

Supporting information for *J. Org. Chem.*

# Reactivity of Molecular Oxygen with Ethoxycarbonyl Derivatives of Tetrathiaatriarylmethyl Radicals

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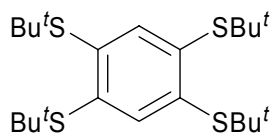
## General Methods.

All reactions were performed under an argon atmosphere. Common solvents were purified before use. Diethyl ether was distilled from sodium-benzophenone ketyl. Toluene and benzene were distilled from calcium hydride. N,N-dimethylformamide (DMF) was dried by molecular sieves. All reagents were reagent grade and purified further when necessary. Reactions were monitored by thin layer chromatography (TLC) using 5×20cm selecto scientific precoated silica gel plates. Flash Column chromatography was performed over silica gel 60A (200-400mesh). HPLC used 1:11 ~ 1:4 ration of water:acetonitrile as eluents and C18 column. Melting points (mp) were measured on an Electrothermal capillary melting point apparatus and are uncorrected. Infrared spectra (IR) were recorded with FT-IR spectrometer and were reported in reciprocal centimeter ( $\text{cm}^{-1}$ ). UV-vis absorption were measured in the concentration 100~200  $\mu\text{M}$  from 200~800 nm at room temperature. Carbon and proton NMR spectra were recorded on 250MHz and 400MHz spectrometer.  $^1\text{H}$  NMR chemical shifts are reported as  $\delta$  values (ppm) relative to deuteriochloroform (7.25 ppm), and splitting patterns are designated as: s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet.  $^{13}\text{C}$  NMR chemical shifts are reported as  $\delta$  values (ppm) relative to deuteriochloroform (77.0 ppm). EPR measurements were carried out on an TMRF 134 EMX instrument at room temperature.

Electrospray ionization (ESI) mass spectrometry analyses were performed with a FTMS Fourier Transform mass spectrometer. Sample was introduced to an electrospray ionization source, and was focused into the FTMS cell using a

home-built set of ion optics. This process generated the sodiated molecular ion (usually as the singly-charged species), denoted as  $((M+Na)^+)$ . But in some cases, acetic acid or trifluoroacetic acid was used to generate the protonated molecular ion  $((M+H)^+)$  instead. Electron impact (EI) ionization was performed with a MS using 70 eV ionization conditions. Matrix assisted laser desorption/ionization time-of-flight (MALDI- TOF) was performed on a mass spectrometer operated in linear, positive ion mode with a  $N_2$  laser. Laser power was used at the threshold level required to generate signal. Accelerating voltage was set to 28 kV. The instrument was calibrated with peptide standards bracketing the molecular weights of the peptide samples (typically mixtures of a Bradykinin fragment 1-5 and Adrenocortico- tropic hormone fragment 18-39).

#### 1,2,4,5-Tetra-tert-butylthiobenzene (5).

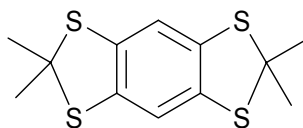


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To a stirred, degassed solution of 2-methyl-2-propanethiol (39 mL, 348 mmol) in dry DMF (20.0 mL) was added small pieces of sodium (8.1 g, 353 mmol) at 0 °C. The mixture was allowed to reach room temperature and stirred 8 h. 1,2,4,5-Tetrachlorobenzene (14.7 g, 68.1 mmol) was added at once, and the resulting mixture was heated to a gentle reflux for 3 h. After being cooled to room temperature, the reaction mixture was poured over ice (200 g). The precipitate was removed by filtration, washed with water, and dried to give 19.8 g (67.5%) of the title compound as an off-white

powder: mp 146-153 °C; <sup>1</sup>H NMR (100 MHz, CDCl<sub>3</sub>) δ 1.35 (s, 36H), 7.94 (s, 2H); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 31.3, 48.1, 139.4, 144.8; IR (CHCl<sub>3</sub>) 2952, 1453, 1416, 1158, 1111, 1052, 883, 725 cm<sup>-1</sup>; MS (ESI, m/z) : 453.176878 (observed, (M+Na<sup>+</sup>)), 453.174848 (exact, (M+Na<sup>+</sup>)).

**2,2,6,6-Tetramethylbenzo[1,2-d;4,5-d']bis[1,3]dithiole (6).**

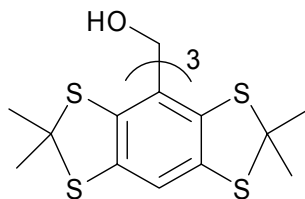


**6**

To a suspension of **5** (8.62 g, 20 mmol) in toluene (80 mL) was added acetone (8 mL) followed by 54% HBF<sub>4</sub> in ether (4.12 mL, 40 mmol) at room temperature. The mixture was stirred at room temperature for 4 h and then heated to reflux for 16 h. After being cooled to room temperature, the resulting black mixture was treated with saturated aqueous NaHCO<sub>3</sub> (80 mL), and the crude product was extracted with ether (2×80 mL). The extracts were dried over MgSO<sub>4</sub> and concentrated in vacuo. The main byproduct of the reaction, *p-tert*-butyltoluene, was also removed under high vacuum at this stage. The resulting pale yellow solid was triturated with MeOH and petroleum ether to give 3.45 g (60%) of the title compound as a white powder: mp 144-147 °C; <sup>1</sup>H NMR (100 MHz, CDCl<sub>3</sub>) δ 1.88 (s, 12H), 7.01 (s, 2H); <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 31.3, 65.7, 116.8, 135.7; IR (CHCl<sub>3</sub>) 2993, 2960, 1449, 1364, 1324, 1166, 1089, 846, 728 cm<sup>-1</sup>; MS (EI, m/z) : 285.9971 (observed, M<sup>+</sup>), 285.997281 (exact, M<sup>+</sup>).

