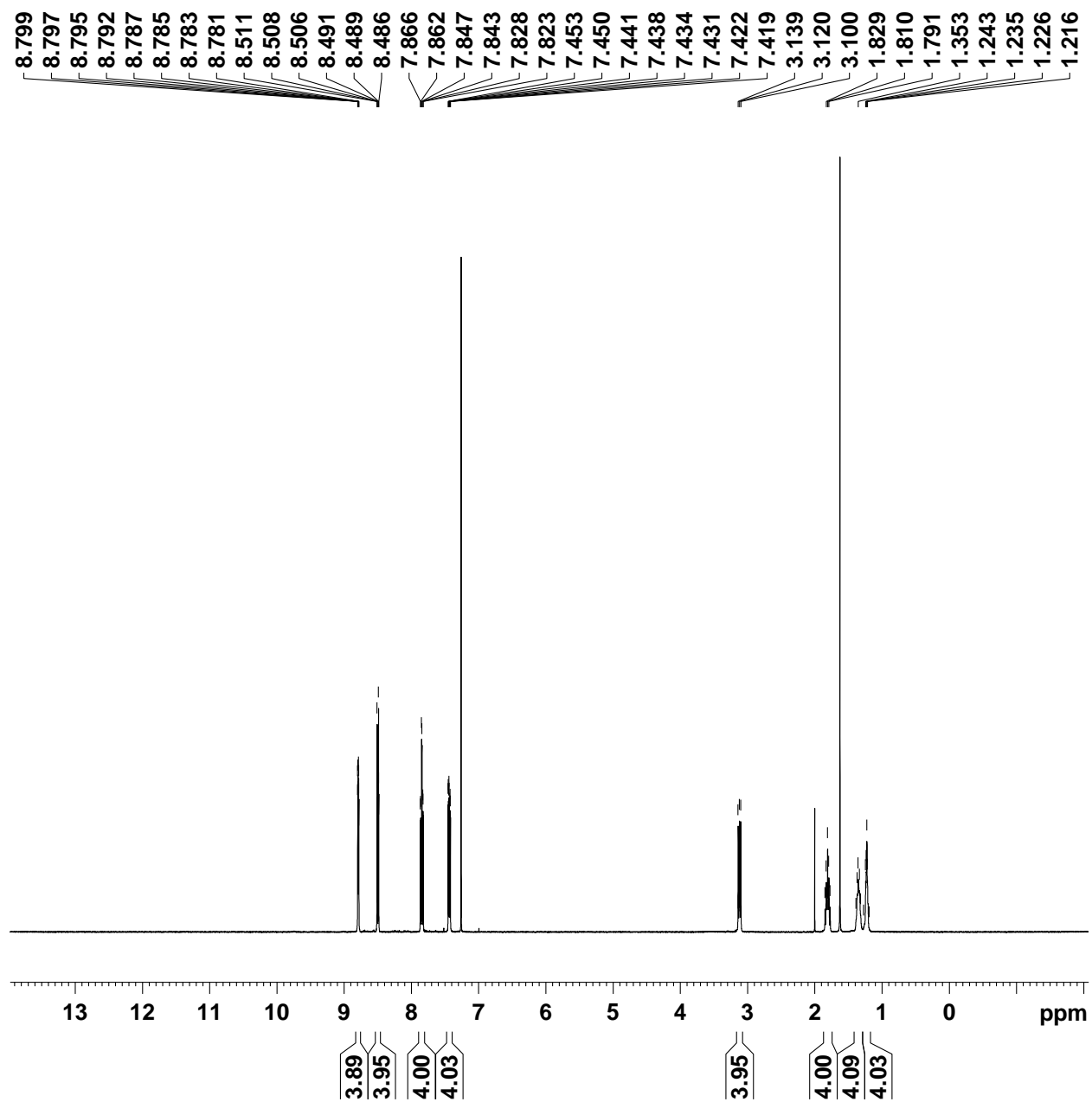


Figure S8. ^1H NMR spectrum of *S,S'*-octyl-bis(Py₂TTA) (11) in CDCl₃.

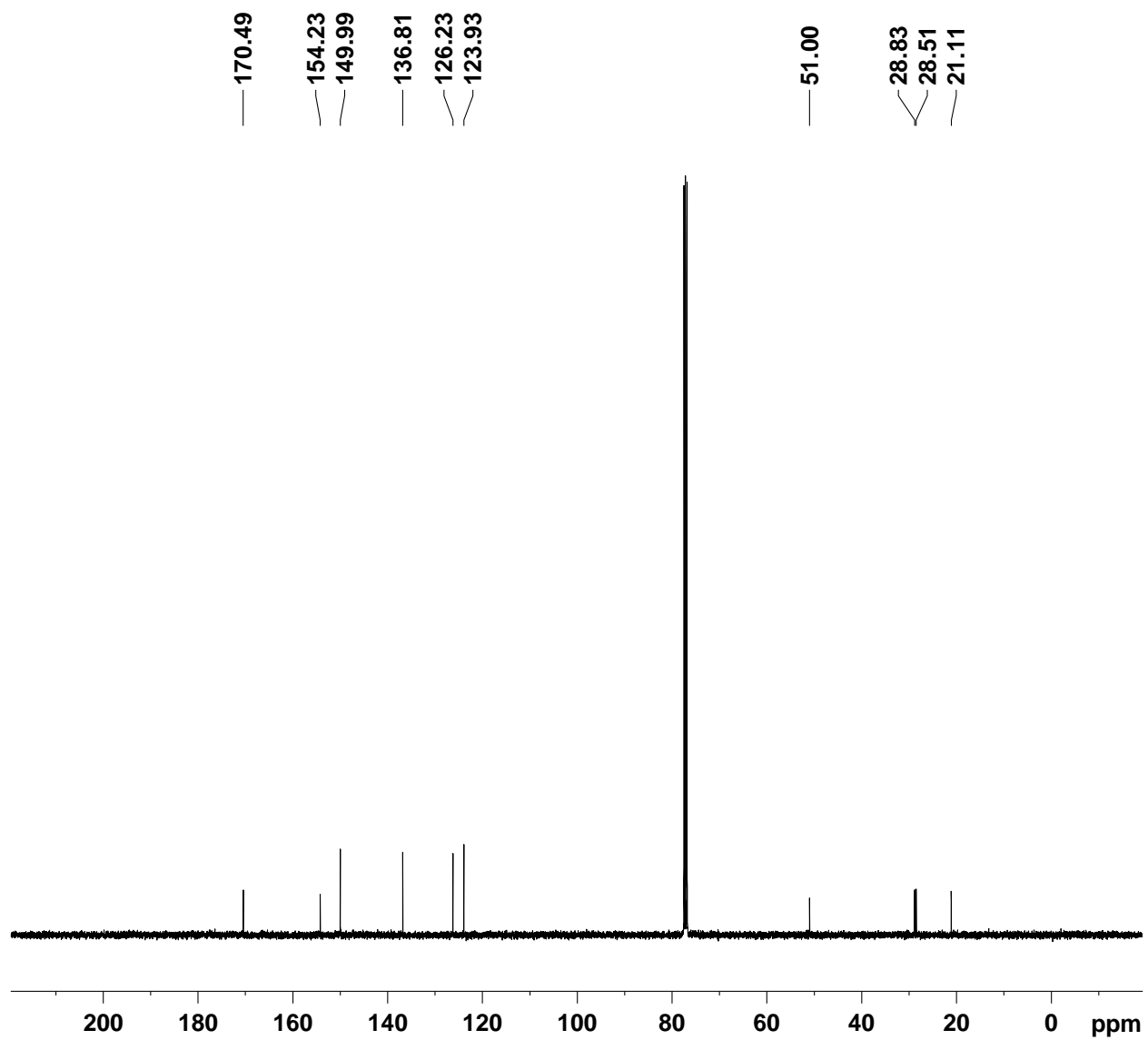


Figure S9. ^{13}C NMR spectrum of *S,S'*-octyl-*bis*(Py₂TTA) (**11**) in CDCl₃.

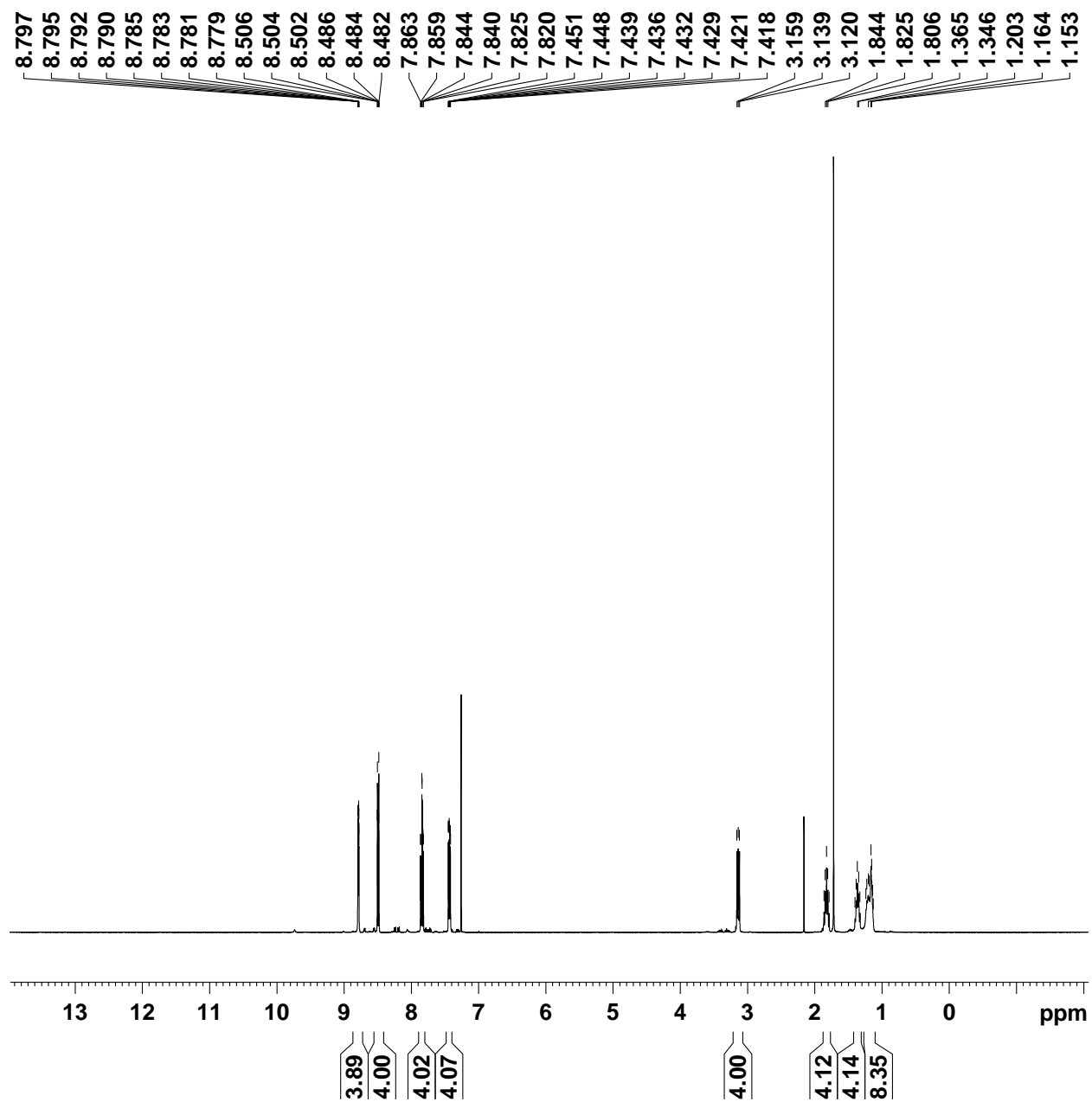


Figure S10. ^1H NMR spectrum of *S,S'*-decyl-*bis*(Py_2TTA) (**12**) in CDCl_3 .

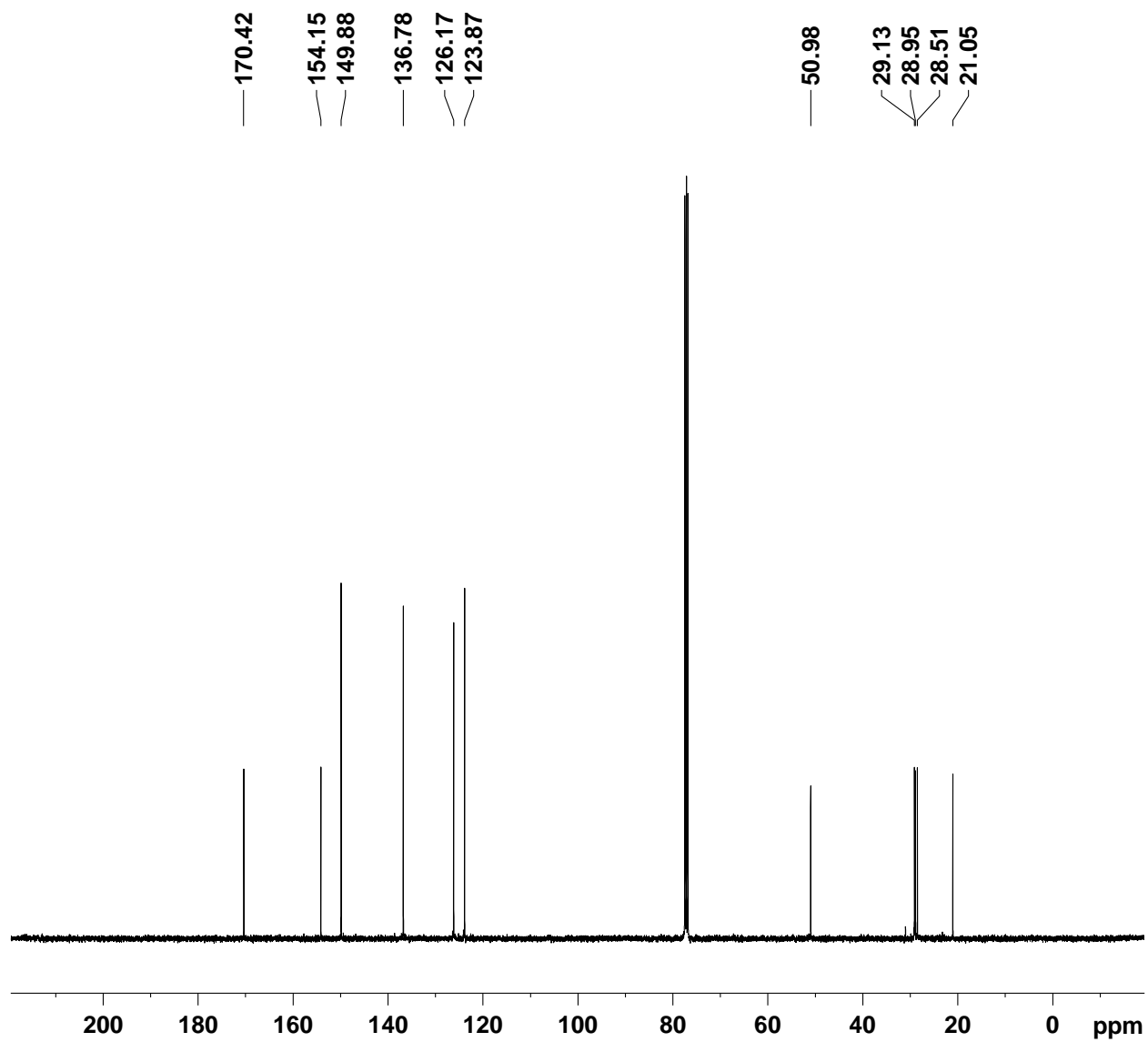


Figure S11. ^{13}C NMR spectrum of *S,S'*-decyl-*bis*(Py_2TTA) (12) in CDCl_3 .

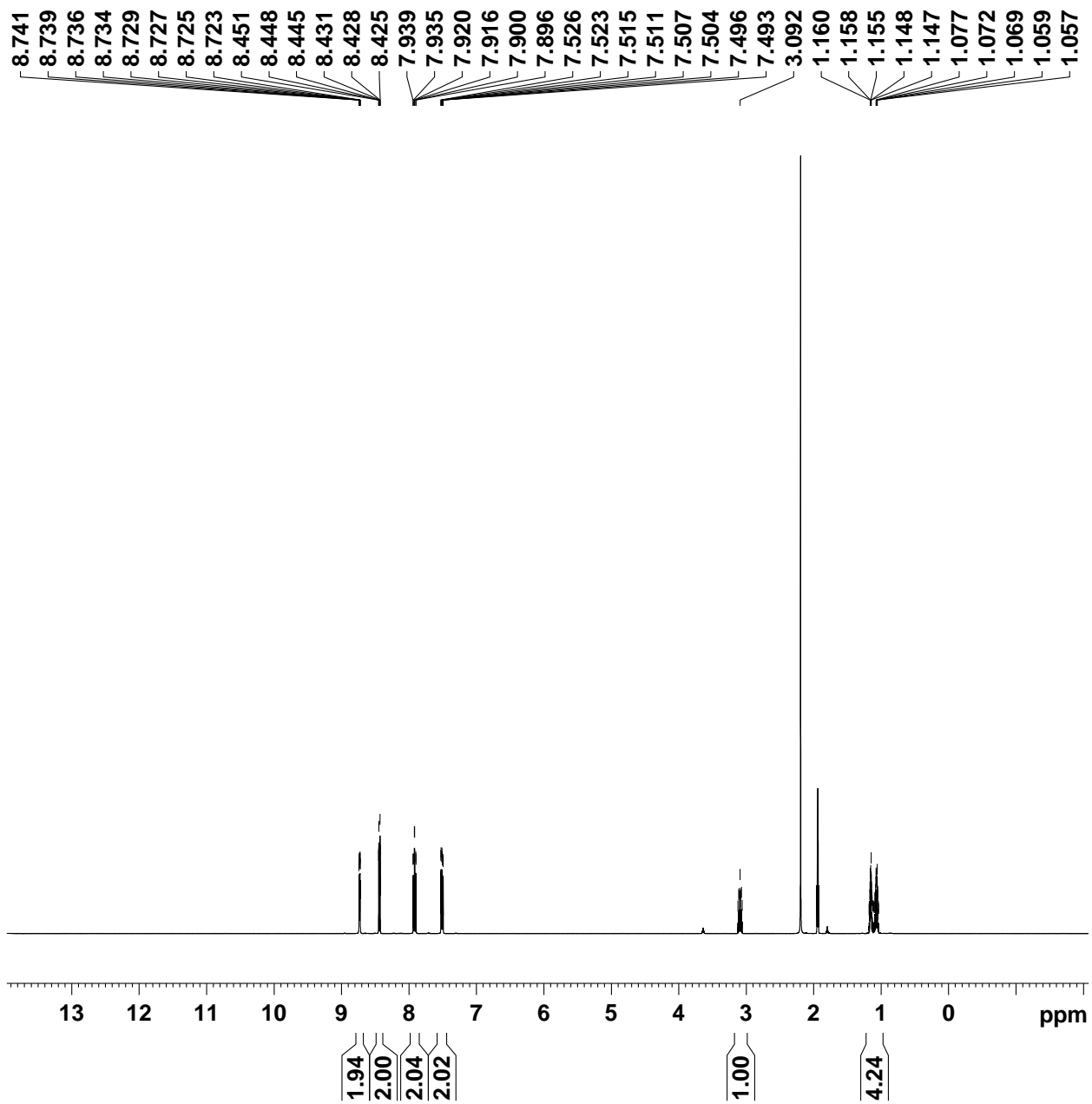


Figure S12. ^1H NMR spectrum of *S*-cyclopropyl-Py₂TTA (**13**) in CD₃CN.