**Tris(2,2,6,6-tetramethylbenzo[1,2-d;4,5-d']bis[1,3]dithiol-4-yl)methanol (7).**

To a stirred suspension of **6** (0.95 g, 3.3 mmol) in ether (40 mL) was added 2.5 M *n*-BuLi in hexane (1.4 mL, 3.3 mmol) dropwise at room temperature. After the mixture was



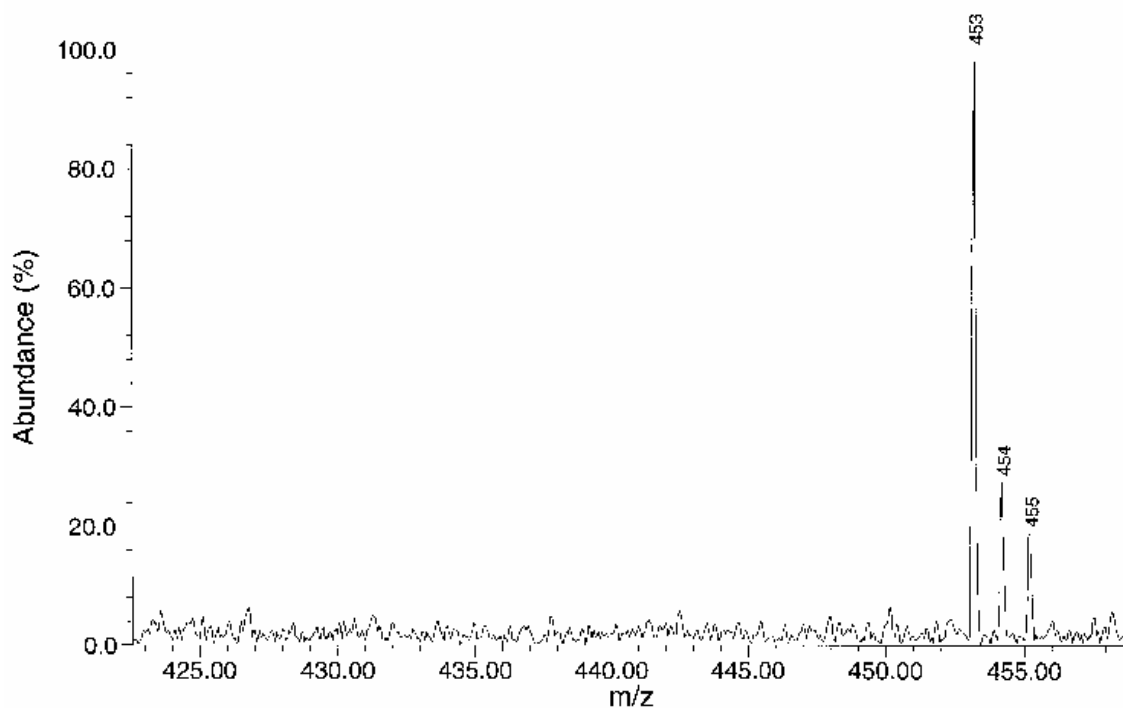
**7**

stirred at 35 °C for 2 h, ClCO<sub>2</sub>Me (77 μL, 0.97 mmol) was added dropwise over 40 min. The resulting orange mixture was stirred and refluxed for 22 h. Saturated aqueous KH<sub>2</sub>PO<sub>4</sub> (15 mL) was added, and the resulting mixture was stirred until the yellow precipitate disappeared. The organic layer was separated, and the aqueous layer was extracted with ether (2×30 mL). The combined organic layers were dried over MgSO<sub>4</sub>, and concentrated in vacuo. The orange residue was crystallized with 5% MeCN in THF (1.5 mL) to give a yellow powder containing THF. The yellow powder was dissolved in benzene and concentrated in vacuo to give 0.38 g (39%) of the title compound as a yellow powder that was a ca. 1:1 mixture of compound **7** / benzene: mp > 290 °C (gradually turned black, dec); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.67 (s, 9H), 1.71 (s, 9H), 1.80 (s, 9H), 1.81 (s, 9H), 6.20 (s, 1H), 7.16 (s, 3H), 7.35 (s, ca. 6H, benzene); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 27.6, 29.1, 32.2, 34.8, 63.3, 64.0, 83.6, 118.1, 128.3 (benzene), 131.8, 137.2, 137.8, 138.3, 139.2; IR (CHCl<sub>3</sub>) 3360, 2960, 2923, 1453, 1361, 1144, 728 cm<sup>-1</sup>; MS (ESI, m/z) : 906.9664 (observed, (M+Na)<sup>+</sup>), 906.961973 (exact, (M+Na)<sup>+</sup>).

# Mass spectra – EI, ESI and MALDI

## Compound 5 (ESI)

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
No. of peaks: 3					
Height and Width: From Spectrum Points	1	455.18001	18.914	0.15943	2855
Peak Fit Type: Lorentzian	2	454.17545	27.514	0.14749	3079
Peak Threshold Set: Automatically	3	453.17688	100.000	0.15265	2969
Min. Peak Width: 3					
Search Start: 99.86000 m/z					
Search Start: 1000.00000 m/z					
Peak Thresh: 7.73 Relative (%)					
Noise Thresh: 1.75 Relative (%)					
Peak S/N: 2.50 (S/N)					



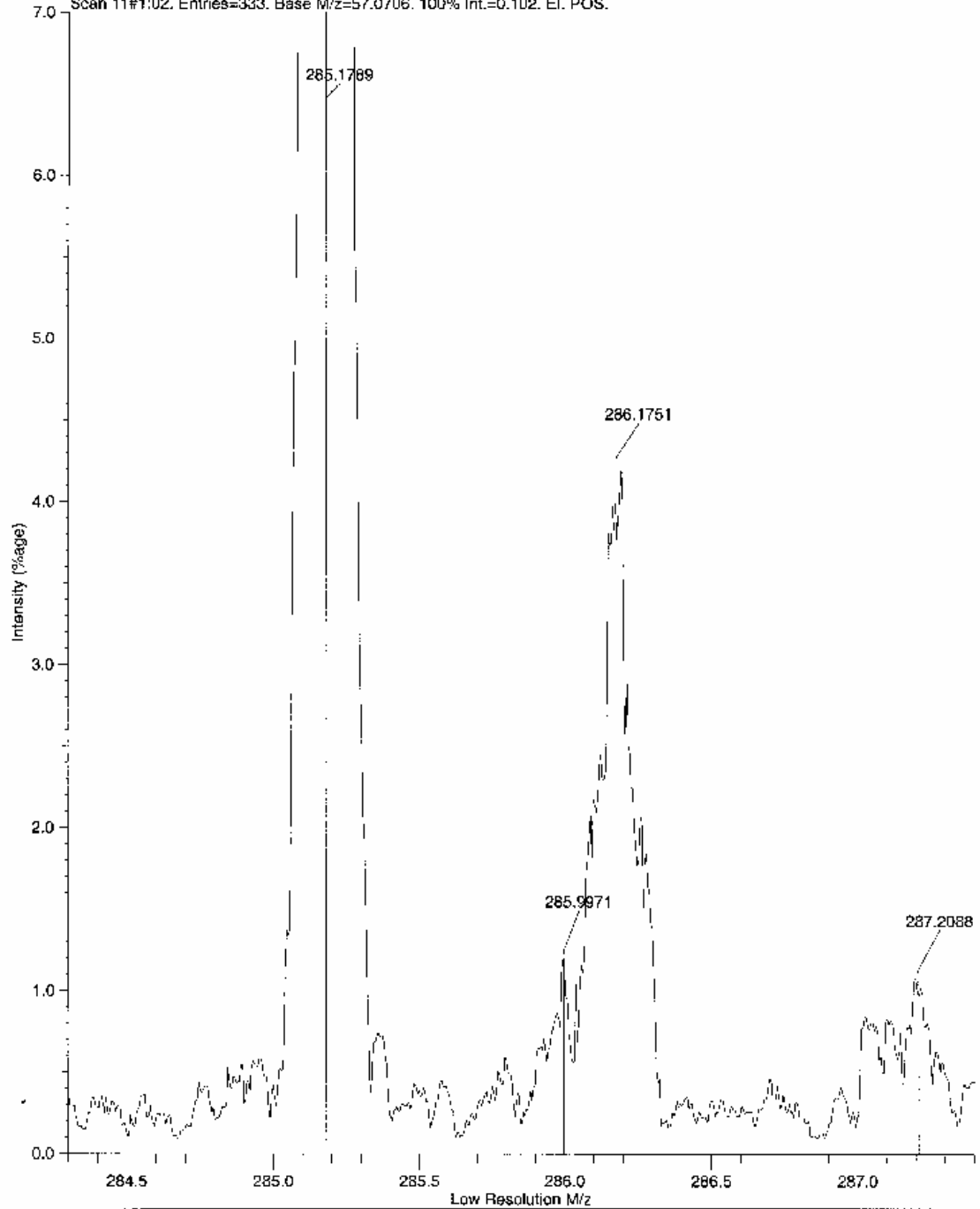
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# Compound 6 (EI)

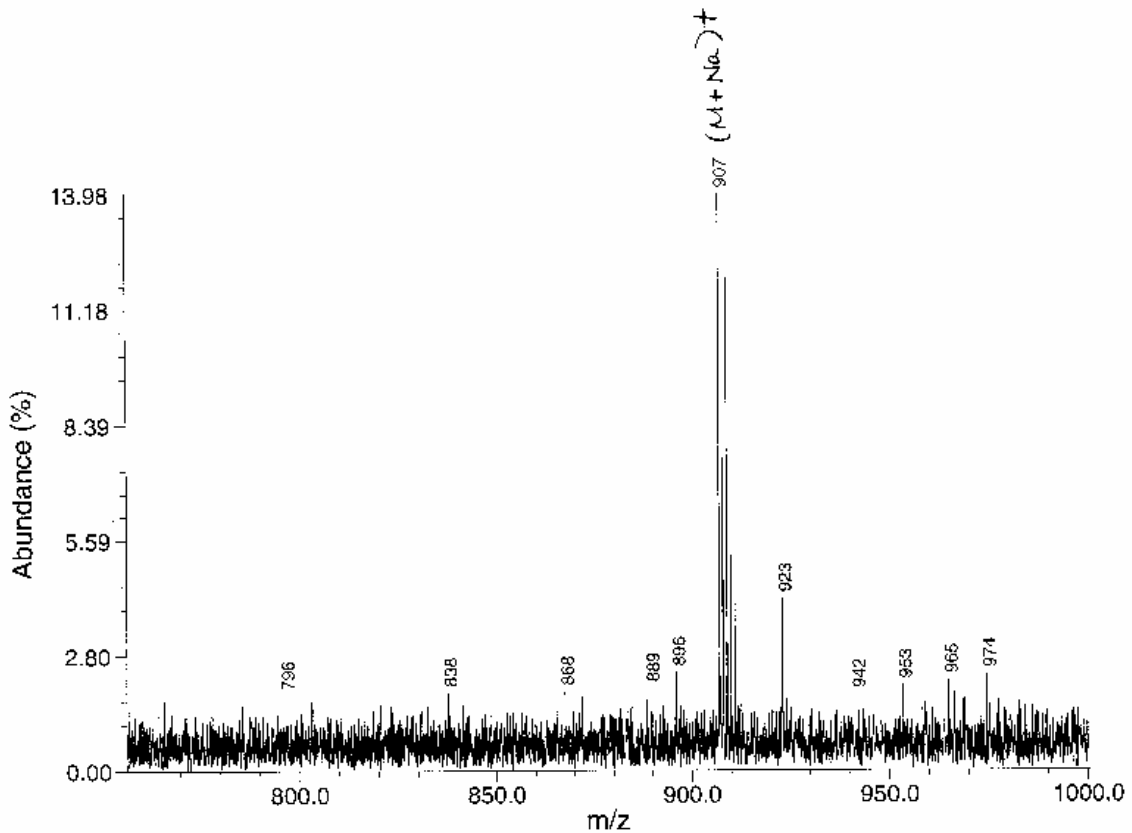
File Name : J:\GCMS Data\Susie\SX-9-16.ms2  
Creation Date/Time : 9/18/03 at 16:36:51  
File Type : Lo-Res Data - Raw (Magnet)  
File Source : Acquired on MASPEC II system [I132/99B4]  
File Title : SX-9-16

SCAN GRAPH. Flagging=Low Resolution M/z. Ctd=(Thr:900 $\mu$ V, Min.Hgt:250 $\mu$ V, Min.Wid(Mlt):12(12), Inc:50%, Res:85%). Highlighting=Sa  
Scan 11#1:02. Entries=333. Base M/z=57.0706. 100% Int.=0.102. EI. POS.



### Compound 7 (ESI)

	Peak Number	Mass (m/z)	Abundance (%)	FWHM (m/z)	Resolving Power
<b>No. of peaks:</b> 17					
<b>Height and Width:</b> From Spectrum Points	1	974.41120	2.317	0.22628	4306
<b>Peak Fit Type:</b> 3-Point Lorentzian	2	966.21204	1.878	0.22338	4326
<b>Peak Threshold Set:</b> Automatically	3	964.85891	2.179	0.11474	8409
<b>Min. Peak Width:</b> 3	4	953.33493	2.058	0.09912	9618
<b>Search Start:</b> 199.71001 m/z	5	941.60861	1.831	0.08256	11405
<b>Search Start:</b> 1000.00000 m/z	6	923.01824	4.168	0.15944	5789
<b>Peak Thresh:</b> 1.80 Relative (%)	7	912.59381	1.865	0.22067	4136
<b>Noise Thresh:</b> 0.41 Relative (%)	8	911.00603	4.036	0.11137	8180
<b>Peak S/N:</b> 2.50 (S/N)	9	909.99275	5.207	0.09306	9779
	10	908.98173	11.929	0.10951	8301
	11	907.97295	7.567	0.17726	5122
	12	906.96640	13.979	0.16276	5572
	13	896.03991	2.382	0.11116	8061
	14	889.34354	1.993	0.08824	10078
	15	867.53592	1.917	0.09428	9202
	16	837.66892	1.894	0.07428	11278
	17	796.48651	1.822	0.07480	10649