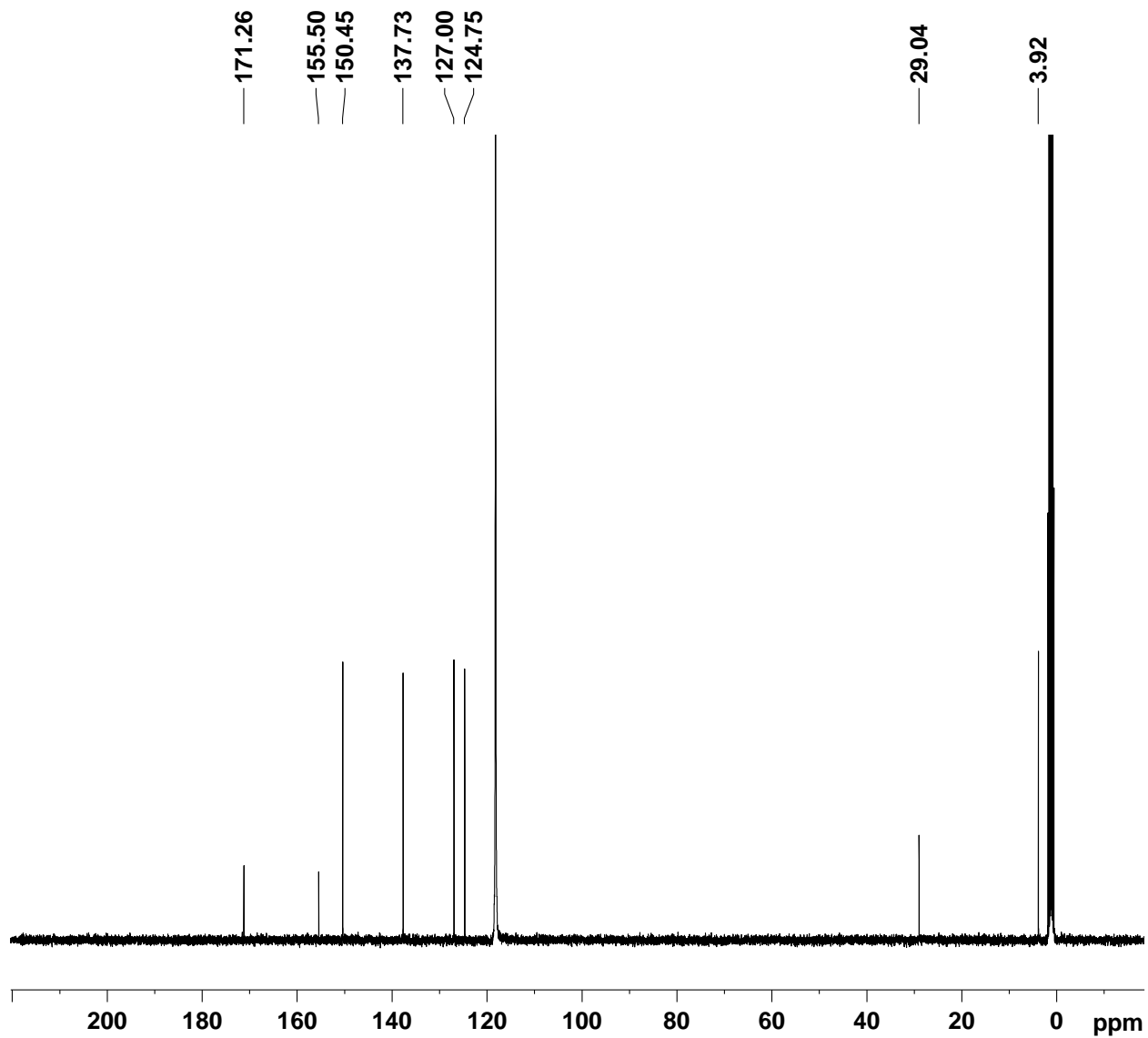


Figure S13. ^{13}C NMR spectrum of *S*-cyclopropyl-Py₂TTA (13) in CD₃CN.

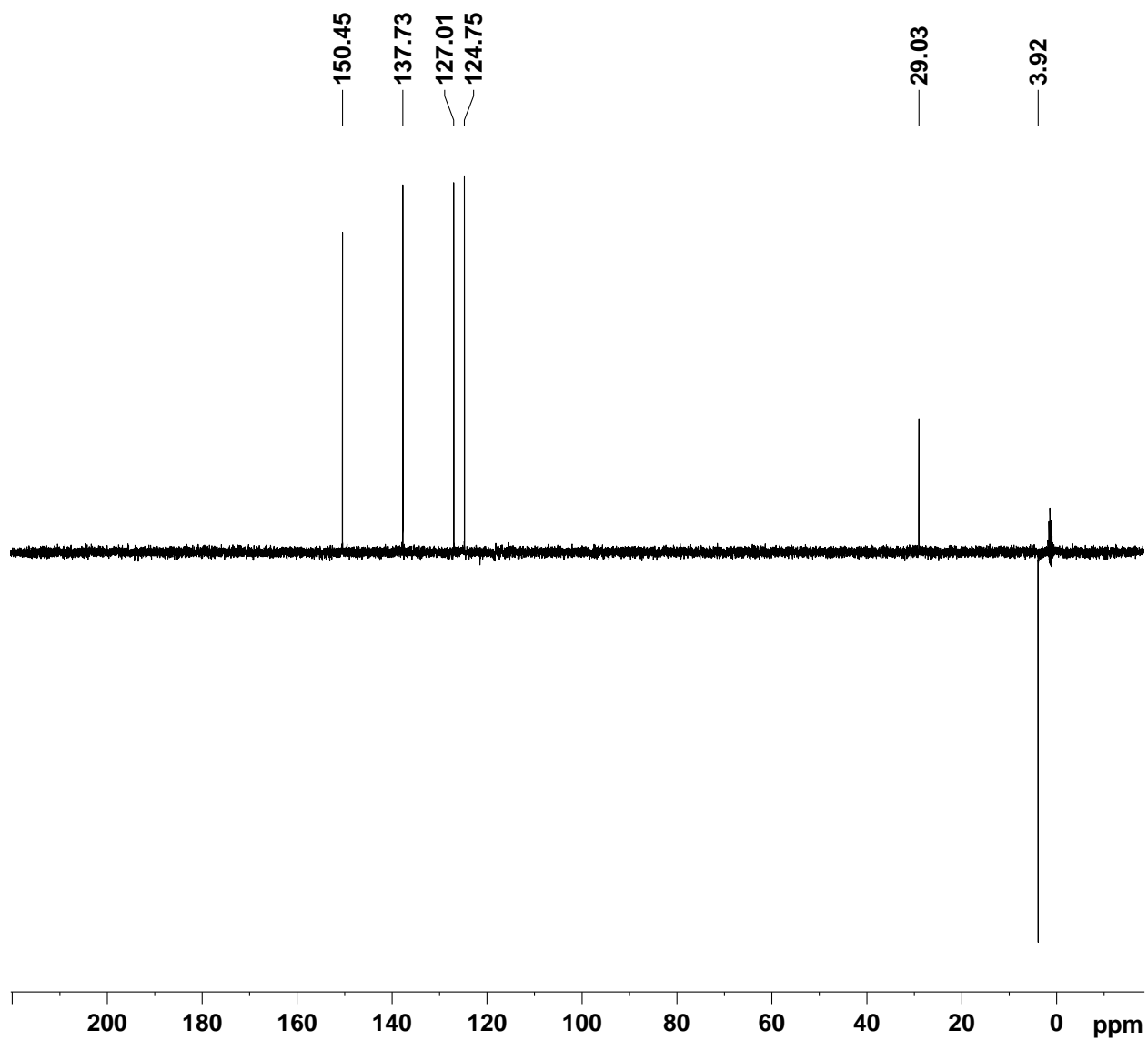


Figure S14. DEPT-135 spectrum of *S*-cyclopropyl-Py₂TTA (13) in CD₃CN.

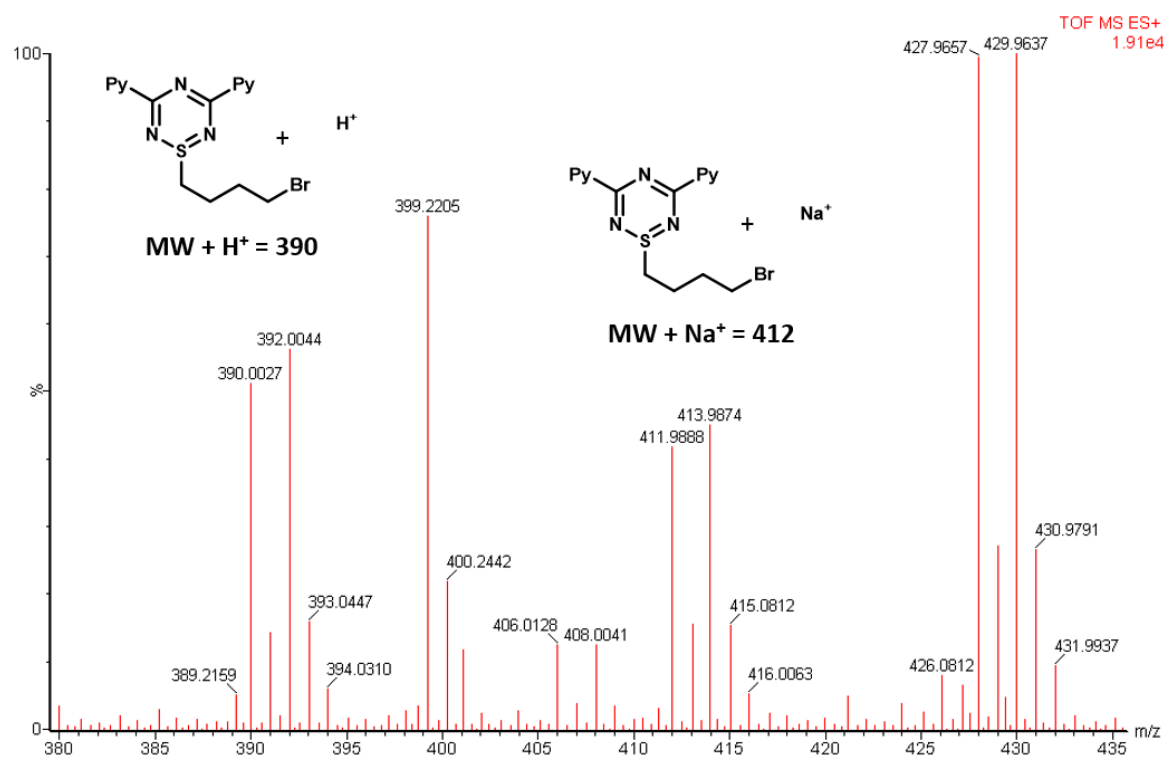
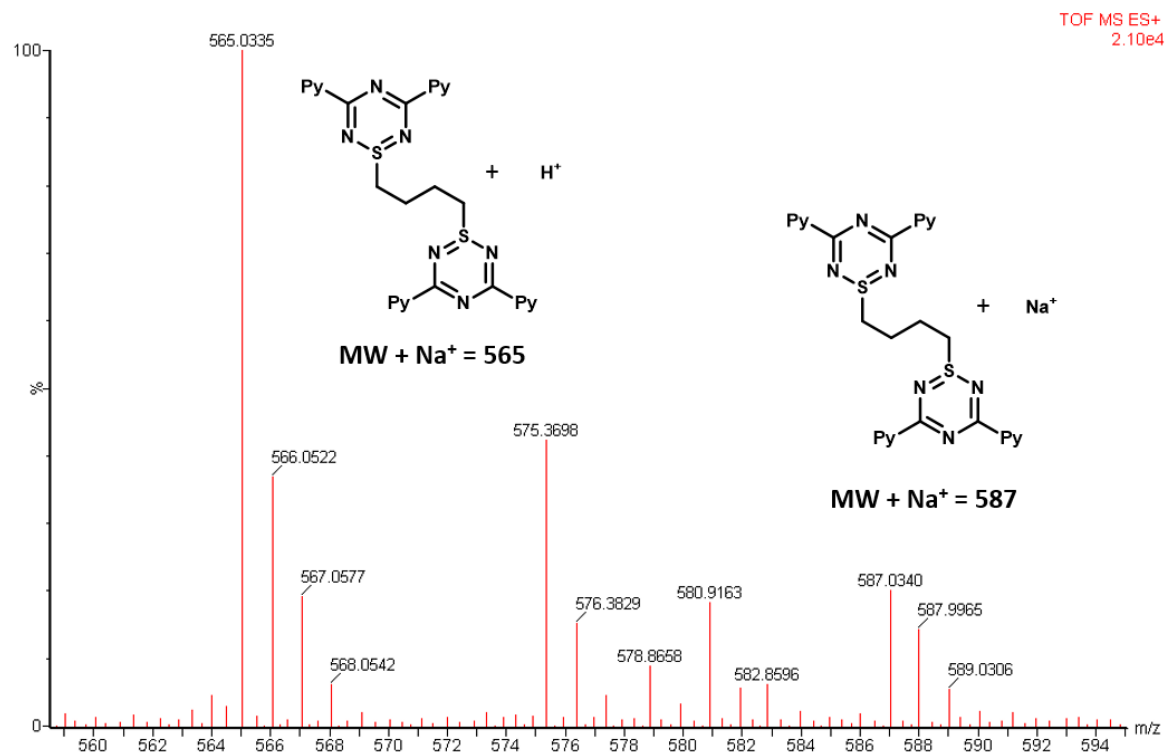


Figure S15. Mass to charge ratios of *S,S'*-butyl-*bis*(Py₂TTA) (**8**) and mono-alkylated intermediate (**16**, where *n* = 4) from electron spray ionization mass spectrometry.

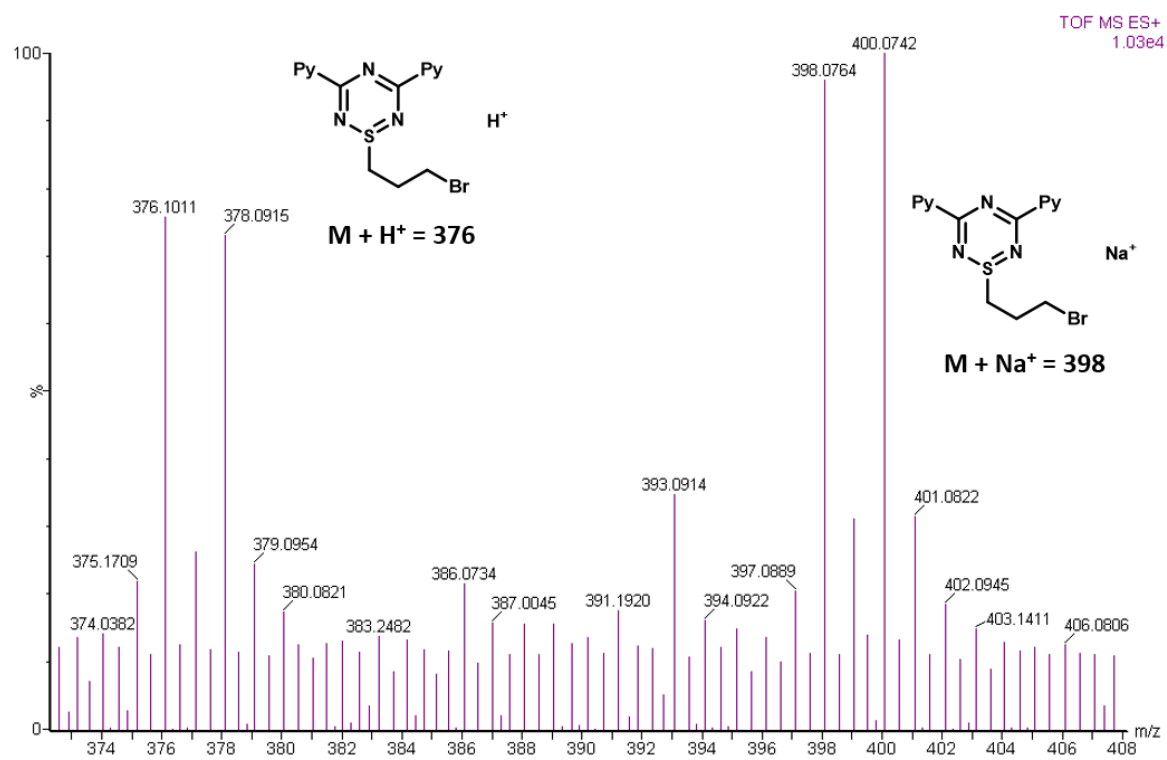
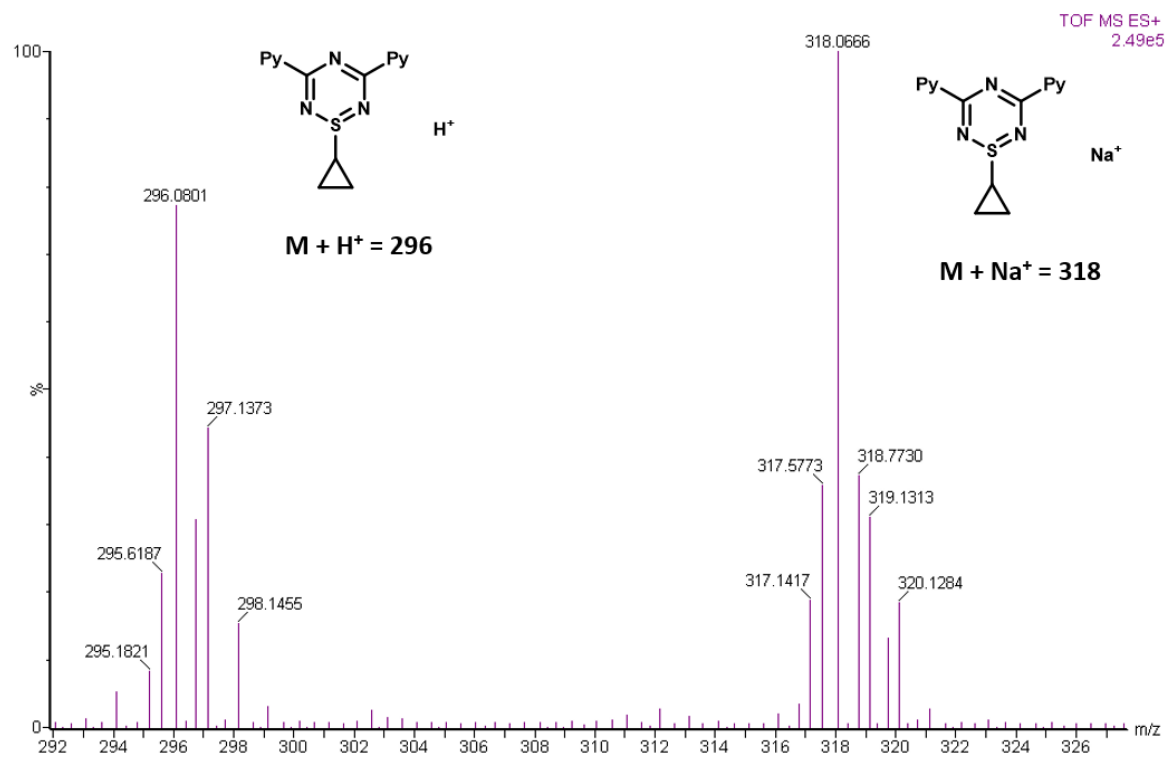