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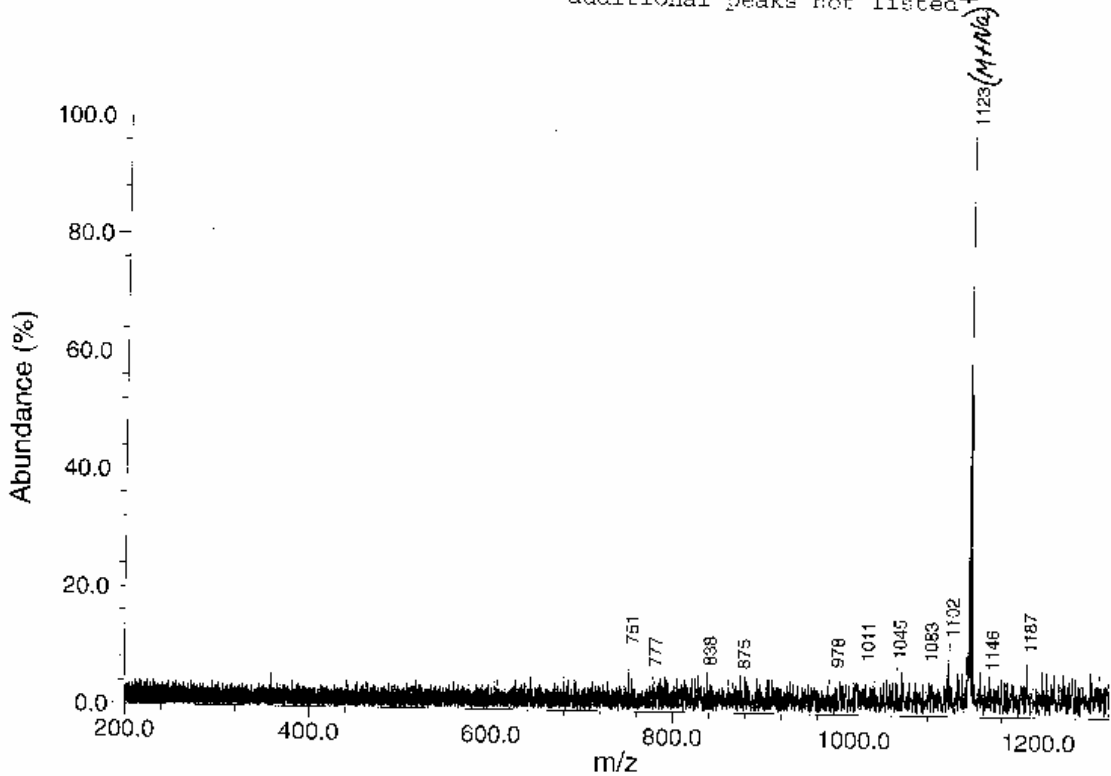
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### Compound 8 (ESI)

<b>No. of peaks:</b> 31		<b>Peak Number</b>	<b>Mass (m/z)</b>	<b>Abundance (%)</b>	<b>FWHH (m/z)</b>	<b>Resolving Power</b>
<b>Height and Width:</b> From Spectrum Points		1	1186.97803	9.930	0.63225	1877
<b>Peak Fit Type:</b> Lorentzian		2	1180.93367	7.019	1.08626	1087
<b>Peak Threshold Set:</b> Automatically		3	1158.52290	6.484	0.51853	2234
<b>Min. Peak Width:</b> 3		4	1153.02855	6.434	0.43776	2634
<b>Search Start:</b> 199.71001 m/z		5	1145.54922	6.927	0.60433	1896
<b>Search Start:</b> 1200.00000 m/z		6	1136.27966	7.643	0.84634	1343
<b>Peak Thresh:</b> 6.27 Relative (%)		7	1128.02331	10.656	0.32164	3507
<b>Noise Thresh:</b> 1.44 Relative (%)		8	1127.02979	19.710	0.40276	2798
<b>Peak S/N:</b> 2.50 (S/N)		9	1126.06245	30.775	0.42020	2680
		10	1125.03879	59.257	0.39504	2848
		11	1124.07490	55.133	0.36345	3093
		12	1123.03005	100.000	0.33109	3392
		13	1120.64447	10.189	0.41254	2716
		14	1116.56449	7.466	0.61514	1815
		15	1112.73540	6.273	1.28687	865
		16	1111.47186	7.346	0.41011	2710
		17	1104.11093	6.555	0.60999	1810
		18	1101.97111	12.378	0.41421	2660
		19	1100.20859	7.046	0.75165	1464
		20	1082.71917	7.677	0.48813	2218
		21	1051.00447	7.556	1.17963	891
		*22	*1045.33090	*8.548	*0.33256	*3142

\* additional peaks not listed†



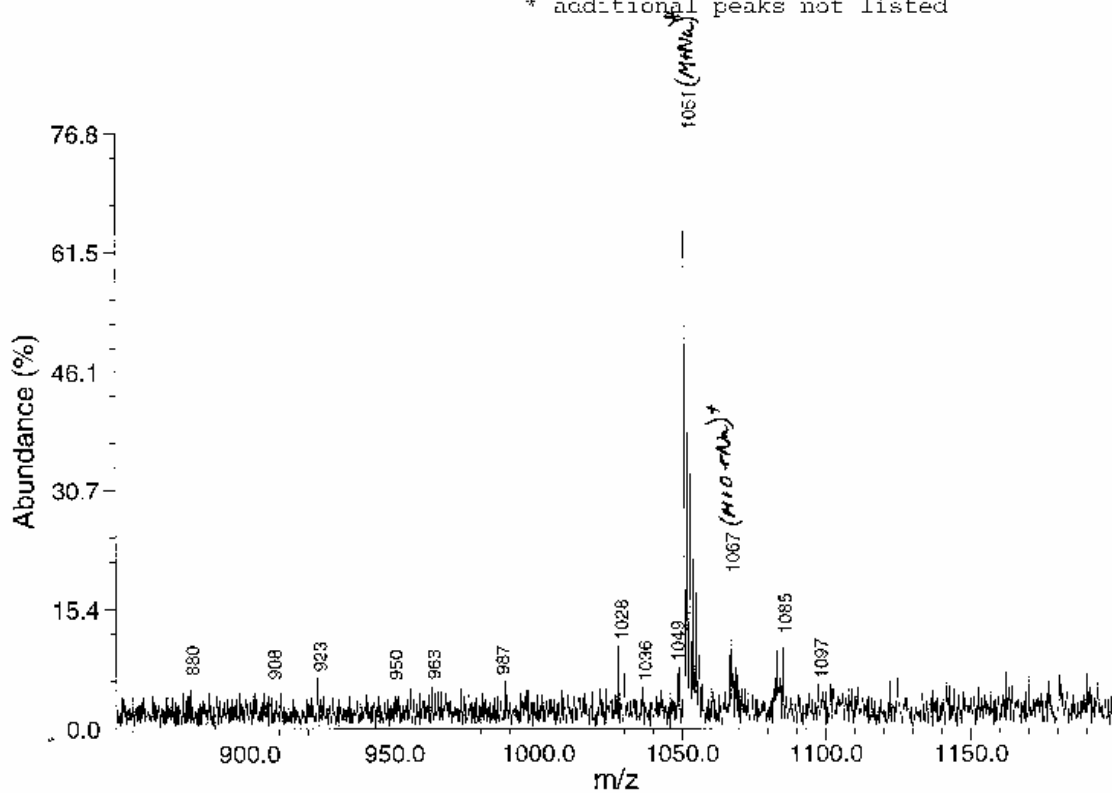
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### Compound 9 (ESI)