Figure S16. Mass to charge ratios of *S,S'*-cyclopropyl-Py₂TTA (**13**) and mono-alkylated intermediate (**16**, where n = 3) from electron spray ionization mass spectrometry.

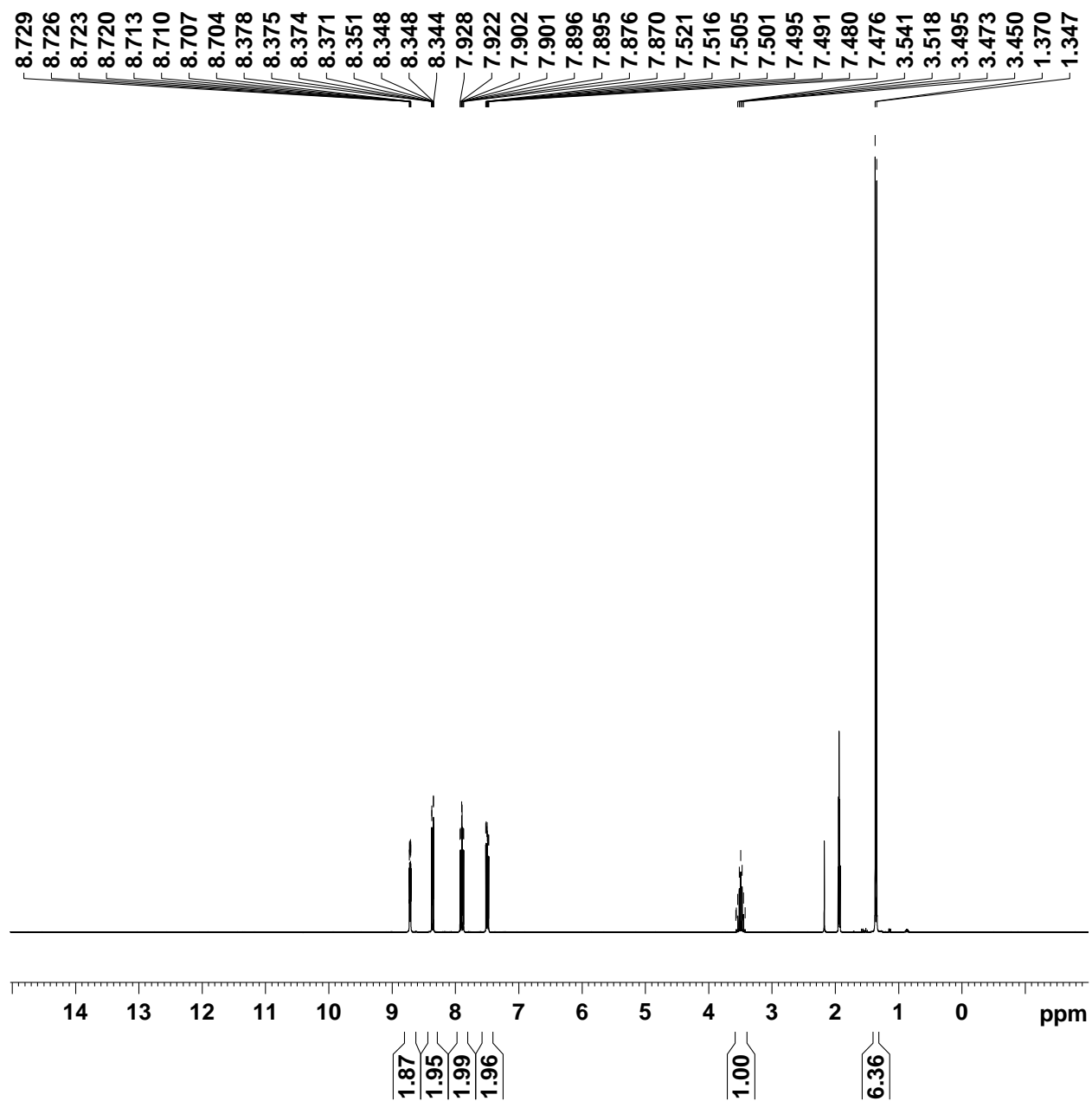


Figure S17. ^1H NMR spectrum of *S*-isopropyl-Py₂TTA (**6**) in CD₃CN.

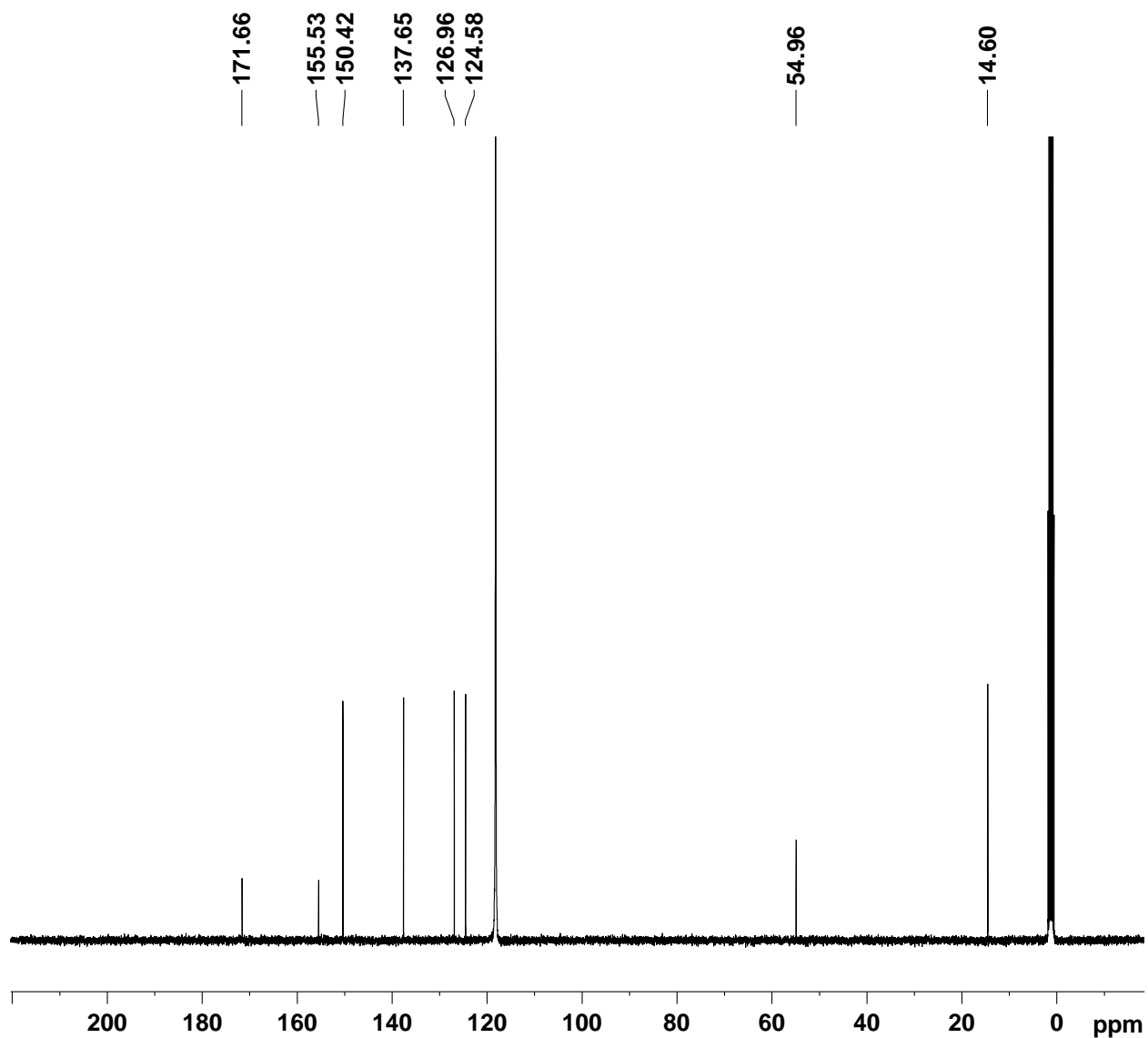


Figure S18. ^{13}C NMR spectrum of *S*-isopropyl-Py₂TTA (6) in CD₃CN.

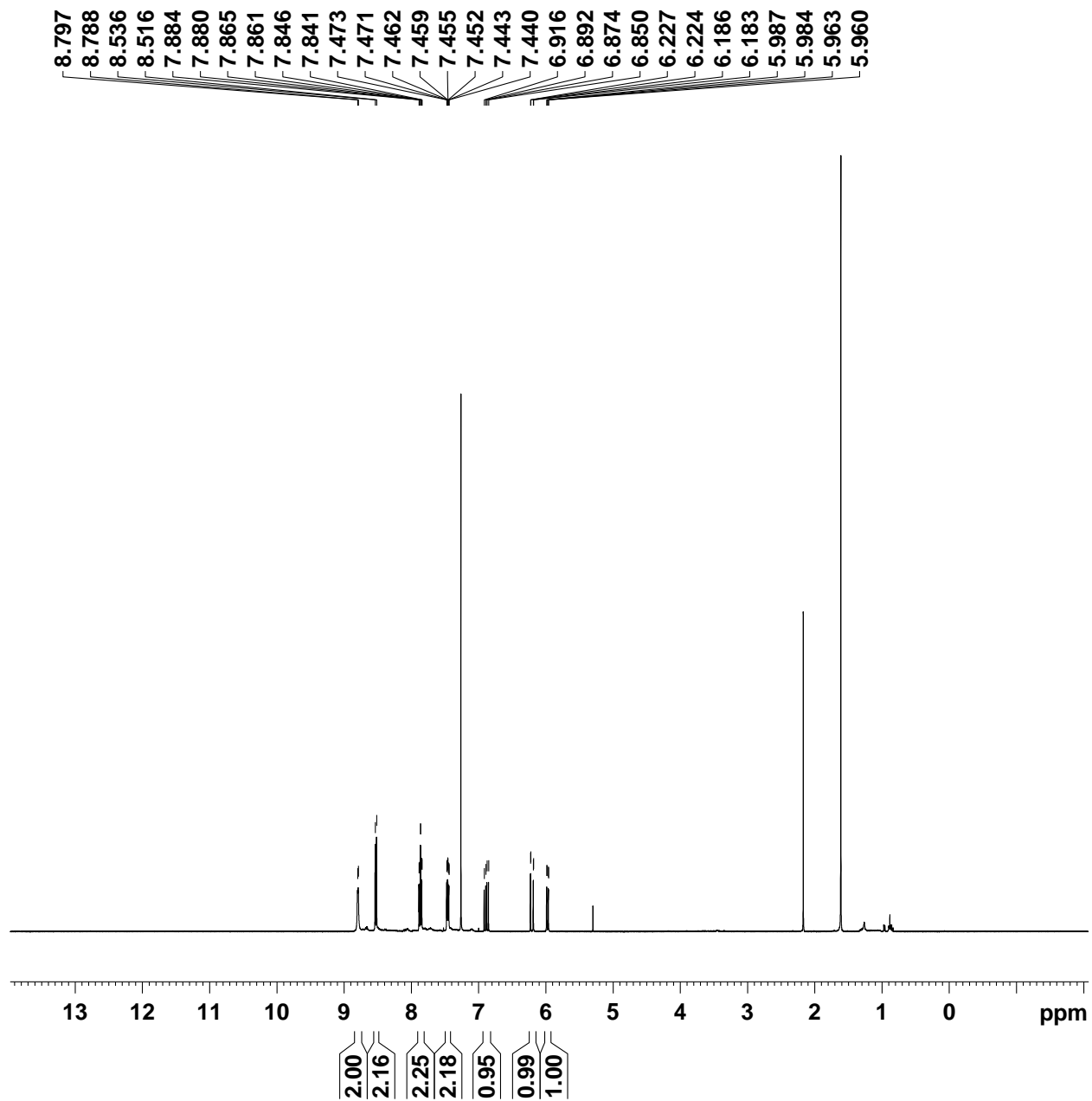


Figure S19. ^1H NMR spectrum of *S*-ethenyl-Py₂TTA (14) in CDCl_3 .

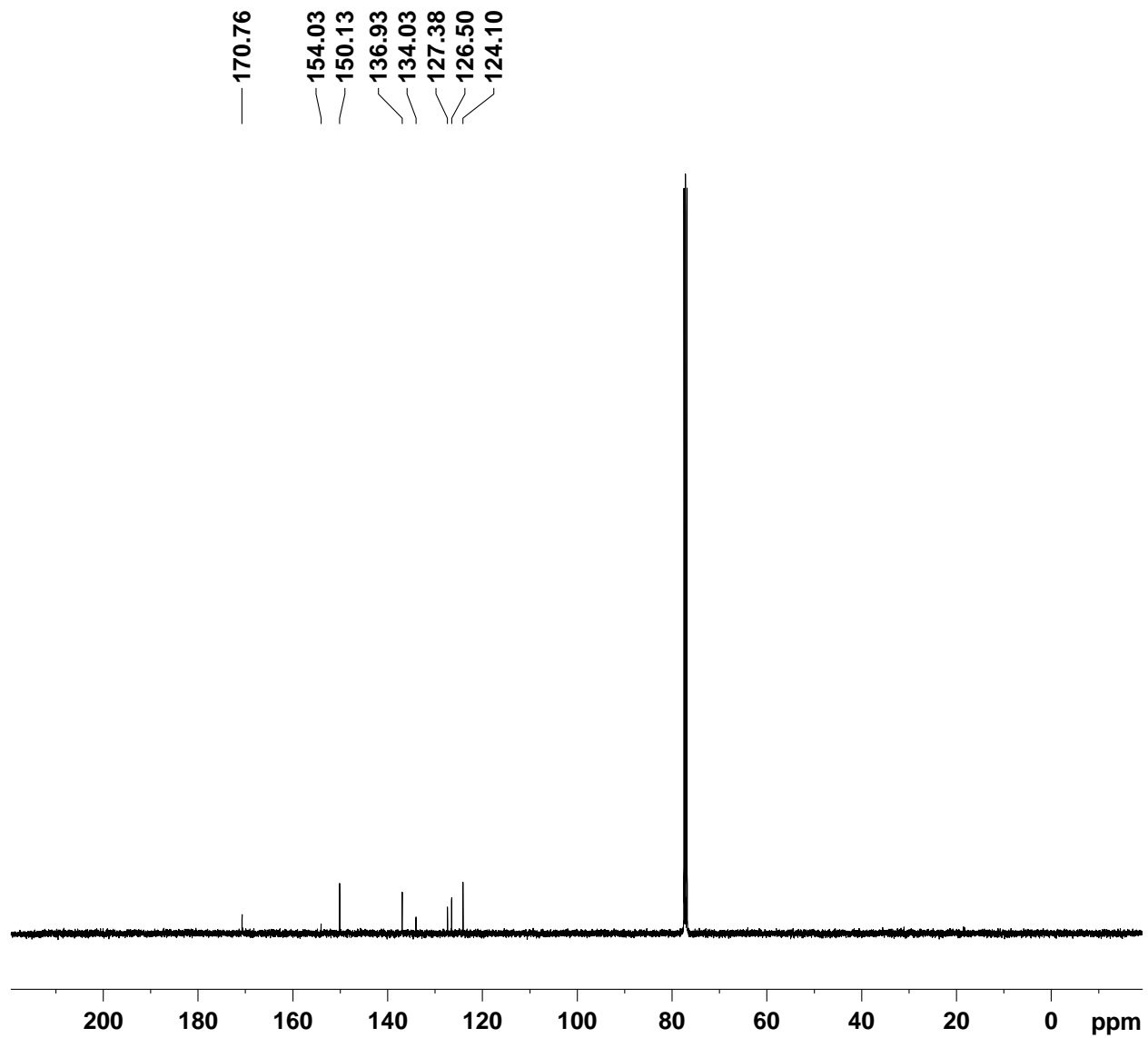


Figure S20. ^{13}C NMR spectrum of *S*-ethenyl-Py₂TTA (**14**) in CDCl₃.

Table S1. Crystallographic data and selected collection parameters for **12** and **13**.

Parameters	12	13
Empirical formula	C ₃₆ H ₄₀ Cl ₄ N ₁₀ S ₂	C ₁₅ H ₁₃ N ₅ S
Formula weight	818.7	295.36
Crystal system	Monoclinic	Monoclinic
a (Å)	18.9919(12)	10.4365(14)
b (Å)	14.2910(8)	15.482(2)
c (Å)	16.4594(16)	9.3960(12)
α (°)	90°	90°
β (°)	122.227(3)°	110.589(1)°
γ (°)	90°	90°
V (Å ³)	3779.1(5)	1421.2(3)
T (K)	200(2)	200(2)
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
Z	4	4
Wavelength	0.71073 Å	0.71073 Å
Density (calculated)	1.439 g/cm ³	1.380 g/cm ³
Absorption coefficient	0.467 mm ⁻¹	0.228 mm ⁻¹
F(000)	1704	616
Crystal size	0.715 x 0.441 x 0.280 mm ³	0.515 x 0.268 x 0.220 mm ³
Theta range for data collection	1.907 to 25.239°	2.085 to 29.130°
Index ranges	-21 ≤ <i>h</i> ≤ 22, -17 ≤ <i>k</i> ≤ 14, -18 ≤ <i>l</i> ≤ 19	-14 ≤ <i>h</i> ≤ 14, -20 ≤ <i>k</i> ≤ 20, -12 ≤ <i>l</i> ≤ 12
Reflections collected	7805	17260
Independent reflections	3374 [<i>R</i> _{int} = 0.0381]	3627 [<i>R</i> _{int} = 0.0278]
Completeness to theta = 25.239°	98.8 %	100.0 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6129	0.7458 and 0.6963
Data / restraints / parameters	3374 / 17 / 245	3627 / 0 / 190
Goodness-of-fit on <i>F</i> ²	1.079	1.034
Final <i>R</i> indices [<i>I</i> > 2σ _{<i>I</i>}]	<i>R</i> ₁ = 0.0872, <i>wR</i> ₂ = 0.2195	<i>R</i> ₁ = 0.0418, <i>wR</i> ₂ = 0.1088
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1292, <i>wR</i> ₂ = 0.2481	<i>R</i> ₁ = 0.0531, <i>wR</i> ₂ = 0.1157
Largest diff. peak and hole	0.756 and -0.608 e ⁻ Å ⁻³	0.305 and -0.203 e ⁻ Å ⁻³

Computation Study

Conformational Analysis

To locate the lowest energy conformations of the mono-alkylated intermediates corresponding to compound **16** ($n = 3, 4$), a molecular mechanics conformational search was performed using Avagadro v1.1.1.¹ All searches started with the fully extended linear chains (all C-C bonds anti-periplanar). The conformational sampling was carried out using MMFF94 and a systematic rotor search.² All conformations that were within 3 kcal/mol of the global minimum were fully optimized in Gaussian09 using B3LYP/6-31G(d) to ensure the global minima were correctly assigned.³

Reaction of second conformation of bromopropyl anion

Deprotonation of **B** leads directly to a conformation of the bromopropyl anion **D1** that is also capable of directly undergoing cyclization (Figure S21). This conformation (**D1**) is 1.2 kcal/mol higher in energy than the lowest energy conformer **D**. The cyclization of this conformer occurs with a barrier of 12.9 kcal/mol. This suggest that cyclization of the bromopropyl anion can occur without any change in conformation and while the transition state from this conformation is higher in energy than that leading from the lowest energy conformation of the anion, it is still 3 kcal/mol lower in energy than the intermolecular substitution.

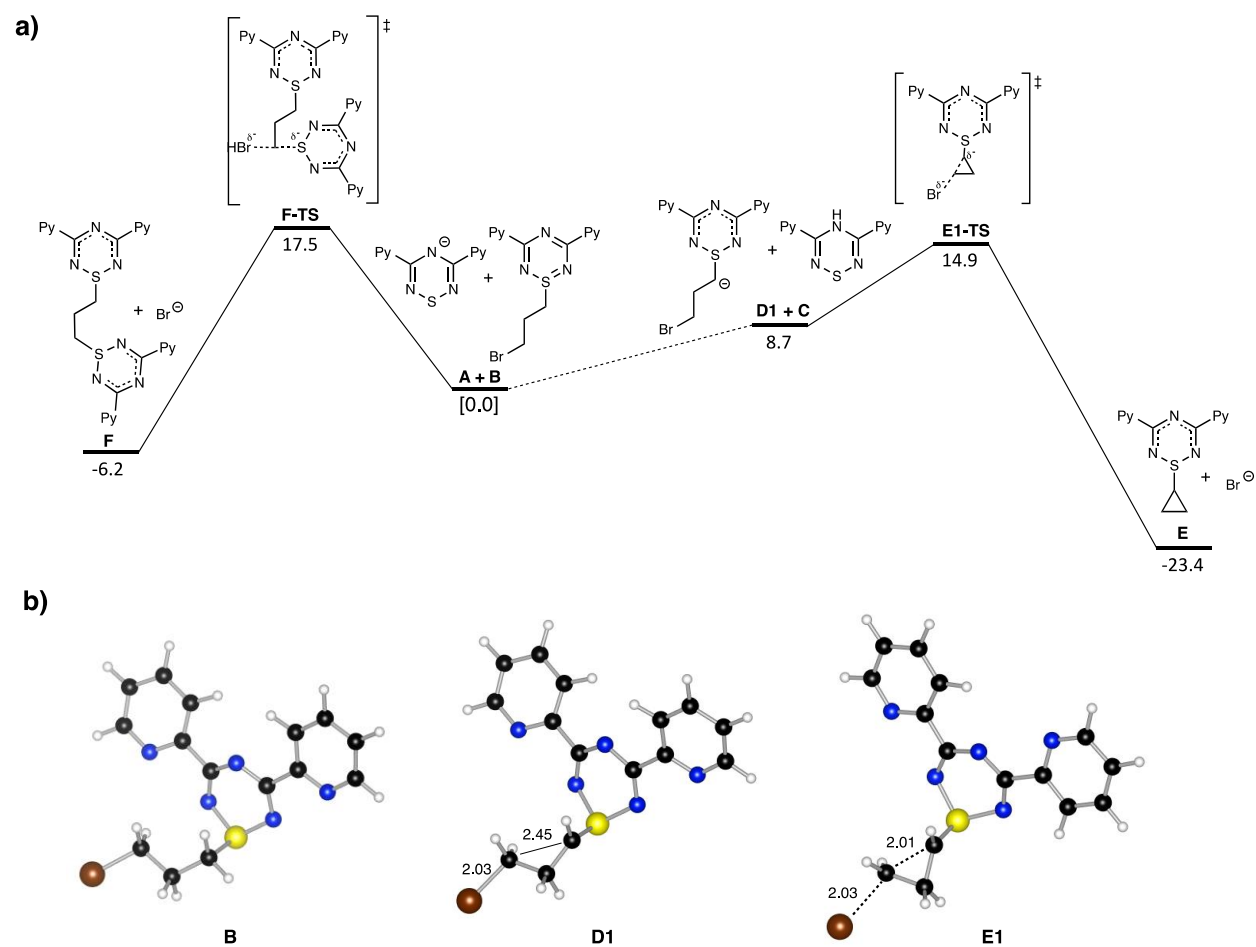
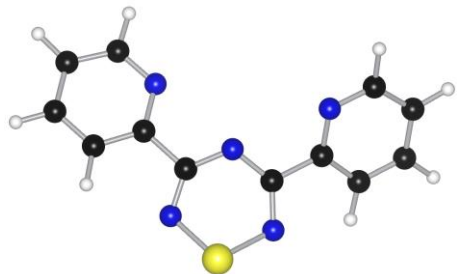


Figure S21. a) Intra- and intermolecular substitution paths for a second conformation of the bromopropyl anion **D1**. Reported values are free energies at 298K and are reported in kcal/mol. Energies for the intramolecular pathways include the energy of **Py₂TTAH** (**C**). b) Structures associated with the cyclization pathway. Distances reported in Angstroms.

Energies and Reaction Coordinates

A



HF (B3LYP/6-31+G(d,p)) = -1134.086189 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -1133.830906 Hartrees

Imaginary Frequencies: none found

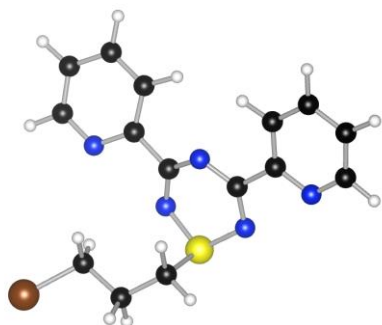
Zero-point correction = 0.18342 (Hartree/Particle)

Thermal correction = 0.139036 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.353696	1.939420	0.124416
2	6	0	1.147595	0.677916	-0.174382
3	6	0	-1.160222	0.644716	-0.140339
4	7	0	-1.400380	1.904364	0.142219
5	16	0	-0.038853	2.945946	-0.170780
6	7	0	-0.002517	0.024217	-0.493061
7	6	0	2.390160	-0.176508	-0.076956
8	6	0	3.484877	0.264962	0.694097
9	6	0	3.531588	-2.084306	-0.670071
10	6	0	4.621323	-0.530791	0.783300
11	1	0	3.407186	1.220667	1.198582
12	1	0	3.518435	-3.013476	-1.240852
13	1	0	5.468976	-0.213547	1.386829
14	6	0	-2.377881	-0.239538	0.002563
15	6	0	-3.662358	0.338156	-0.070034
16	6	0	-3.298518	-2.327238	0.304818
17	6	0	-4.785065	-0.471888	0.053033
18	1	0	-3.737280	1.409136	-0.215722
19	1	0	-3.113502	-3.391279	0.456336
20	1	0	-5.783019	-0.042614	-0.003168
21	6	0	4.654743	-1.742673	0.084551
22	1	0	5.519369	-2.400411	0.120718
23	6	0	-4.607390	-1.846516	0.246429
24	1	0	-5.451589	-2.523943	0.346244
25	7	0	2.423276	-1.338803	-0.750061
26	7	0	-2.208367	-1.560257	0.185267

B



HF (B3LYP/6-31+G(d,p)) = -3823.686609 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3823.3798886 Hartrees

Imaginary Frequencies: none found

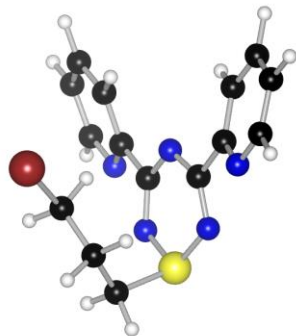
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Thermal correction = 0.219264 Hartrees

Coordinates from last standard orientation:

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1	7	0	-1.764057	-1.595935	1.058787
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3	6	0	-0.319346	0.822647	0.578658
4	7	0	0.397639	0.056763	1.395156
5	16	0	-0.119419	-1.542102	1.425968
6	7	0	-1.492520	0.549002	-0.027307
7	6	0	-3.609673	-0.616550	-0.119359
8	6	0	-5.512723	0.412355	-1.173148
9	6	0	-5.563603	-1.809296	-0.277284
10	1	0	-5.982403	1.252994	-1.675671
11	1	0	-6.083395	-2.742697	-0.069840
12	6	0	0.231052	2.199950	0.346033
13	6	0	-0.077576	4.526335	-0.176703
14	6	0	2.073410	3.566885	0.272171
15	1	0	-0.715834	5.370044	-0.422619
16	1	0	3.153755	3.650363	0.370526
17	6	0	-6.225670	-0.759142	-0.923421
18	1	0	-7.264232	-0.865657	-1.221086
19	6	0	1.301454	4.688922	-0.045885
20	1	0	1.773538	5.655960	-0.188507
21	6	0	0.601988	-2.243467	-0.135431
22	6	0	2.134286	-2.322411	-0.130960
23	1	0	0.213328	-1.647216	-0.966484
24	1	0	0.157409	-3.243002	-0.185557
25	6	0	2.809303	-0.968079	-0.325223
26	1	0	2.493645	-2.796190	0.790124
27	1	0	2.421121	-2.988110	-0.952802
28	1	0	2.433633	-0.454047	-1.210427
29	1	0	2.716056	-0.302708	0.529504
30	35	0	4.737665	-1.199824	-0.643325
31	6	0	-0.625249	3.258913	0.015382
32	1	0	-1.688189	3.075201	-0.078463
33	6	0	-4.181526	0.489016	-0.765314
34	1	0	-3.580027	1.371745	-0.938524
35	7	0	1.560325	2.349274	0.470213
36	7	0	-4.289775	-1.750306	0.115546

B1 (conformation leading directly to D)



HF (B3LYP/6-31+G(d,p)) = -3823.684044 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3823.3781037 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.272014 (Hartree/Particle)

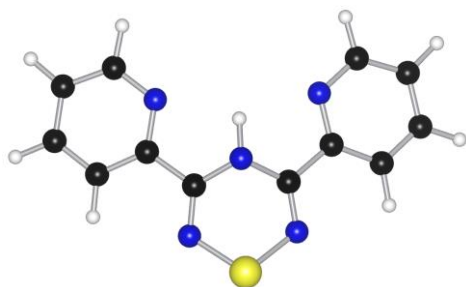
Thermal correction = 0.220059 Hartrees

Coordinates from last standard orientation:

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			X	Y	Z
1	7	0	1.045393	-0.650522	2.068753
2	6	0	0.788544	-1.114804	0.852700
3	6	0	-1.496220	-0.629889	0.747525
4	7	0	-1.636934	-0.004085	1.901863
5	16	0	-0.212309	0.197428	2.790739
6	7	0	-0.375963	-1.127986	0.168640
7	6	0	1.948615	-1.760811	0.150144
8	6	0	2.809773	-3.265713	-1.514954
9	6	0	4.220738	-1.981496	-0.062884
10	1	0	2.662478	-3.985203	-2.315159
11	1	0	5.205680	-1.674279	0.283059
12	6	0	-2.752863	-0.802276	-0.058504
13	6	0	-3.842530	-1.112476	-2.180013
14	6	0	-5.042683	-0.901341	-0.116051
15	1	0	-3.807314	-1.241413	-3.257903
16	1	0	-5.973002	-0.873432	0.447901
17	6	0	4.093159	-2.912961	-1.098918
18	1	0	4.976600	-3.341596	-1.561882
19	6	0	-5.061392	-1.079094	-1.503761
20	1	0	-6.004817	-1.186453	-2.030041
21	6	0	0.225757	1.989921	2.475638
22	6	0	0.985880	2.331571	1.190589
23	1	0	0.830761	2.253377	3.349150
24	1	0	-0.741636	2.498352	2.559552
25	6	0	0.144101	2.260572	-0.075463
26	1	0	1.359767	3.354946	1.313817
27	1	0	1.864044	1.684548	1.098687
28	1	0	-0.133171	1.247919	-0.351436
29	1	0	-0.745356	2.888208	-0.019059
30	35	0	1.155277	2.931486	-1.627532
31	7	0	-3.922977	-0.757081	0.597187
32	7	0	3.181064	-1.417244	0.556520
33	6	0	-2.663994	-0.975754	-1.447611
34	1	0	-1.690903	-0.999135	-1.922653
35	6	0	1.714698	-2.675887	-0.885535

36 1 0 0.695545 -2.905653 -1.170398

C



HF (B3LYP/6-31+G(d,p)) = -1134.6646995 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -1134.3367957 Hartrees

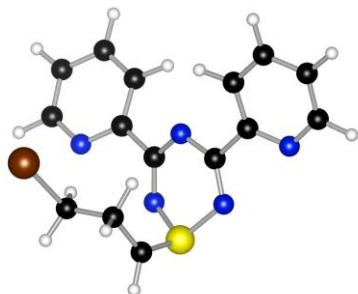
Imaginary Frequencies: none found

Zero point correction = 0.198665 (Hartree/Particle)

Thermal correction = 0.156254 Hartrees

Coordinates from last standard orientation:

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			X	Y	Z
1	7	0	1.369993	2.029866	0.079119
2	6	0	1.207247	0.780002	-0.171120
3	6	0	-1.207253	0.780062	-0.171193
4	7	0	-1.369941	2.029913	0.079047
5	16	0	0.000098	3.054907	-0.120160
6	7	0	0.000030	0.202203	-0.584158
7	6	0	2.355477	-0.156814	-0.027201
8	6	0	3.629792	0.312371	0.324034
9	6	0	3.098401	-2.329035	-0.159127
10	6	0	4.664868	-0.610600	0.432385
11	1	0	3.777377	1.370855	0.502773
12	1	0	2.848300	-3.368192	-0.359759
13	1	0	5.664300	-0.283775	0.703812
14	6	0	-2.355483	-0.156757	-0.027242
15	6	0	-3.629669	0.312395	0.324484
16	6	0	-3.098632	-2.328871	-0.159800
17	6	0	-4.664785	-0.610542	0.432829
18	1	0	-3.777146	1.370834	0.503583
19	1	0	-2.848676	-3.367981	-0.360857
20	1	0	-5.664105	-0.283728	0.704677
21	6	0	4.399234	-1.961588	0.187427
22	1	0	5.178797	-2.712952	0.261519
23	6	0	-4.399325	-1.961461	0.187330
24	1	0	-5.178894	-2.712815	0.261457
25	7	0	2.093203	-1.451691	-0.266446
26	7	0	-2.093394	-1.451572	-0.267051
27	1	0	0.000017	-0.816774	-0.615052

D

HF (B3LYP/6-31+G(d,p)) = -3823.1183083 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3822.8687052 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.257261 (Hartree/Particle)