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolution Power
No. of peaks: 35					
Height and Width: From Spectrum Points	1	1097.36316	5.547	0.43700	2511
Peak Fit Type: Lorentzian	2	1085.06229	11.282	0.40760	2662
Peak Threshold Set: Automatically	3	1084.03681	6.453	2.06594	525
Min. Peak Width: 3	4	1083.60629	5.213	2.16689	500
Search Start: 199.71001 m/z	5	1083.15119	9.868	0.47644	2273
Search Start: 1100.00000 m/z	6	1082.67556	6.503	2.05388	527
Peak Thresh: 5.19 Relative (%)	7	1070.99639	5.517	0.33680	3180
Noise Thresh: 1.19 Relative (%)	8	1070.07575	6.592	0.38347	2791
Peak S/N: 2.50 (S/N)	9	1068.98107	8.217	0.75774	1411
	10	1067.98917	12.605	0.24555	4349
	11	1067.75161	6.899	1.68847	632
	12	1067.39529	5.258	2.15231	496
	13	1066.97859	19.188	0.23640	4514
	14	1066.74429	9.326	0.63235	1687
	15	1057.07389	5.600	0.24311	4348
	16	1055.96088	9.326	0.62121	1700
	17	1055.04603	18.173	0.31474	3352
	18	1054.64617	5.384	5.44908	194
	19	1054.03915	22.843	0.36739	2869
	20	1053.03136	40.984	0.41052	2565
	21	1052.01939	38.304	0.40164	2619
	*22	*1051.00782	*76.821	*0.34714	*3028

\* additional peaks not listed



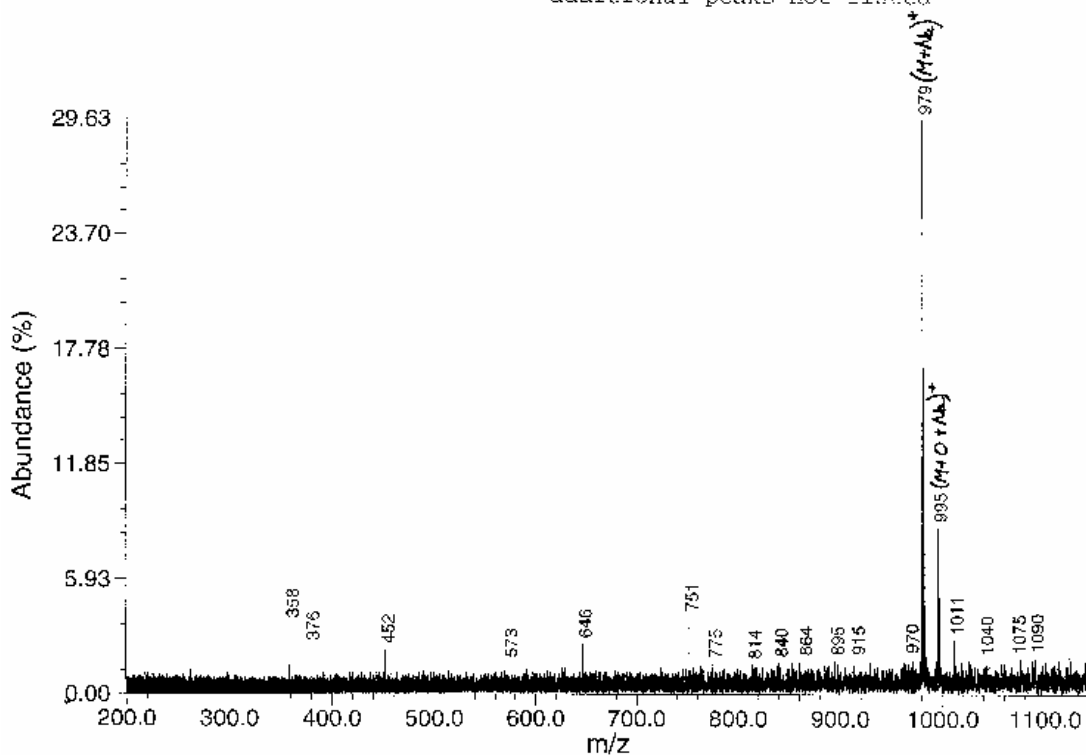
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### Compound 10 (ESI)

No. of peaks: 73		Peak Number	Mass (m/z)	Abundance (%)	FWHM (m/z)	Resolution Power
Height and Width:	From Spectrum Points	1	1099.89431	1.808	0.29587	3718
Peak Fit Type:	Lorentzian	2	1099.55037	1.502	0.20481	5369
Peak Threshold Set:	Automatically	3	1097.06186	1.496	0.35882	1963
Min. Peak Width:	3	4	1090.17777	1.611	0.41709	2614
Search Start:	199.71001 m/z	5	1089.64152	1.849	0.13875	7653
Search Start:	1100.00000 m/z	6	1086.98139	1.761	0.15890	6841
Peak Thresh:	1.48 Relative (%)	7	1082.10952	1.485	0.19818	5460
Noise Thresh:	0.34 Relative (%)	8	1075.12215	1.809	0.34400	3125
Peak S/N:	2.50 (S/N)	9	1059.69531	1.587	0.36476	2905
		10	1056.27281	1.585	0.21752	4856
		11	1045.60899	1.479	0.14380	7271
		12	1044.53301	1.588	0.36019	2900
		13	1042.64183	1.529	0.31496	3310
		14	1040.34648	1.752	0.31676	3284
		15	1028.84968	1.700	0.19062	5397
		16	1026.67961	1.574	0.25699	3995
		17	1025.66930	1.576	0.17463	5873
		18	1025.04490	1.746	0.10863	9436
		19	1017.80045	1.677	0.28861	3527
		20	1017.46763	1.629	0.19223	5293
		21	1012.99806	2.626	0.10575	9580
		*22	*1011.59024	*1.504	*0.10810	*9358