Thermal correction = 0.204351 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.957029	-0.641792	1.769706
2	6	0	-1.891316	0.083824	0.673279
3	6	0	0.199947	1.025837	1.005683
4	7	0	0.463999	0.501205	2.186022
5	16	0	-0.453424	-0.927688	2.587538
6	7	0	-0.872122	0.844831	0.198244
7	6	0	-3.128473	0.117300	-0.190867
8	6	0	-4.164543	0.563017	-2.326841
9	6	0	-5.385978	-0.247477	-0.438158
10	1	0	-4.103091	0.881790	-3.364824
11	1	0	-6.315086	-0.567682	0.033923
12	6	0	1.199064	2.024415	0.485840
13	6	0	1.702784	4.018941	-0.776225
14	6	0	3.383364	2.731646	0.339340
15	1	0	1.390444	4.861953	-1.388241
16	1	0	4.423204	2.541050	0.603885
17	6	0	-5.382820	0.157719	-1.775042
18	1	0	-6.300538	0.152328	-2.356944
19	6	0	3.048590	3.838617	-0.443280
20	1	0	3.817699	4.525716	-0.785267
21	6	0	0.270842	-2.259102	1.891918
22	6	0	0.666986	-2.405191	0.449637
23	1	0	0.579699	-2.997345	2.625674
24	6	0	2.101369	-1.913216	0.282006
25	1	0	0.603718	-3.455298	0.134259
26	1	0	0.002692	-1.837181	-0.210205
27	1	0	2.231893	-0.856638	0.504986
28	1	0	2.806937	-2.504869	0.864332
29	35	0	2.785141	-2.118431	-1.619570
30	6	0	0.767563	3.098669	-0.313771
31	1	0	-0.286331	3.175532	-0.553775
32	6	0	-3.025891	0.549974	-1.527081
33	1	0	-2.055630	0.858018	-1.896948
34	7	0	2.494305	1.845613	0.800442
35	7	0	-4.299108	-0.278306	0.339135

D 1

HF (B3LYP/6-31+G(d,p)) = -3823.115956 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3822.862049 Hartrees

Imaginary Frequencies: none found

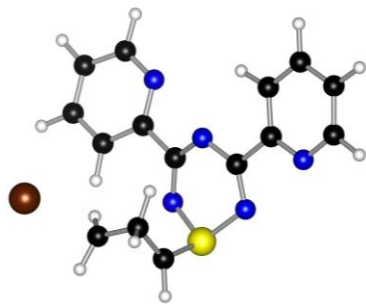
Zero point correction = 0.257082 (Hartree/Particle)

Thermal correction = 0.203907 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.145499	0.722812	1.439125
2	6	0	0.761022	1.144790	0.564956
3	6	0	2.040466	-0.802366	0.399633
4	7	0	1.333332	-1.584914	1.201320
5	16	0	-0.161077	-0.945777	1.638774
6	7	0	1.771002	0.460584	-0.012310
7	6	0	0.689029	2.604467	0.219269
8	6	0	1.746815	4.650294	-0.472115
9	6	0	-0.598288	4.490253	-0.000239
10	1	0	2.626863	5.214447	-0.767108
11	1	0	-1.590006	4.932935	0.067647
12	6	0	3.341983	-1.372879	-0.095654
13	6	0	5.368718	-1.163420	-1.375954
14	6	0	4.803800	-3.140755	-0.146483
15	1	0	6.030073	-0.594850	-2.023414
16	1	0	5.023642	-4.154142	0.184010
17	6	0	0.498826	5.267111	-0.386426
18	1	0	0.371030	6.320789	-0.614362
19	6	0	5.699803	-2.457202	-0.976196
20	1	0	6.622498	-2.931382	-1.296149
21	6	0	-1.218413	-1.496826	0.214872
22	6	0	-2.666888	-1.031241	0.400311
23	1	0	-1.124176	-2.588335	0.218923
24	1	0	-0.759702	-1.101275	-0.696335
25	6	0	-3.518890	-1.562157	-0.740739
26	1	0	-3.060745	-1.397453	1.355236
27	1	0	-2.707149	0.061591	0.426720
28	1	0	-3.190378	-1.179959	-1.708038
29	1	0	-3.530764	-2.652486	-0.770791
30	35	0	-5.406821	-1.029014	-0.591196
31	6	0	4.170713	-0.607376	-0.929073
32	1	0	3.862550	0.391047	-1.210884
33	6	0	1.846012	3.292881	-0.171139
34	1	0	2.788411	2.762352	-0.226678
35	7	0	3.651938	-2.622796	0.284296
36	7	0	-0.515691	3.191626	0.302223

E-TS



HF (B3LYP/6-31+G(d,p)) = -3823.105861 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3822.855421 Hartrees

Imaginary Frequencies: 1 (-409.33 cm⁻¹)

Zero-point correction = 0.256476 (Hartree/Particle)

Thermal Correction = 0.204000 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.948553	-0.992927	1.607581
2	6	0	-2.018833	-0.190092	0.562734
3	6	0	-0.062812	0.997873	0.896551
4	7	0	0.356753	0.388953	1.999586
5	16	0	-0.401093	-1.110908	2.345197
6	7	0	-1.125774	0.728192	0.122212
7	6	0	-3.301945	-0.222333	-0.230400
8	6	0	-4.717544	0.737032	-1.929602
9	6	0	-5.326544	-1.210520	-0.679107
10	1	0	-4.915917	1.489566	-2.688754
11	1	0	-6.020746	-2.017507	-0.445601
12	6	0	0.772346	2.188338	0.495655
13	6	0	2.878692	3.361404	0.517422
14	6	0	0.946357	4.181848	-0.631207
15	1	0	3.922235	3.433417	0.811445
16	1	0	0.446862	4.930854	-1.245133
17	6	0	-5.645144	-0.273069	-1.665527
18	1	0	-6.585512	-0.339414	-2.205811
19	6	0	2.287136	4.346624	-0.275123
20	1	0	2.844956	5.214351	-0.615741
21	6	0	0.494608	-2.326044	1.535044
22	6	0	0.799836	-2.387373	0.064677
23	1	0	0.647455	-3.200385	2.158242
24	6	0	2.135081	-1.924426	0.477149
25	1	0	0.768745	-3.388613	-0.369268
26	1	0	0.248266	-1.683006	-0.556969
27	1	0	2.292378	-0.878201	0.679080
28	1	0	2.818684	-2.626655	0.928198
29	35	0	3.720614	-1.785413	-1.475311
30	6	0	2.111061	2.270468	0.913745
31	1	0	2.520933	1.480603	1.530716
32	6	0	-3.529434	0.766597	-1.204544
33	1	0	-2.767497	1.520829	-1.361329
34	7	0	0.199451	3.134794	-0.266900
35	7	0	-4.190735	-1.197558	0.024499

E1-TS



HF (B3LYP/6-31+G(d,p)) = -3823.1056158 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3822.8510794 Hartrees

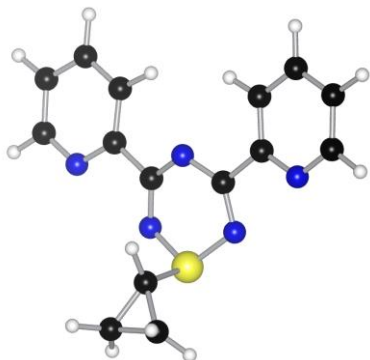
Imaginary Frequencies: 1 (-409.87 cm⁻¹)

Zero point correction = 0.256199 (Hartree/Particle)

Thermal correction = 0.202835 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.094154	1.015866	1.043449
2	6	0	-1.011441	1.212691	0.350972
3	6	0	-1.822163	-0.952028	0.327968
4	7	0	-0.863472	-1.516185	1.054466
5	16	0	0.598222	-0.613898	1.131838
6	7	0	-1.911214	0.311719	-0.115956
7	6	0	-1.396019	2.648749	0.096729
8	6	0	-3.004988	4.265547	-0.682064
9	6	0	-0.865989	4.881889	0.197210
10	1	0	-3.973414	4.514143	-1.109222
11	1	0	-0.124158	5.632535	0.468168
12	6	0	-2.983814	-1.860508	0.017183
13	6	0	-3.902389	-4.086386	-0.143940
14	6	0	-5.173262	-2.119381	-0.634046
15	1	0	-3.800075	-5.165343	-0.059659
16	1	0	-6.098856	-1.631387	-0.938484
17	6	0	-2.093734	5.269391	-0.347051
18	1	0	-2.320445	6.320530	-0.502638
19	6	0	-5.112055	-3.511997	-0.541857
20	1	0	-5.982282	-4.119084	-0.774988
21	6	0	1.471482	-0.899073	-0.305716
22	6	0	2.756065	-1.685130	-0.271892
23	1	0	1.000349	-0.656879	-1.252476
24	6	0	3.410415	-0.370301	-0.256556
25	1	0	2.937674	-2.289222	-1.162323
26	1	0	2.923244	-2.279498	0.628024
27	1	0	3.489908	0.163337	0.677675
28	1	0	3.436067	0.218485	-1.160190
29	35	0	5.907818	-0.543953	-0.338076
30	6	0	-2.824779	-3.252888	0.139179
31	1	0	-1.863759	-3.640861	0.454572
32	6	0	-2.656165	2.936154	-0.458148
33	1	0	-3.317492	2.110674	-0.692932
34	7	0	-4.146799	-1.305515	-0.366497
35	7	0	-0.515374	3.611677	0.415954

E

HF (B3LYP/6-31+G(d,p)) = -1251.3139237 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -1250.942544 Hartrees

Imaginary Frequencies: none found

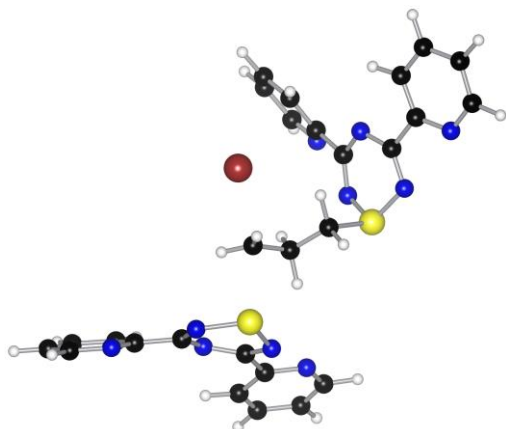
Zero point correction = 0.258159 (Hartree/Particle)

Thermal correction = 0.208643 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.372318	1.186439	-0.843694
2	6	0	-1.166952	0.001110	-0.286409
3	6	0	1.166880	0.000960	-0.286523
4	7	0	1.372362	1.186237	-0.843886
5	16	0	0.000085	2.159484	-0.895396
6	7	0	-0.000050	-0.574972	0.083046
7	6	0	-2.395220	-0.845709	-0.087512
8	6	0	-3.424695	-2.967858	0.393261
9	6	0	-4.686153	-0.978565	-0.042547
10	1	0	-3.356751	-4.026215	0.628276
11	1	0	-5.633737	-0.453755	-0.148991
12	6	0	2.395074	-0.845955	-0.087662
13	6	0	3.424419	-2.968588	0.391234
14	6	0	4.685987	-0.978602	-0.041095
15	1	0	3.356416	-4.027256	0.624829
16	1	0	5.633592	-0.453548	-0.146131
17	6	0	-4.664606	-2.344731	0.258143
18	1	0	-5.592515	-2.894179	0.383751
19	6	0	4.664362	-2.345146	0.257859
20	1	0	5.592237	-2.894648	0.383487
21	6	0	0.000244	2.924118	0.747226
22	6	0	0.752975	4.222478	0.909164
23	6	0	-0.752283	4.222585	0.909271
24	1	0	0.000255	2.197417	1.554696
25	1	0	1.261272	4.629763	0.039425
26	1	0	1.286405	4.361518	1.844185
27	1	0	-1.285558	4.361703	1.844369
28	1	0	-1.260646	4.629941	0.039604
29	6	0	2.268474	-2.208794	0.218508
30	1	0	1.281267	-2.641263	0.314863
31	6	0	-2.268702	-2.208158	0.220435
32	1	0	-1.281518	-2.640378	0.318111
33	7	0	3.587103	-0.239949	-0.210857
34	7	0	-3.587225	-0.239998	-0.212360

F-TS



HF (B3LYP/6-31+G(d,p)) = -4957.7780916 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -4957.202743 Hartrees

Imaginary Frequencies: 1 (-311.31 cm⁻¹)

Zero point correction = 0.455755 (Hartree/Particle)

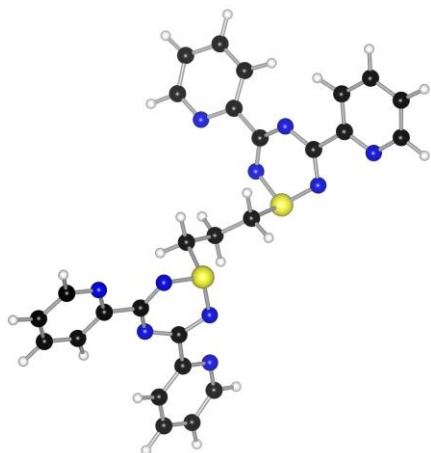
Thermal correction = 0.378200 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.708982	1.855322	-0.950028
2	6	0	4.395476	0.787118	-0.568390
3	6	0	3.174708	0.221674	1.329485
4	7	0	2.281462	1.195770	1.299941
5	16	0	2.196716	1.968751	-0.199889
6	7	0	4.131930	-0.090092	0.424212
7	6	0	1.231890	0.749190	-1.207318
8	6	0	-0.136193	0.435004	-0.601037
9	1	0	1.841949	-0.156132	-1.263170
10	1	0	1.158700	1.215600	-2.195729
11	6	0	-0.754155	-0.760390	-1.269759
12	1	0	-0.031855	0.213105	0.464763
13	1	0	-0.801642	1.307685	-0.682769
14	1	0	-1.581802	-1.276361	-0.810659
15	1	0	-0.416470	-1.113923	-2.230523
16	35	0	0.766976	-2.517963	-0.266010
17	7	0	-2.847955	1.816076	-1.605750
18	6	0	-3.557286	1.567427	-0.525036
19	6	0	-4.473474	-0.493346	-1.143060
20	7	0	-3.892966	-0.653266	-2.303822
21	16	0	-2.609031	0.444687	-2.609684
22	7	0	-4.260414	0.458568	-0.181898
23	6	0	3.152490	-0.653183	2.549403
24	6	0	3.331199	-2.841807	3.520796
25	6	0	2.818484	-0.883097	4.803335
26	6	0	3.037775	-2.262000	4.756450
27	1	0	3.489022	-3.912880	3.431172
28	1	0	2.590941	-0.393133	5.748849
29	1	0	2.970923	-2.858781	5.661646
30	6	0	5.676519	0.521967	-1.316531
31	6	0	7.545103	-0.917192	-1.799637
32	6	0	7.234362	1.209014	-2.855381
33	6	0	7.994741	0.045535	-2.704121
34	1	0	8.098243	-1.840309	-1.648701
35	1	0	7.551236	1.986087	-3.549625

36	1	0	8.905084	-0.095436	-3.279563
37	6	0	-3.655342	2.701526	0.462122
38	6	0	-4.800337	3.804537	2.273661
39	6	0	-2.765876	4.636206	1.325056
40	6	0	-3.798398	4.776144	2.257084
41	1	0	-5.623190	3.866684	2.981377
42	1	0	-1.957292	5.364975	1.288030
43	1	0	-3.806438	5.614554	2.947690
44	6	0	-5.551610	-1.486744	-0.793685
45	6	0	-6.918236	-2.572185	0.870548
46	6	0	-7.038958	-3.106043	-1.458569
47	6	0	-7.488290	-3.329787	-0.153879
48	1	0	-7.227728	-2.711005	1.903348
49	1	0	-7.460367	-3.672928	-2.288144
50	1	0	-8.255644	-4.072491	0.045368
51	7	0	2.862239	-0.086903	3.729353
52	7	0	6.101891	1.448949	-2.189492
53	6	0	3.401002	-2.025018	2.395945
54	1	0	3.601299	-2.423562	1.409495
55	6	0	6.371690	-0.676519	-1.088781
56	1	0	5.976865	-1.381956	-0.368938
57	6	0	-5.942104	-1.632381	0.548752
58	1	0	-5.467857	-1.011593	1.298556
59	6	0	-4.727873	2.749033	1.367502
60	1	0	-5.468032	1.959021	1.338170
61	7	0	-6.094741	-2.217958	-1.781216
62	7	0	-2.687131	3.633303	0.446288

F



HF (B3LYP/6-31+G(d,p)) = -2385.9639024 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -2385.270823 Hartrees

Imaginary Frequencies: none found

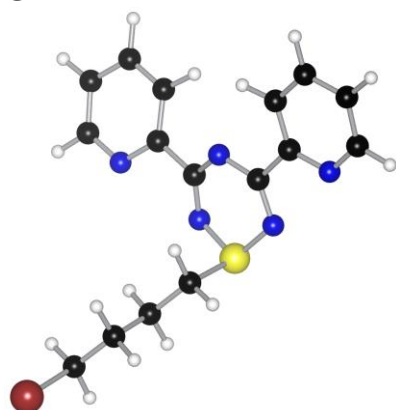
Zero point correction = 0.457825 (Hartree/Particle)

Thermal correction = 0.383757 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.544646	-1.905008	0.258085
2	6	0	4.398753	-0.928311	0.521649
3	6	0	3.861986	0.513918	-1.234818
4	7	0	2.947950	-0.232745	-1.843520