\* additional peaks not listed



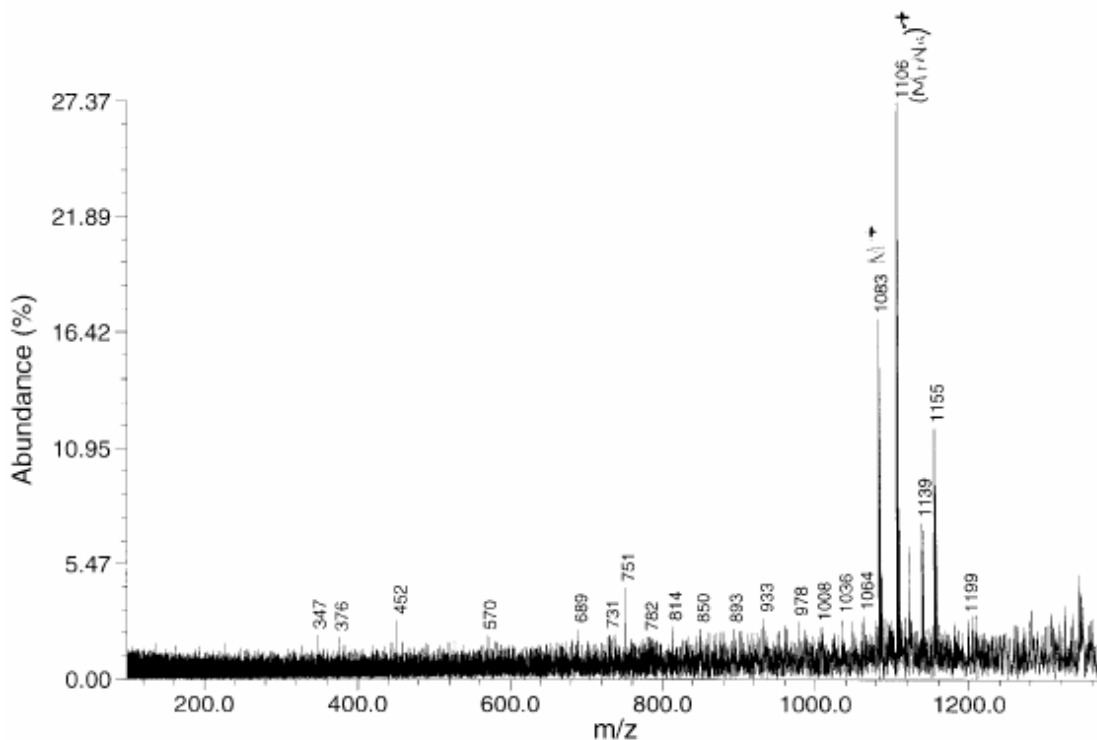
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### Triester radical 1-CO<sub>2</sub>Et without O<sub>2</sub> (ESI)

No. of peaks: 122	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
Height and Width: From Spectrum Points	1	1199.25512	2.050	1.50063	799
Peak Fit Type: Lorentzian	2	1198.52206	2.904	1.30170	921
Peak Threshold Set: Automatically	3	1197.70554	2.383	0.50584	2368
Min. Peak Width: 3	4	1190.16684	2.224	0.97354	1223
Search Start: 99.86000 m/z	5	1185.71091	2.371	0.84431	1404
Search Start: 1200.00000 m/z	6	1182.39214	2.105	1.32427	893
Peak Thresh: 1.99 Relative (%)	7	1181.28624	2.006	0.61215	1930
Noise Thresh: 0.46 Relative (%)	8	1180.67664	2.716	0.41880	2819
Peak S/N: 2.50 (S/N)	9	1179.76873	2.020	1.11712	1056
	10	1172.92283	2.149	0.62122	1888
	11	1170.29007	2.153	1.41233	829
	12	1167.47258	2.315	0.85067	1372
	13	1164.97084	2.144	0.84165	1384
	14	1162.28074	2.228	0.92659	1254
	15	1160.53412	2.623	0.53039	2188
	16	1158.05818	5.402	0.51629	2243
	17	1157.02293	9.259	0.50770	2279
	18	1156.02925	8.814	0.55545	2081
	19	1155.01118	11.945	0.47317	2441
	20	1153.65199	2.580	1.22278	943
	21	1150.52516	2.228	0.63760	1804
	*22	*1146.70260	*2.434	*0.80606	*1423

\* additional peaks not listed

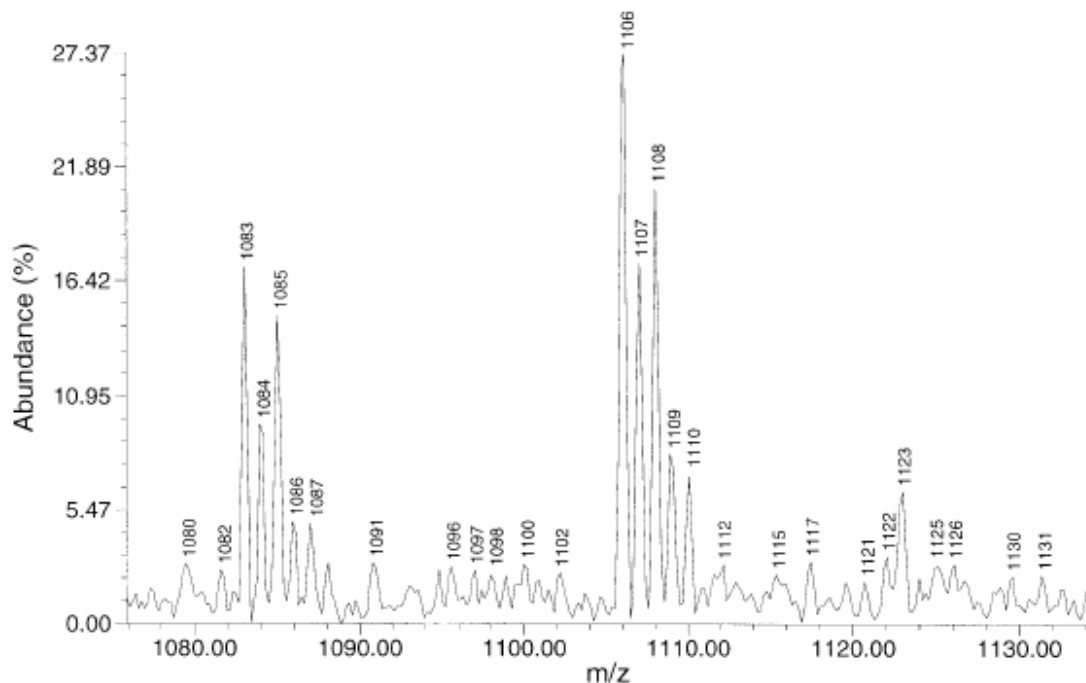


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SX-5-1.pro

### Triester radical 1-CO<sub>2</sub>Et without O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHM (m/z)	Resolving Power
<b>No. of peaks:</b> 35					
<b>Height and Width:</b> From Spectrum Points	1	1131.39752	2.304	0.56557	2000
<b>Peak Fit Type:</b> Lorentzian	2	1129.50523	2.272	0.48096	2348
<b>Peak Threshold Set:</b> Automatically	3	1126.70600	2.065	3.37251	334
<b>Min. Peak Width:</b> 3	4	1126.01990	2.851	2.42388	465
<b>Search Start:</b> 99.86000 m/z	5	1125.04798	2.736	2.45109	459
<b>Search Start:</b> 1200.00000 m/z	6	1123.99079	2.192	3.32583	338
<b>Peak Thresh:</b> 1.99 Relative (%)	7	1122.91994	6.353	0.55125	2037
<b>Noise Thresh:</b> 0.46 Relative (%)	8	1121.97925	3.215	1.56728	716
<b>Peak S/N:</b> 2.50 (S/N)	9	1120.70672	1.999	0.52258	2145
	10	1117.39540	2.966	0.54025	2068
	11	1115.35538	2.347	1.66664	669
	12	1112.04616	2.808	0.96655	1151
	13	1111.62401	2.365	1.04057	1068
	14	1110.02921	7.119	0.44113	2516
	15	1109.00819	8.157	0.47947	2313
	16	1108.04540	20.848	0.42866	2585
	17	1107.00473	17.220	0.41938	2640
	18	1106.02081	27.366	0.45540	2429
	19	1102.14936	2.414	0.65232	1690
	20	1100.82387	2.077	0.71215	1546
	21	1100.05352	2.826	0.96264	1143
	*22	*1098.87555	*2.299	*0.51298	*2142
	* additional peaks not listed				

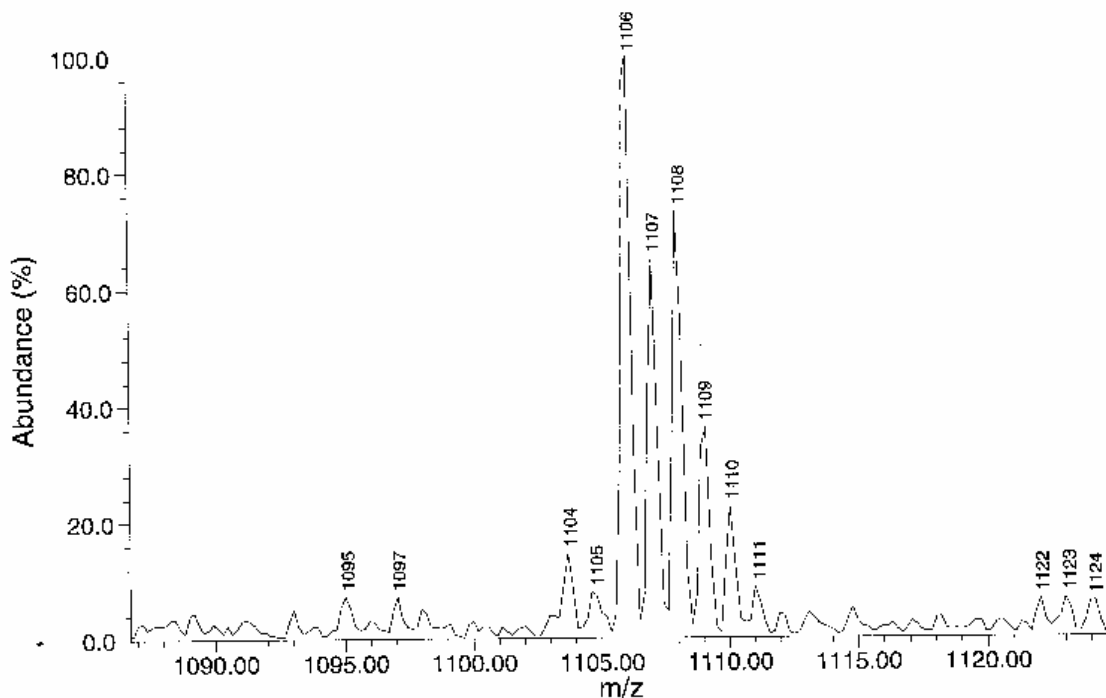


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SX-5-1.pro

### Triester radical 1-CO<sub>2</sub>Et with O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHM (m/z)	Resolving Power
<b>No. of peaks:</b> 13					
<b>Height and Width:</b> From Spectrum Points	1	1124.07015	6.075	0.55023	2043
<b>Peak Fit Type:</b> Lorentzian	2	1123.05385	6.712	0.50744	2213
<b>Peak Threshold Set:</b> Automatically	3	1121.99766	6.462	0.41838	2682
<b>Min. Peak Width:</b> 3	4	1111.07467	8.637	0.43601	2548
<b>Search Start:</b> 99.86000 m/z	5	1110.04015	22.506	0.42635	2604
<b>Search Start:</b> 1200.00000 m/z	6	1109.02775	36.164	0.44764	2478
<b>Peak Thresh:</b> 6.02 Relative (%)	7	1108.04848	73.121	0.43716	2535
<b>Noise Thresh:</b> 0.79 Relative (%)	8	1107.03027	65.080	0.44438	2491
<b>Peak S/N:</b> 5.00 (S/N)	9	1106.02565	100.000	0.45643	2423
	10	1104.70961	7.900	0.64932	1701
	11	1103.69059	14.484	0.46467	2375
	12	1096.98570	7.301	0.40460	2711
	13	1095.00658	7.346	0.54830	1997