5	16	0	2.392264	-1.515158	-0.906244
6	7	0	4.530028	0.276595	-0.086839
7	6	0	1.092197	-0.689337	0.133460
8	6	0	-0.053938	-0.185492	-0.748128
9	1	0	1.590366	0.118309	0.679123
10	1	0	0.782476	-1.464254	0.841781
11	6	0	-1.069391	0.675715	0.007673
12	1	0	0.356521	0.433942	-1.554029
13	1	0	-0.571319	-1.030360	-1.215394
14	1	0	-1.837483	1.065777	-0.665835
15	1	0	-0.602399	1.512874	0.537188
16	7	0	-2.692946	-1.505074	0.453412
17	6	0	-3.844421	-1.151151	-0.105734
18	6	0	-4.230308	0.825683	1.078853
19	7	0	-3.125727	0.852647	1.809248
20	16	0	-1.965960	-0.273132	1.336274
21	7	0	-4.582265	-0.039074	0.095654
22	6	0	4.253911	1.769458	-1.961342
23	6	0	5.865462	3.481450	-2.468211
24	6	0	3.675380	3.424828	-3.440735
25	6	0	4.922442	4.047390	-3.325903
26	1	0	6.847197	3.930211	-2.347313
27	1	0	2.909757	3.842590	-4.091580
28	1	0	5.139443	4.948319	-3.891415
29	6	0	5.386980	-1.198608	1.624291
30	6	0	7.208160	-0.485866	3.026490
31	6	0	6.194738	-2.649233	3.207947
32	6	0	7.155559	-1.732137	3.648832
33	1	0	7.933488	0.260813	3.336796
34	1	0	6.119169	-3.631827	3.669820
35	1	0	7.833872	-1.992806	4.455405
36	6	0	-4.438857	-2.162342	-1.044201
37	6	0	-6.342654	-3.152111	-2.130295
38	6	0	-4.099823	-3.927176	-2.470315
39	6	0	-5.465874	-4.043750	-2.747649
40	1	0	-7.411598	-3.205308	-2.315507
41	1	0	-3.383329	-4.597401	-2.941049
42	1	0	-5.823282	-4.809525	-3.429110
43	6	0	-5.258675	1.875217	1.405507
44	6	0	-7.393582	2.911925	1.007249
45	6	0	-5.867306	3.678632	2.687215
46	6	0	-7.097017	3.809114	2.032102
47	1	0	-8.333142	2.976432	0.465979
48	1	0	-5.596387	4.361823	3.489971
49	1	0	-7.791742	4.592348	2.319372
50	7	0	3.339952	2.311546	-2.782665
51	7	0	5.326896	-2.397109	2.226266
52	7	0	-3.588855	-3.015551	-1.638447
53	7	0	-4.964521	2.743043	2.386842
54	6	0	-6.461900	1.925383	0.686367
55	1	0	-6.639112	1.205292	-0.101856
56	6	0	-5.822525	-2.188744	-1.267316
57	1	0	-6.456252	-1.469304	-0.764125
58	6	0	6.311738	-0.211090	1.994404
59	1	0	6.306968	0.740072	1.478075
60	6	0	5.526094	2.325539	-1.767090
61	1	0	6.217018	1.846309	-1.084855

G

HF (B3LYP/6-31+G(d,p)) = -3863.002696 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3862.672959 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.300591 (Hartree/Particle)

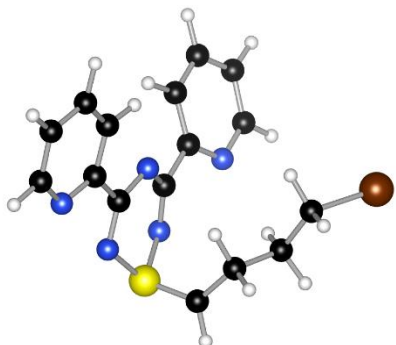
Thermal correction = 0.244850 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.678526	-1.546330	1.368893
2	6	0	-2.354050	-0.908626	0.425122
3	6	0	-1.337003	1.187250	0.596453
4	7	0	-0.512834	0.935555	1.606579
5	16	0	-0.332747	-0.705218	1.932416
6	7	0	-2.173936	0.348543	-0.050034
7	6	0	-3.505673	-1.662790	-0.183487
8	6	0	-4.772374	-3.574977	-0.242976
9	6	0	-5.312739	-1.806344	-1.766158
10	1	0	-4.948839	-4.566983	0.168536
11	1	0	-5.910809	-1.382290	-2.567642
12	6	0	-1.392576	2.621968	0.153954
13	6	0	-2.578082	4.465418	-0.836617
14	6	0	-0.334611	4.650725	-0.013426
15	1	0	-3.465217	4.887890	-1.299535
16	1	0	0.570473	5.227440	0.166906
17	6	0	-5.583006	-3.081326	-1.271369
18	1	0	-6.394659	-3.683595	-1.667736
19	6	0	-1.446725	5.249912	-0.613581
20	1	0	-1.418692	6.297411	-0.897290
21	6	0	0.955532	-1.206994	0.695570
22	6	0	2.293936	-0.532491	0.992251
23	1	0	0.567810	-0.952163	-0.295235
24	1	0	1.006930	-2.297366	0.788449
25	6	0	3.385289	-1.000932	0.011664
26	1	0	2.172297	0.554662	0.930740
27	1	0	2.602292	-0.763488	2.020599
28	1	0	3.517247	-2.086814	0.082172
29	1	0	3.083543	-0.780482	-1.018673
30	6	0	4.699097	-0.304786	0.317619
31	1	0	5.061646	-0.534419	1.320295
32	1	0	4.626181	0.777018	0.200969
33	35	0	6.147252	-0.861400	-0.896043
34	6	0	-2.551539	3.125612	-0.453062
35	1	0	-3.399478	2.469805	-0.606110

36	6	0	-4.258576	-1.080048	-1.213471
37	1	0	-4.003177	-0.087187	-1.560384
38	7	0	-0.298576	3.370983	0.368478
39	7	0	-3.755958	-2.893944	0.289780

H



HF (B3LYP/6-31+G(d,p)) = -3862.4278005 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3862.1579702Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.285468 (Hartree/Particle)

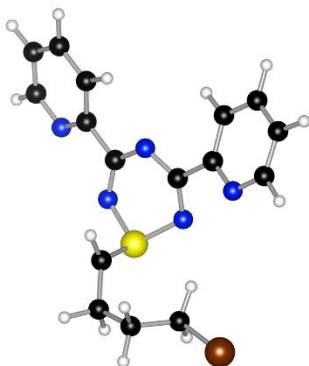
Thermal correction = 0.229649 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.158002	0.761522	2.276080
2	6	0	0.307889	1.143440	1.024193
3	6	0	2.263173	-0.015311	0.553865
4	7	0	2.416340	-0.615140	1.716415
5	16	0	1.002078	-0.703924	2.719723
6	7	0	1.248082	0.775508	0.117573
7	6	0	-0.647645	2.195689	0.524315
8	6	0	-2.714005	3.202948	0.635940
9	6	0	-1.127497	4.061587	-0.934224
10	1	0	-3.699656	3.211777	1.101069
11	1	0	-0.831236	4.759880	-1.713750
12	6	0	3.387129	-0.175748	-0.443047
13	6	0	5.482550	-0.979493	-0.956052
14	6	0	4.290884	0.209157	-2.652492
15	1	0	6.360801	-1.523182	-0.606678
16	1	0	4.201986	0.615494	-3.657531
17	6	0	-2.399402	4.131726	-0.358670
18	1	0	-3.127856	4.874829	-0.671406
19	6	0	5.441562	-0.479990	-2.260239
20	1	0	6.278291	-0.629473	-2.937317
21	6	0	0.130957	-2.037181	2.243153
22	6	0	-0.379792	-2.308508	0.858048
23	1	0	-0.166589	-2.664723	3.078086
24	6	0	-1.850074	-1.852730	0.612108
25	1	0	0.270693	-1.819617	0.122138
26	1	0	-0.317411	-3.387689	0.643583
27	1	0	-2.526730	-2.474671	1.209749
28	1	0	-1.973910	-0.819594	0.947663
29	6	0	-2.179022	-1.977469	-0.859637
30	1	0	-2.015458	-2.987499	-1.239715

31	1	0	-1.623998	-1.264159	-1.469318
32	35	0	-4.090385	-1.607859	-1.308425
33	6	0	3.255806	0.367844	-1.736281
34	1	0	2.341513	0.893251	-1.981829
35	6	0	-0.244375	3.081024	-0.493881
36	1	0	0.749896	2.972240	-0.909965
37	7	0	4.493242	-0.843826	-0.068490
38	7	0	-1.872657	2.261800	1.075839

H1 (productive conformer – leading to I-TS)



HF (B3LYP/6-31+G(d,p)) = -3862.4290752 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3862.1559194 Hartrees

Imaginary Frequencies: 1 (-470.37 cm⁻¹)

Zero point correction = 0.285442 (Hartree/Particle)

Thermal correction = 0.230384 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.385318	-2.172954	0.632963
2	6	0	1.637781	-2.999046	0.745367
3	6	0	2.961069	-2.226395	1.013890
4	1	0	1.529038	-3.731088	1.562281
5	1	0	1.769232	-3.595247	-0.170660
6	1	0	2.875052	-1.655671	1.946649
7	1	0	3.776454	-2.950710	1.149305
8	6	0	3.301642	-1.282628	-0.127336
9	35	0	5.142063	-0.535792	0.068951
10	1	0	-0.000496	-1.660861	1.512639
11	7	0	0.225162	0.032472	-1.092896
12	6	0	-0.584197	0.848786	-0.449323
13	6	0	-2.405417	-0.579451	-0.295686
14	7	0	-1.857287	-1.667352	-0.801957
15	16	0	-0.137575	-1.669296	-0.864056
16	7	0	-1.843109	0.619967	-0.000290
17	1	0	3.327591	-1.792530	-1.091193
18	1	0	2.646948	-0.414649	-0.194235
19	6	0	-3.886656	-0.646943	-0.016038
20	6	0	-5.860381	0.295155	1.012970
21	6	0	-5.900457	-1.737929	-0.243046
22	6	0	-6.591610	-0.782825	0.506519
23	1	0	-6.346117	1.065626	1.607526
24	1	0	-6.431305	-2.594229	-0.659917
25	1	0	-7.658670	-0.884976	0.684950

26	6	0	-0.081965	2.246364	-0.221346
27	6	0	-0.492026	4.615536	0.003227
28	6	0	1.696808	3.658559	0.153592
29	6	0	0.883648	4.794197	0.179511
30	1	0	-1.168742	5.466969	0.017697
31	1	0	2.772678	3.749996	0.301066
32	1	0	1.315039	5.778781	0.338499
33	7	0	-4.589775	-1.687461	-0.498173
34	7	0	1.241532	2.417347	-0.046047
35	6	0	-4.497016	0.369055	0.745396
36	1	0	-3.879650	1.182613	1.105433
37	6	0	-0.982296	3.328169	-0.191014
38	1	0	-2.039201	3.126729	-0.320766

H2 (conformation of H leading from direct deprotonation of G)



HF (B3LYP/6-31+G(d,p)) = -3863.002696 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3862.151835 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.28536 (Hartree/Particle)

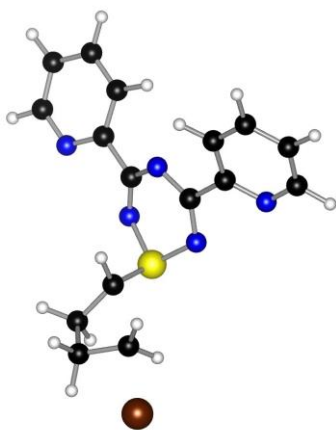
Thermal correction = 0.244857 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.349401	-1.538934	1.197086
2	6	0	-2.248893	-1.012369	0.390476
3	6	0	-1.524988	1.189261	0.487737
4	7	0	-0.495759	1.016653	1.293148
5	16	0	0.107379	-0.603744	1.383624
6	7	0	-2.353019	0.263592	-0.059318
7	6	0	-3.376690	-1.913583	-0.040597
8	6	0	-4.206824	-4.037880	-0.352965
9	6	0	-5.637621	-2.188953	-0.852390
10	1	0	-4.013691	-5.109590	-0.297328
11	1	0	-6.585069	-1.771504	-1.185962
12	6	0	-1.881977	2.613575	0.141129
13	6	0	-1.608476	4.870651	0.501334
14	6	0	-3.136119	4.183563	-1.203339
15	1	0	-1.106399	5.647083	1.079226
16	1	0	-3.850455	4.397851	-1.995170
17	6	0	-5.449007	-3.572766	-0.791558
18	1	0	-6.232883	-4.270081	-1.074769
19	6	0	-2.520765	5.220853	-0.497120
20	1	0	-2.735308	6.264649	-0.710048

21	6	0	1.098010	-0.859159	0.075717
22	6	0	2.467341	-1.442569	0.267096
23	1	0	0.711059	-0.691529	-0.926630
24	6	0	3.630193	-0.512500	-0.181470
25	1	0	2.609645	-1.690742	1.328949
26	1	0	2.573272	-2.396004	-0.281725
27	1	0	3.505648	-0.250024	-1.238309
28	1	0	3.591317	0.419027	0.391738
29	6	0	4.948096	-1.225902	0.032698
30	1	0	5.016290	-2.150198	-0.542398
31	1	0	5.131325	-1.444383	1.085511
32	35	0	6.557832	-0.193674	-0.526564
33	6	0	-2.820051	2.868060	-0.878895
34	1	0	-3.268167	2.023503	-1.387270
35	6	0	-4.592804	-1.351119	-0.476679
36	1	0	-4.679328	-0.271946	-0.505475
37	7	0	-1.285204	3.612887	0.815786
38	7	0	-3.194616	-3.245996	0.013921

I-TS



HF (B3LYP/6-31+G(d,p)) = -3862.409378 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3862.131257 Hartrees

Imaginary Frequencies: 1 (-470.37 cm⁻¹)

Zero point correction = 0.284916 (Hartree/Particle)

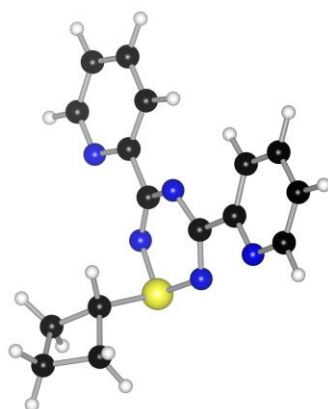
Thermal correction = 0.230405 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.137224	-1.387475	0.031476
2	6	0	-1.851553	-2.732695	0.044959
3	6	0	-3.201774	-2.325213	-0.560507
4	1	0	-1.337567	-3.550865	-0.481443
5	1	0	-1.996892	-3.061866	1.082728
6	1	0	-3.193158	-2.380118	-1.654580
7	1	0	-4.062001	-2.903470	-0.211897
8	6	0	-3.279602	-0.866845	-0.128655
9	35	0	-5.647625	-0.458849	-0.468654
10	1	0	-0.705794	-1.069965	-0.919334
11	7	0	-0.083644	0.746662	1.258196
12	6	0	0.901035	1.168050	0.492122
13	6	0	2.166981	-0.775395	0.392328

14	7	0	1.438366	-1.510319	1.210344
15	16	0	-0.188914	-0.955552	1.399491
16	7	0	1.933121	0.480322	-0.059915
17	1	0	-3.381794	-0.622945	0.916877
18	1	0	-3.070720	-0.049660	-0.796426
19	6	0	3.490229	-1.355671	-0.031732
20	6	0	5.756091	-1.046085	-0.803555
21	6	0	4.816696	-3.202974	-0.368042
22	6	0	5.911094	-2.433985	-0.772592
23	1	0	6.576533	-0.401867	-1.110238
24	1	0	4.892293	-4.289656	-0.337898
25	1	0	6.846292	-2.909976	-1.053922
26	6	0	0.921130	2.647354	0.196520
27	6	0	1.625238	4.481028	-1.203186
28	6	0	0.250815	4.778674	0.732007
29	6	0	0.918837	5.340502	-0.359115
30	1	0	2.159046	4.866248	-2.068486
31	1	0	-0.307995	5.413198	1.419069
32	1	0	0.882103	6.411574	-0.536807
33	7	0	3.636698	-2.691825	-0.004535
34	7	0	0.238863	3.471264	1.008087
35	6	0	4.531040	-0.498738	-0.433306
36	1	0	4.349401	0.568957	-0.442346
37	6	0	1.634808	3.117969	-0.919871
38	1	0	2.172887	2.405231	-1.532609

I



HF (B3LYP/6-31+G(d,p)) = -1290.6366098 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -1290.239968 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.287415 (Hartree/Particle)

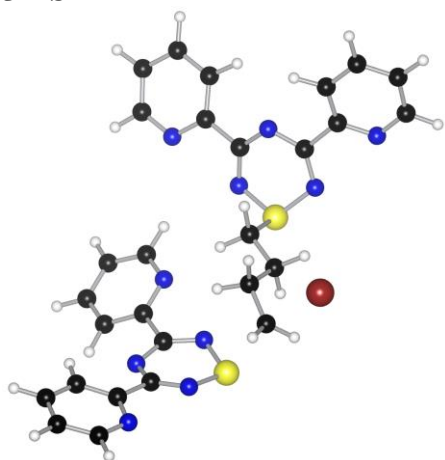
Thermal correction = 0.236029 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.376288	0.884389	1.020540
2	6	0	1.167973	-0.249217	0.366490
3	6	0	-1.167848	-0.249358	0.366310
4	7	0	-1.376393	0.884051	1.020647
5	16	0	-0.000162	1.846556	1.165599
6	7	0	0.000114	-0.794531	-0.046367
7	6	0	2.395809	-1.075372	0.092761
8	6	0	3.426006	-3.164570	-0.513731

9	6	0	4.685498	-1.187388	-0.020275
10	1	0	3.359078	-4.211559	-0.795313
11	1	0	5.632077	-0.660277	0.083689
12	6	0	-2.395477	-1.075885	0.092879
13	6	0	-3.425281	-3.166143	-0.510596
14	6	0	-4.685052	-1.187824	-0.022417
15	1	0	-3.358186	-4.213702	-0.790008
16	1	0	-5.631674	-0.660385	0.079459
17	6	0	4.664885	-2.538468	-0.382472
18	1	0	5.592736	-3.074333	-0.557485
19	6	0	-4.664218	-2.539620	-0.381911
20	1	0	-5.591951	-3.075715	-0.556859
21	6	0	-0.000377	2.761849	-0.437564
22	6	0	-1.091939	3.847866	-0.606378
23	6	0	1.090709	3.848337	-0.606452
24	1	0	-0.000250	2.013644	-1.234678
25	6	0	-0.000833	4.759360	-1.238211
26	1	0	-1.438292	4.233716	0.358434
27	1	0	-1.962903	3.578895	-1.207234
28	1	0	1.436959	4.234342	0.358335
29	1	0	1.961748	3.579750	-1.207373
30	1	0	-0.001047	5.812752	-0.944702
31	1	0	-0.000857	4.699556	-2.330618
32	7	0	3.586617	-0.466294	0.213893
33	7	0	-3.586331	-0.466417	0.211584
34	6	0	2.270020	-2.422426	-0.276623
35	1	0	1.283282	-2.856644	-0.370177
36	6	0	-2.269458	-2.423662	-0.273763
37	1	0	-1.282681	-2.858207	-0.365404

J-TS



HF (B3LYP/6-31+G(d,p)) = -4997.0940673 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -4996.497142 Hartrees

Imaginary Frequencies: 1 (-315.30 cm^{-1})

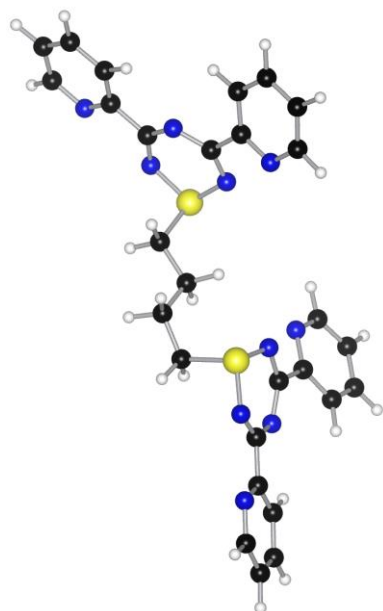
Zero point correction = 0.484541 (Hartree/Particle)

Thermal correction = 0.405664 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.538042	-0.940937	-1.364793
2	6	0	4.311221	-0.618682	-0.345455

3	6	0	3.677203	1.608387	-0.096165
4	7	0	2.790537	1.685263	-1.072972
5	16	0	2.302150	0.173187	-1.671579
6	7	0	4.355583	0.534047	0.368362
7	6	0	0.256584	-1.572786	-0.878073
8	6	0	-0.923973	-1.822976	0.075030
9	1	0	0.922387	-2.441331	-0.873349
10	1	0	-0.130787	-1.442238	-1.895179
11	6	0	-1.894500	-2.835614	-0.452725
12	1	0	-0.564425	-2.155550	1.053837
13	1	0	-1.451740	-0.872507	0.235595
14	1	0	-2.738178	-3.149604	0.144561
15	1	0	-1.707693	-3.365938	-1.371927
16	35	0	-0.747322	-5.001525	0.477421
17	7	0	-2.518747	0.139996	-1.591646
18	6	0	-3.168829	1.141646	-1.047770
19	6	0	-5.010646	-0.006930	-0.195613
20	7	0	-4.684893	-1.226011	-0.546184
21	16	0	-3.393051	-1.335279	-1.670881
22	7	0	-4.405823	1.183896	-0.486017
23	6	0	0.988027	-0.294832	-0.469334
24	1	0	0.308743	0.567261	-0.508964
25	1	0	1.460587	-0.365065	0.515625
26	6	0	-6.206963	0.114520	0.714773
27	6	0	-7.541857	1.414354	2.246165
28	6	0	-8.074893	-0.841130	1.651381
29	6	0	-8.384558	0.310485	2.381923
30	1	0	-7.737853	2.333954	2.791943
31	1	0	-8.709936	-1.723451	1.723514
32	1	0	-9.256397	0.334712	3.029604
33	6	0	-2.426264	2.453389	-1.017005
34	6	0	-2.445447	4.860702	-0.991725
35	6	0	-0.415331	3.583067	-0.992323
36	6	0	-1.049794	4.829054	-0.988890
37	1	0	-2.979633	5.807728	-0.987838
38	1	0	0.670803	3.509009	-0.966644
39	1	0	-0.460602	5.741401	-0.979924
40	6	0	5.316903	-1.658368	0.073538
41	6	0	6.775361	-2.592188	1.745069
42	6	0	6.475234	-3.576528	-0.417189
43	6	0	7.082878	-3.609653	0.841805
44	1	0	7.217014	-2.577281	2.737791
45	1	0	6.691252	-4.349433	-1.152831
46	1	0	7.768532	-4.411063	1.100373
47	6	0	4.045889	2.918290	0.552335
48	6	0	5.528412	4.227424	1.926805
49	6	0	3.556387	5.132339	0.914314
50	6	0	4.689246	5.320905	1.711630
51	1	0	6.421054	4.323346	2.539026
52	1	0	2.872238	5.958808	0.728604
53	1	0	4.898491	6.293097	2.148019
54	6	0	-3.147563	3.657209	-0.992728
55	1	0	-4.230081	3.618197	-0.975464
56	6	0	-6.439225	1.319414	1.399740
57	1	0	-5.749683	2.140693	1.251197
58	6	0	5.885055	-1.593623	1.355207
59	1	0	5.612133	-0.778699	2.014030
60	6	0	5.203218	3.005513	1.341415
61	1	0	5.814416	2.121714	1.473357
62	7	0	3.234400	3.968324	0.344188
63	7	0	5.609144	-2.634779	-0.798752
64	7	0	-7.021100	-0.947438	0.838601
65	7	0	-1.082943	2.421749	-1.016808

J

HF (B3LYP/6-31+G(d,p)) = -2425.2797189 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -2424.566392 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.486086 (Hartree/Particle)

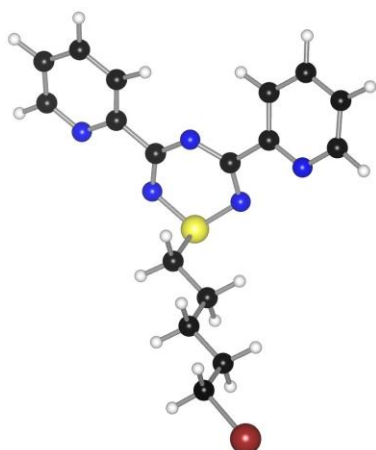
Thermal correction = 0.409675 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.726311	0.884544	0.708890
2	6	0	3.776725	1.055720	-0.083375
3	6	0	4.888658	-0.952989	0.341158
4	7	0	4.021236	-1.498243	1.179162
5	16	0	2.536573	-0.698781	1.247609
6	7	0	4.788173	0.203831	-0.357743
7	6	0	0.167550	-1.090433	-0.206038
8	6	0	-0.522596	-1.679619	-1.450171
9	1	0	0.075990	-0.000031	-0.199448
10	1	0	-0.336121	-1.442402	0.701914
11	6	0	-2.050194	-1.572425	-1.469415
12	1	0	-0.111721	-1.215654	-2.356279
13	1	0	-0.288333	-2.750588	-1.524072
14	1	0	-2.516897	-2.018349	-0.585692
15	1	0	-2.467747	-2.041629	-2.366573
16	7	0	-2.566707	0.716329	0.007283
17	6	0	-3.602287	0.373655	0.763304
18	6	0	-5.081648	-0.275840	-0.921245
19	7	0	-4.295338	-0.098435	-1.971432
20	16	0	-2.676342	0.174999	-1.580838
21	7	0	-4.785919	-0.160868	0.396991
22	6	0	1.641372	-1.496920	-0.168624
23	1	0	1.773726	-2.570426	0.007050
24	1	0	2.182552	-1.216991	-1.078075
25	6	0	-6.516118	-0.618480	-1.224588
26	6	0	-8.734743	-1.184063	-0.483459
27	6	0	-8.142932	-0.999208	-2.797503

28	6	0	-9.114411	-1.253863	-1.823063
29	1	0	-9.452009	-1.378289	0.308860
30	1	0	-8.398398	-1.046321	-3.854470
31	1	0	-10.131188	-1.500648	-2.112760
32	6	0	-3.455927	0.682337	2.225841
33	6	0	-4.415157	1.257146	4.354233
34	6	0	-2.058278	0.967168	4.022615
35	6	0	-3.122802	1.266776	4.878921
36	1	0	-5.271890	1.483487	4.982444
37	1	0	-1.036654	0.953884	4.396891
38	1	0	-2.937370	1.496941	5.923518
39	6	0	3.890737	2.414832	-0.714960
40	6	0	5.220359	4.185502	-1.654281
41	6	0	2.835404	4.314053	-1.451236
42	6	0	4.040824	4.905585	-1.842938
43	1	0	6.179994	4.604865	-1.942703
44	1	0	1.892613	4.839331	-1.591038
45	1	0	4.047114	5.897966	-2.283212
46	6	0	6.187968	-1.693808	0.164312
47	6	0	8.354864	-1.905186	-0.862003
48	6	0	7.497549	-3.498476	0.707791
49	6	0	8.532774	-3.082379	-0.136575
50	1	0	9.127867	-1.543869	-1.534274
51	1	0	7.595879	-4.413707	1.288685
52	1	0	9.443041	-3.668245	-0.219488
53	6	0	5.147092	2.914667	-1.086248
54	1	0	6.030108	2.310105	-0.921061
55	6	0	7.164794	-1.194935	-0.710286
56	1	0	6.972783	-0.276994	-1.250467
57	6	0	-4.589229	0.952742	3.005105
58	1	0	-5.569850	0.926348	2.546144
59	6	0	-7.414662	-0.858551	-0.174519
60	1	0	-7.064802	-0.791764	0.847511
61	7	0	-6.874585	-0.693899	-2.516285
62	7	0	-2.209648	0.683753	2.725741
63	7	0	2.751786	3.101643	-0.897025
64	7	0	6.350903	-2.832163	0.857526

K



HF (B3LYP/6-31+G(d,p)) = -3902.3205639 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3901.969343 Hartrees

Imaginary Frequencies: none found

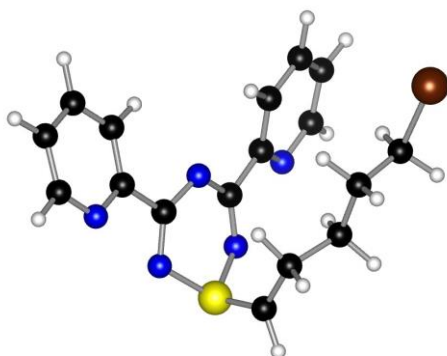
Zero point correction = 0.329090 (Hartree/Particle)

Thermal correction = 0.271126 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.907102	0.825001	1.570667
2	6	0	1.743895	1.147529	0.592301
3	6	0	2.865165	-0.890625	0.382614
4	7	0	2.199986	-1.589026	1.289817
5	16	0	0.802544	-0.831878	1.848556
6	7	0	2.637789	0.371566	-0.056976
7	6	0	1.741585	2.597153	0.196823
8	6	0	2.864940	4.528359	-0.694048
9	6	0	0.588713	4.575543	0.055532
10	1	0	3.744651	5.009170	-1.112086
11	1	0	-0.349889	5.100422	0.222341
12	6	0	4.062749	-1.571917	-0.224007
13	6	0	5.409978	-3.426680	-0.326093
14	6	0	5.912968	-1.576982	-1.763110
15	1	0	5.617674	-4.426615	0.050204
16	1	0	6.512537	-1.096376	-2.530886
17	6	0	1.688528	5.248258	-0.486575
18	1	0	1.617124	6.301842	-0.738411
19	6	0	6.224322	-2.858909	-1.312373
20	1	0	7.070247	-3.410726	-1.710552
21	6	0	-0.438257	-1.364006	0.576149
22	6	0	-1.814345	-0.766000	0.868533
23	1	0	-0.433858	-2.457796	0.640356
24	1	0	-0.046508	-1.063296	-0.400385
25	6	0	-2.872356	-1.245926	-0.135719
26	1	0	-2.127312	-1.044420	1.883744
27	1	0	-1.747143	0.327264	0.845760
28	1	0	-2.564311	-0.964360	-1.151974
29	1	0	-2.925851	-2.343246	-0.117859
30	6	0	-4.262603	-0.657253	0.162709
31	1	0	-4.215938	0.437662	0.144009
32	1	0	-4.582892	-0.945554	1.170787
33	6	0	-5.276431	-1.144742	-0.854758
34	1	0	-5.024132	-0.829036	-1.868003
35	1	0	-5.386346	-2.229879	-0.835773
36	35	0	-7.088901	-0.439683	-0.535347
37	6	0	4.815730	-0.917744	-1.210290
38	1	0	4.527713	0.077199	-1.524107
39	6	0	2.893348	3.177045	-0.353271
40	1	0	3.777896	2.569157	-0.496860
41	7	0	4.353067	-2.810059	0.206459
42	7	0	0.604856	3.283793	0.396241

L



HF (B3LYP/6-31+G(d,p)) = -3901.7453839 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3901.4554370 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.314151 (Hartree/Particle)

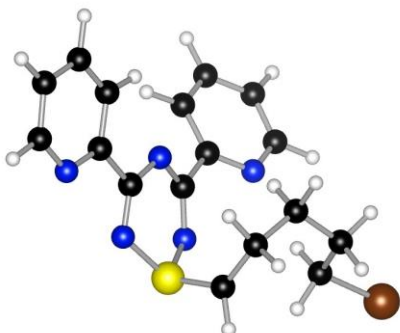
Thermal correction = 0.257895 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	0.903816	2.383006	1.116227
2	6	0	0.704849	1.694715	0.009636
3	6	0	2.525942	0.267125	0.178206
4	7	0	3.012451	0.708921	1.319816
5	16	0	1.895034	1.592081	2.317492
6	7	0	1.387592	0.625904	-0.471078
7	6	0	-0.434128	2.138089	-0.876624
8	6	0	-1.992874	3.727657	-1.461487
9	6	0	-2.021032	1.644686	-2.634329
10	1	0	-2.383604	4.729796	-1.283168
11	1	0	-2.433806	0.967412	-3.378321
12	6	0	3.378307	-0.722244	-0.576842
13	6	0	5.082664	-2.268695	-0.585674
14	6	0	3.975271	-1.806215	-2.653458
15	1	0	5.832599	-2.802463	-0.001298
16	1	0	3.835291	-1.956476	-3.721553
17	6	0	-2.568650	2.916108	-2.442292
18	1	0	-3.413531	3.269160	-3.027187
19	6	0	4.958693	-2.512883	-1.955694
20	1	0	5.607430	-3.230381	-2.450914
21	6	0	0.991812	0.486812	3.174115
22	6	0	0.191048	-0.647034	2.600084
23	1	0	0.991753	0.691228	4.240334
24	6	0	-1.256389	-0.274830	2.186579
25	1	0	0.703061	-1.057350	1.718633
26	1	0	0.147301	-1.468719	3.331877
27	1	0	-1.835339	-0.022312	3.085893
28	1	0	-1.215145	0.637712	1.584543
29	6	0	-1.971450	-1.387593	1.395952
30	1	0	-2.170297	-2.254682	2.038525
31	1	0	-1.323486	-1.731570	0.580985
32	6	0	-3.264788	-0.849163	0.823165
33	1	0	-3.953175	-0.508631	1.597475
34	1	0	-3.095919	-0.046249	0.106473
35	35	0	-4.325868	-2.197239	-0.197257

36	6	0	3.175770	-0.904003	-1.959009
37	1	0	2.395304	-0.330787	-2.443986
38	6	0	-0.937217	1.254774	-1.852958
39	1	0	-0.464993	0.286535	-1.965290
40	7	0	4.324134	-1.404047	0.094696
41	7	0	-0.965931	3.359645	-0.688965

L1 (productive conformer – leading to M-TS)



HF (B3LYP/6-31+G(d,p)) = -3901.7492789 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3901.4567362 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.314549 (Hartree/Particle)

Thermal correction = 0.259971 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	2.127290	-1.392581	-1.342668
2	6	0	2.443508	-0.401280	-0.536816
3	6	0	0.482267	0.819357	-0.735238
4	7	0	-0.168538	0.028246	-1.562652
5	16	0	0.434522	-1.606855	-1.676530
6	7	0	1.694875	0.668935	-0.154266
7	6	0	-0.266366	-2.521262	-0.474146
8	6	0	-0.124046	-2.362819	1.019122
9	6	0	-0.962250	-1.267304	1.721054
10	1	0	-0.379527	-3.330591	1.476919
11	1	0	0.929116	-2.177162	1.288392
12	1	0	-0.725575	-1.303844	2.796077
13	1	0	-0.637567	-0.280809	1.377240
14	6	0	-2.496562	-1.366483	1.583309
15	1	0	-2.950068	-0.669085	2.298544
16	1	0	-2.837446	-2.372748	1.865792
17	6	0	-2.997365	-1.023208	0.189676
18	1	0	-2.784025	-1.786976	-0.550575
19	35	0	-5.004762	-0.861397	0.178008
20	1	0	-2.645112	-0.054441	-0.162262
21	1	0	-0.682901	-3.437917	-0.881302
22	6	0	3.854726	-0.382490	0.002162
23	6	0	5.545051	0.642639	1.393383
24	6	0	5.955855	-1.317843	0.089440
25	6	0	6.433277	-0.354726	0.982085
26	1	0	5.861186	1.415141	2.090808
27	1	0	6.614050	-2.114836	-0.257654
28	1	0	7.459093	-0.390474	1.338878
29	6	0	-0.194338	2.128052	-0.422162

30	6	0	-0.082141	4.511504	-0.062594
31	6	0	-2.138183	3.287423	0.008279
32	6	0	-1.471043	4.510286	0.099955
33	1	0	0.483402	5.437947	0.005298
34	1	0	-3.217159	3.235343	0.148955
35	1	0	-2.021241	5.425152	0.301826
36	6	0	4.244752	0.632413	0.898206
37	1	0	3.511658	1.378352	1.178539
38	6	0	0.566157	3.306186	-0.313421
39	1	0	1.641877	3.243897	-0.431045
40	7	0	-1.529028	2.126170	-0.257381
41	7	0	4.708935	-1.345207	-0.389321

L2 (conformation of L leading directly from direct deprotonation of G)



HF (B3LYP/6-31+G(d,p)) = -3901.7430179 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3901.4474875 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.314074 (Hartree/Particle)

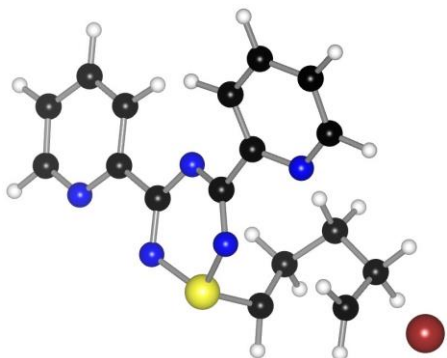
Thermal correction = 0.257226 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.565332	0.273907	-1.383752
2	6	0	-1.368492	0.929069	-0.574106
3	6	0	-2.942832	-0.751817	-0.290983
4	7	0	-2.335101	-1.730998	-0.934062
5	16	0	-0.661661	-1.484699	-1.218480
6	7	0	-2.505494	0.492124	0.027947
7	6	0	-1.052501	2.378429	-0.329053
8	6	0	-1.790712	4.642574	0.081843
9	6	0	0.517660	4.049056	-0.121701
10	1	0	-2.583435	5.371285	0.235751
11	1	0	1.575857	4.311530	-0.116617
12	6	0	-4.360146	-1.030076	0.147468
13	6	0	-6.262797	-2.317177	0.014383
14	6	0	-6.269275	-0.455052	1.512930
15	1	0	-6.752806	-3.174487	-0.447826

16	1	0	-6.750502	0.177528	2.255414
17	6	0	-0.449238	5.037408	0.076758
18	1	0	-0.158132	6.073214	0.228870
19	6	0	-6.945029	-1.545293	0.957782
20	1	0	-7.963864	-1.792924	1.243295
21	6	0	0.084182	-2.036091	0.174008
22	6	0	1.550167	-2.376328	0.093326
23	1	0	-0.306418	-1.669343	1.123423
24	6	0	2.489754	-1.151458	0.233784
25	1	0	1.803474	-3.105169	0.880525
26	1	0	1.768319	-2.874086	-0.864198
27	1	0	2.260649	-0.450007	-0.576968
28	1	0	2.238948	-0.623785	1.164304
29	6	0	3.990619	-1.498466	0.232627
30	1	0	4.250904	-2.053270	-0.677735
31	1	0	4.235360	-2.145635	1.084419
32	6	0	4.793765	-0.218699	0.302465
33	1	0	4.629120	0.418466	-0.565910
34	1	0	4.588891	0.347753	1.210956
35	35	0	6.770085	-0.491543	0.341271
36	7	0	0.239733	2.757381	-0.326701
37	7	0	-5.008017	-2.082999	-0.381508
38	6	0	-2.095984	3.299772	-0.114531
39	1	0	-3.115827	2.933418	-0.108805
40	6	0	-4.967578	-0.188851	1.100145
41	1	0	-4.396863	0.646789	1.485952

M-TS



HF (B3LYP/6-31+G(d,p)) = -3901.7346138 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -3901.4402083 Hartrees

Imaginary Frequencies: 1 (-394.78 cm⁻¹)

Zero point correction = 0.314106 (Hartree/Particle)

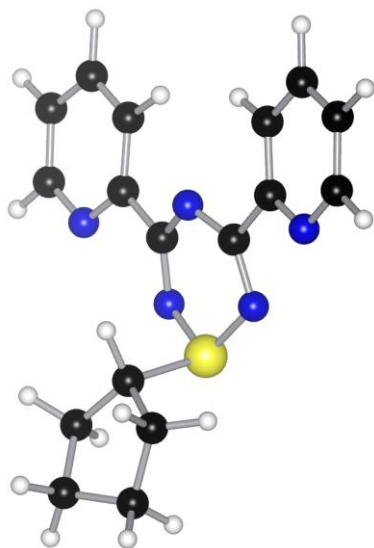
Thermal correction = 0.259673 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.964787	-1.470887	-1.219166
2	6	0	2.396977	-0.454718	-0.501294
3	6	0	0.511388	0.888759	-0.640008
4	7	0	-0.233861	0.114732	-1.401720
5	16	0	0.263919	-1.525833	-1.498963
6	7	0	1.743004	0.675854	-0.124311
7	6	0	-0.518324	-2.333343	-0.198477
8	6	0	-0.121615	-2.187188	1.255729

9	6	0	-1.007062	-1.146782	1.958684
10	1	0	-0.263425	-3.162622	1.742953
11	1	0	0.941232	-1.934635	1.380703
12	1	0	-0.876310	-1.180187	3.050731
13	1	0	-0.720079	-0.139862	1.637215
14	6	0	-2.485647	-1.382734	1.599164
15	1	0	-3.085327	-0.574567	2.027361
16	1	0	-2.845393	-2.317618	2.047231
17	6	0	-2.723801	-1.414710	0.108587
18	1	0	-2.997625	-2.318465	-0.402570
19	35	0	-5.106233	-0.857762	-0.002291
20	1	0	-2.461839	-0.555417	-0.490011
21	1	0	-0.759085	-3.337379	-0.546707
22	6	0	3.845323	-0.499877	-0.074484
23	6	0	5.692112	0.459900	1.148928
24	6	0	5.888413	-1.554325	-0.124721
25	6	0	6.486638	-0.596706	0.698946
26	1	0	6.105472	1.229946	1.795815
27	1	0	6.471232	-2.396108	-0.498322
28	1	0	7.533829	-0.682117	0.975475
29	6	0	-0.082996	2.238643	-0.341441
30	6	0	0.142804	4.604402	0.043778
31	6	0	-1.977009	3.485461	0.039665
32	6	0	-1.247318	4.670659	0.167843
33	1	0	0.751747	5.500146	0.139076
34	1	0	-3.060659	3.485291	0.145222
35	1	0	-1.754873	5.610839	0.364828
36	6	0	4.357460	0.513442	0.756509
37	1	0	3.692898	1.307880	1.071876
38	6	0	0.737666	3.369514	-0.204353
39	1	0	1.811396	3.255066	-0.297984
40	7	0	-1.418550	2.298516	-0.214390
41	7	0	4.607793	-1.520726	-0.502935

M



HF (B3LYP/6-31+G(d,p)) = -1329.9831698 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -1329.5669773 Hartrees

Imaginary Frequencies: none found

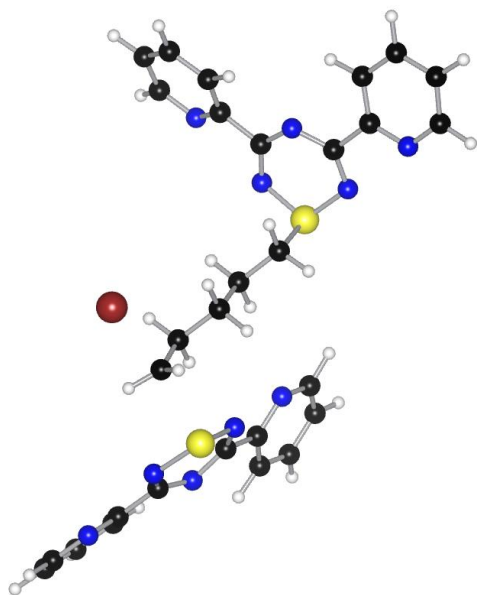
Zero point correction = 0.317296 (Hartree/Particle)

Thermal correction = 0.265125 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	1.362252	0.679506	0.993476
2	6	0	1.182809	-0.465686	0.350635
3	6	0	-1.150426	-0.521993	0.358468
4	7	0	-1.383078	0.613953	0.998802
5	16	0	-0.032027	1.612830	1.130992
6	7	0	0.028927	-1.046136	-0.050288
7	6	0	2.432232	-1.259566	0.079894
8	6	0	3.519050	-3.325701	-0.506076
9	6	0	4.723523	-1.306813	-0.044996
10	1	0	3.480898	-4.377679	-0.774128
11	1	0	5.655081	-0.751433	0.046785
12	6	0	-2.359720	-1.378990	0.097204
13	6	0	-3.343341	-3.500296	-0.473838
14	6	0	-4.646174	-1.541928	-0.019825
15	1	0	-3.253140	-4.550542	-0.736196
16	1	0	-5.604093	-1.033356	0.071929
17	6	0	4.740026	-2.662456	-0.389817
18	1	0	5.682075	-3.173442	-0.563345
19	6	0	-4.595702	-2.898571	-0.357408
20	1	0	-5.511355	-3.457172	-0.525394
21	6	0	-0.067546	2.532416	-0.497002
22	6	0	-1.345401	3.413606	-0.566022
23	6	0	1.143750	3.493635	-0.582699
24	1	0	-0.040434	1.749523	-1.258861
25	6	0	-0.836684	4.838297	-0.883343
26	1	0	-1.873372	3.406187	0.395512
27	1	0	-2.054861	3.032083	-1.304199
28	6	0	0.566412	4.882136	-0.256257
29	1	0	1.523814	3.475336	-1.610986
30	1	0	1.976202	3.191021	0.060364
31	1	0	-0.760815	4.979351	-1.969101
32	1	0	-1.508332	5.613130	-0.500288
33	1	0	1.188055	5.696565	-0.641611
34	1	0	0.489216	5.015869	0.830607
35	6	0	-2.204205	-2.729491	-0.247342
36	1	0	-1.208150	-3.144217	-0.330488
37	6	0	2.343461	-2.614269	-0.271576
38	1	0	1.369058	-3.077833	-0.353539
39	7	0	-3.563588	-0.793336	0.204225
40	7	0	3.605514	-0.614651	0.186224

N-TS



HF (B3LYP/6-31+G(d,p)) = -5036.408744 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -5035.789274 Hartrees

Imaginary Frequencies: 1 (-307.94 cm⁻¹)

Zero point correction = 0.512392 (Hartree/Particle)

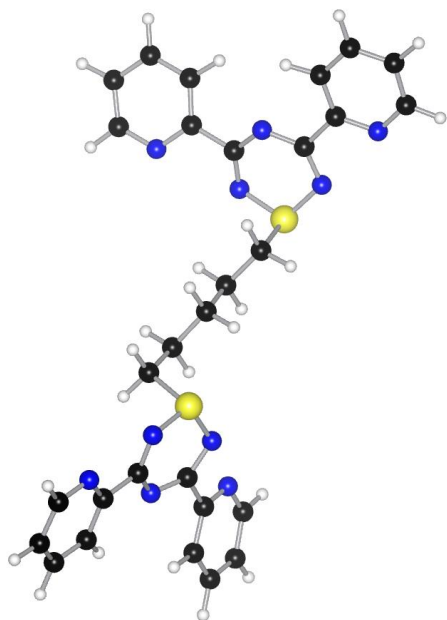
Thermal correction = 0.428167 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-4.326424	-2.019084	-0.336538
2	6	0	-5.256184	-1.077552	-0.336535
3	6	0	-4.448177	0.236796	1.410698
4	7	0	-3.369188	-0.461638	1.716426
5	16	0	-2.942174	-1.603040	0.544970
6	7	0	-5.323307	0.060985	0.390890
7	6	0	0.115458	0.698314	-1.173834
8	6	0	1.442124	1.225447	-0.616888
9	1	0	-0.474416	1.547156	-1.539744
10	1	0	0.323228	0.040824	-2.028703
11	6	0	2.288018	1.898389	-1.652975
12	1	0	1.260406	1.931068	0.200589
13	1	0	1.996501	0.375763	-0.189786
14	1	0	3.160354	2.469857	-1.370937
15	1	0	1.990650	1.922880	-2.688493
16	35	0	1.076205	4.214656	-1.706309
17	7	0	3.168588	-1.238774	-1.313745
18	6	0	3.957717	-1.744022	-0.394593
19	6	0	5.700905	-0.188567	-0.482332
20	7	0	5.231458	0.614681	-1.401512
21	16	0	3.827742	0.058417	-2.219606
22	7	0	5.204907	-1.370554	-0.006102
23	6	0	-0.670953	-0.091672	-0.117068
24	1	0	-0.063963	-0.942438	0.217366
25	1	0	-0.862597	0.544505	0.754773
26	6	0	-1.998248	-0.593183	-0.684592

27	1	0	-1.851971	-1.284504	-1.522305
28	1	0	-2.657009	0.220035	-1.004501
29	6	0	6.968915	0.265136	0.196346
30	6	0	8.517883	0.117440	2.039446
31	6	0	8.814036	1.634229	0.212771
32	6	0	9.272751	1.120357	1.429843
33	1	0	8.829732	-0.315263	2.986792
34	1	0	9.376531	2.413837	-0.299877
35	1	0	10.188985	1.495911	1.876663
36	6	0	3.400352	-2.922071	0.365760
37	6	0	3.759766	-4.862409	1.751912
38	6	0	1.588785	-4.180845	1.012173
39	6	0	2.381413	-5.081181	1.729344
40	1	0	4.420033	-5.533289	2.295804
41	1	0	0.507933	-4.310661	0.977535
42	1	0	1.927793	-5.918295	2.252047
43	6	0	-4.781351	1.375309	2.337645
44	6	0	-5.879115	3.477940	2.743040
45	6	0	-4.503155	2.391461	4.374813
46	6	0	-5.313808	3.473591	4.018174
47	1	0	-6.508441	4.300984	2.416048
48	1	0	-4.045579	2.348653	5.361690
49	1	0	-5.486775	4.284992	4.718745
50	6	0	-6.449768	-1.337177	-1.218249
51	6	0	-8.722453	-0.862767	-1.856087
52	6	0	-7.381221	-2.516080	-2.953394
53	6	0	-8.601423	-1.841806	-2.842389
54	1	0	-9.650102	-0.311032	-1.730689
55	1	0	-7.243468	-3.282139	-3.714736
56	1	0	-9.423077	-2.078715	-3.511799
57	7	0	-6.328149	-2.278814	-2.167556
58	7	0	-4.230671	1.368272	3.561061
59	7	0	2.072984	-3.131524	0.340295
60	7	0	7.696931	1.227513	-0.394878
61	6	0	-7.630318	-0.601879	-1.030739
62	1	0	-7.664064	0.147581	-0.250209
63	6	0	-5.618646	2.408115	1.888995
64	1	0	-6.032514	2.358232	0.889605
65	6	0	4.277830	-3.764741	1.068796
66	1	0	5.336015	-3.535029	1.058887
67	6	0	7.352685	-0.321464	1.414334
68	1	0	6.726730	-1.097973	1.835343

N



HF (B3LYP/6-31+G(d,p)) = -2464.6003596 Hartrees

HF (M062X/6-31+G(d,p)//B3LYP/6-31+G(d,p)) = -2463.8650475 Hartrees

Imaginary Frequencies: none found

Zero point correction = 0.514736 (Hartree/Particle)

Thermal correction = 0.436576 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	4.805241	-1.945447	0.298872
2	6	0	5.603948	-0.935180	0.605619
3	6	0	5.047252	0.515695	-1.137927
4	7	0	4.172914	-0.250819	-1.776799
5	16	0	3.658796	-1.581564	-0.881616
6	7	0	5.699119	0.284618	0.021929
7	6	0	-0.044523	0.134303	0.103608
8	6	0	-1.263072	0.485211	-0.763071
9	1	0	0.313045	1.036007	0.620080
10	1	0	-0.335353	-0.579445	0.885279
11	6	0	-2.402515	1.181252	-0.015263
12	1	0	-0.951954	1.162386	-1.569707
13	1	0	-1.650468	-0.419200	-1.245819
14	1	0	-3.219811	1.461035	-0.685937
15	1	0	-2.068694	2.072045	0.528158
16	7	0	-3.669665	-1.231766	0.416974
17	6	0	-4.854611	-1.066138	-0.157244
18	6	0	-5.561890	0.831883	1.006711
19	7	0	-4.488121	1.031352	1.755064
20	16	0	-3.155722	0.103626	1.302585
21	7	0	-5.759911	-0.081159	0.023943
22	6	0	1.098988	-0.465406	-0.729693
23	1	0	0.729911	-1.348561	-1.267259
24	1	0	1.425362	0.257943	-1.485798
25	6	0	2.291211	-0.859996	0.142220
26	1	0	2.043295	-1.653974	0.855203

27	1	0	2.714783	-0.010839	0.687442
28	6	0	-6.745579	1.711593	1.309509
29	6	0	-9.017468	2.385119	0.888272
30	6	0	-7.637340	3.426262	2.546750
31	6	0	-8.870258	3.343456	1.889981
32	1	0	-9.953925	2.285511	0.346911
33	1	0	-7.480698	4.163755	3.331749
34	1	0	-9.681388	4.013279	2.158392
35	6	0	-5.275159	-2.165584	-1.091441
36	6	0	-6.994117	-3.450726	-2.177617
37	6	0	-4.655886	-3.861963	-2.506693
38	6	0	-5.984873	-4.195034	-2.787925
39	1	0	-8.040496	-3.673622	-2.365362
40	1	0	-3.840540	-4.412803	-2.971550
41	1	0	-6.213790	-5.011049	-3.466352
42	6	0	5.414184	1.794543	-1.838096
43	6	0	6.971391	3.578879	-2.261296
44	6	0	4.833380	3.434227	-3.334250
45	6	0	6.045200	4.109919	-3.158674
46	1	0	7.926191	4.068588	-2.092720
47	1	0	4.081254	3.822636	-4.018304
48	1	0	6.248561	5.023416	-3.708936
49	6	0	6.572038	-1.182223	1.731992
50	6	0	8.346783	-0.429325	3.172801
51	6	0	7.373517	-2.612057	3.338109
52	6	0	8.305855	-1.675008	3.797368
53	1	0	9.049996	0.332580	3.496782
54	1	0	7.307041	-3.594608	3.801588
55	1	0	8.971374	-1.920001	4.619388
56	7	0	-6.596282	2.638942	2.268960
57	7	0	-4.298605	-2.876896	-1.678074
58	7	0	4.516745	2.302985	-2.698121
59	7	0	6.522936	-2.380130	2.336391
60	6	0	7.467883	-0.175308	2.120626
61	1	0	7.454716	0.774444	1.601973
62	6	0	6.650896	2.404077	-1.583128
63	1	0	7.330129	1.949805	-0.872863
64	6	0	-7.939545	1.552263	0.590826
65	1	0	-7.996936	0.793970	-0.179142
66	6	0	-6.636270	-2.412769	-1.318819
67	1	0	-7.377898	-1.799835	-0.822184

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2. T. A. Halgren, *J. Comp. Chem.*, 1996, **17**, 490-519.
3. (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648–5652. (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 1372–1377. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785–789. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* 1994, **98**, 11623–11627.