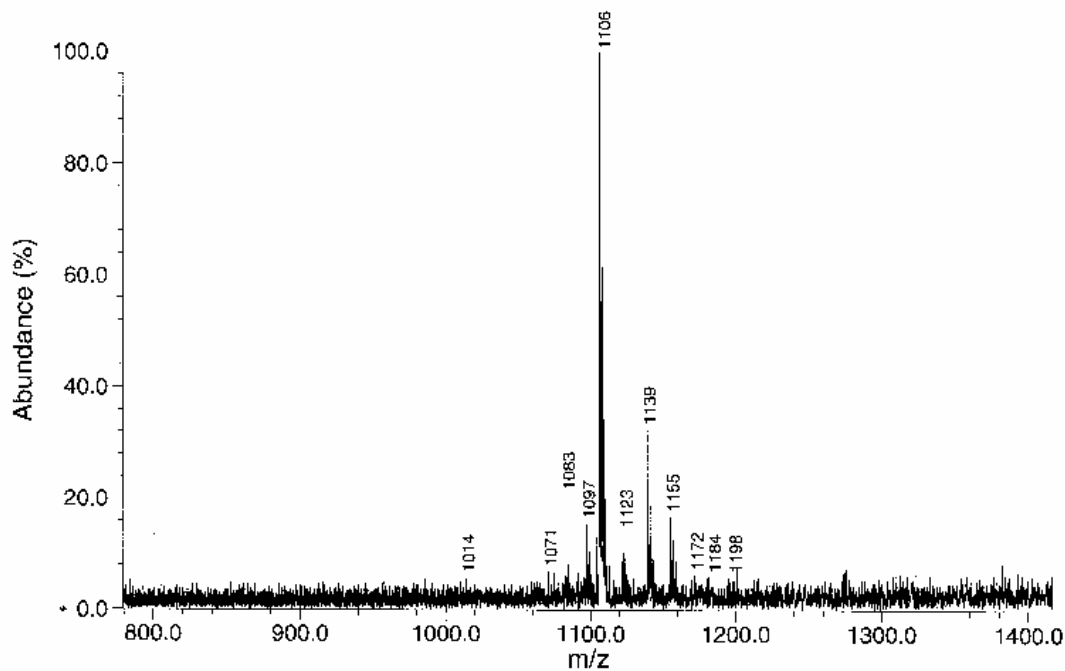
Slide 20

sx-5-1-O2.pro

## Triester radical 1-CO<sub>2</sub>Et with <sup>18</sup>O<sub>2</sub> (ESI) spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHM (m/z)	Resolving Power
<b>No. of peaks:</b> 58					
<b>Height and Width:</b> From Spectrum Points	1	1198.15752	5.689	0.23537	5091
<b>Peak Fit Type:</b> 3-Point Quadratic	2	1194.94140	5.698	0.21802	5481
<b>Peak Threshold Set:</b> Automatically	3	1183.83926	5.753	0.17285	6849
<b>Min. Peak Width:</b> 2	4	1181.05705	6.004	0.19871	5944
<b>Search Start:</b> 199.71001 m/z	5	1180.08671	5.654	0.22798	5176
<b>Search Start:</b> 1200.00000 m/z	6	1171.84857	6.144	0.25856	4532
<b>Peak Thresh:</b> 5.50 Relative (%)	7	1158.99194	8.622	0.14901	7778
<b>Noise Thresh:</b> 1.10 Relative (%)	8	1157.95081	5.635	0.23504	4927
<b>Peak S/N:</b> 3.00 (S/N)	9	1157.02738	12.568	0.26028	4445
	10	1156.03351	9.063	0.37193	3108
	11	1155.02559	16.671	0.30853	3744
	12	1143.19495	5.886	0.44798	2552
	13	1143.00847	9.063	0.15914	7182
	14	1142.07308	8.769	0.47647	2397
	15	1141.94984	9.306	0.45021	2536
	16	1141.02966	18.734	0.35773	3190
	17	1140.02537	16.246	0.18345	6214
	18	1139.86438	8.207	0.60044	1898
	19	1139.02588	32.327	0.22009	5175
	20	1129.61361	5.504	0.20919	5400
	21	1124.99737	6.457	0.45122	2493
	*22	*1123.96386	*9.376	*0.40508	*2775

\* additional peaks not listed

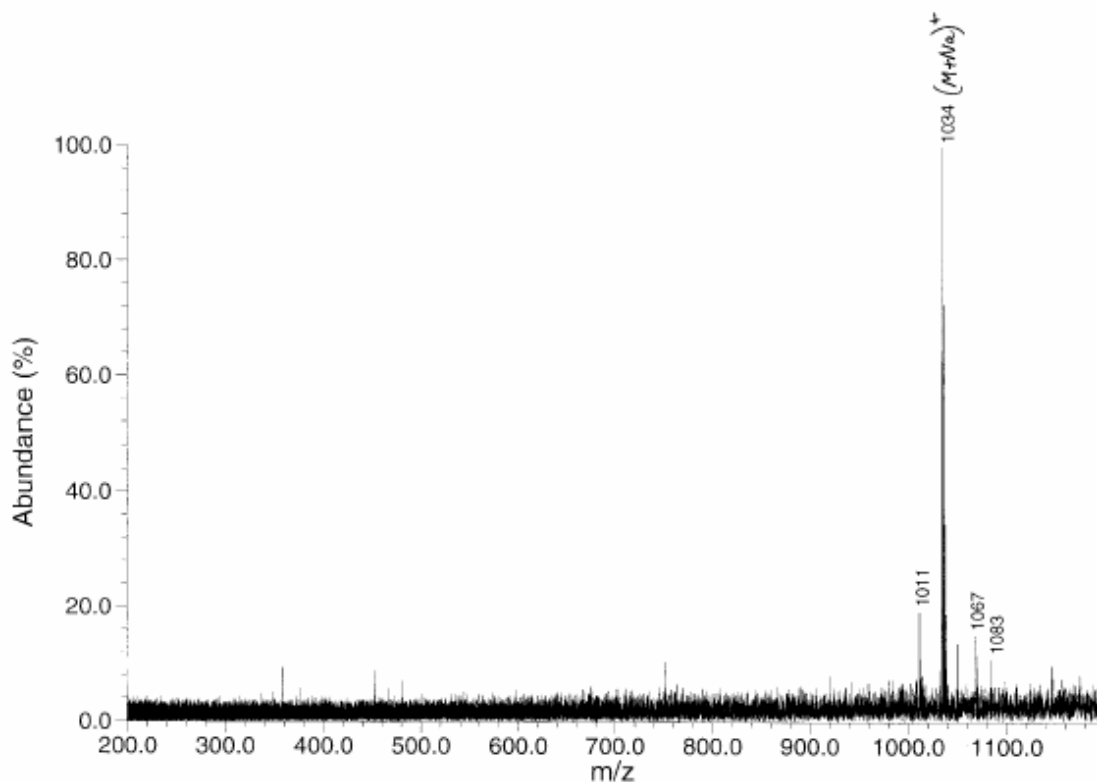


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SX-5-1-O18.pro

### Diester radical 2-CO<sub>2</sub>Et without O<sub>2</sub> (ESI)

No. of peaks: 11		Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
Height and Width:	From Spectrum Points	1	1082.99920	10.866	0.19302	5611
Peak Fit Type:	Lorentzian	2	1069.00764	11.695	0.19842	5388
Peak Threshold Set:	Automatically	3	1066.97563	15.025	0.19144	5574
Min. Peak Width:	3	4	1049.99333	13.623	0.21163	4961
Search Start:	199.71001 m/z	5	1038.00374	18.885	0.19597	5297
Search Start:	1100.00000 m/z	6	1037.01090	34.468	0.16241	6385
Peak Thresh:	10.62 Relative (%)	7	1035.97883	72.591	0.15389	6732
Noise Thresh:	1.38 Relative (%)	8	1034.99812	62.687	0.14853	6968
Peak S/N:	5.00 (S/N)	9	1034.00046	100.000	0.16692	6195
		10	1013.00398	10.961	0.13165	7695
		11	1011.00321	19.127	0.12644	7996



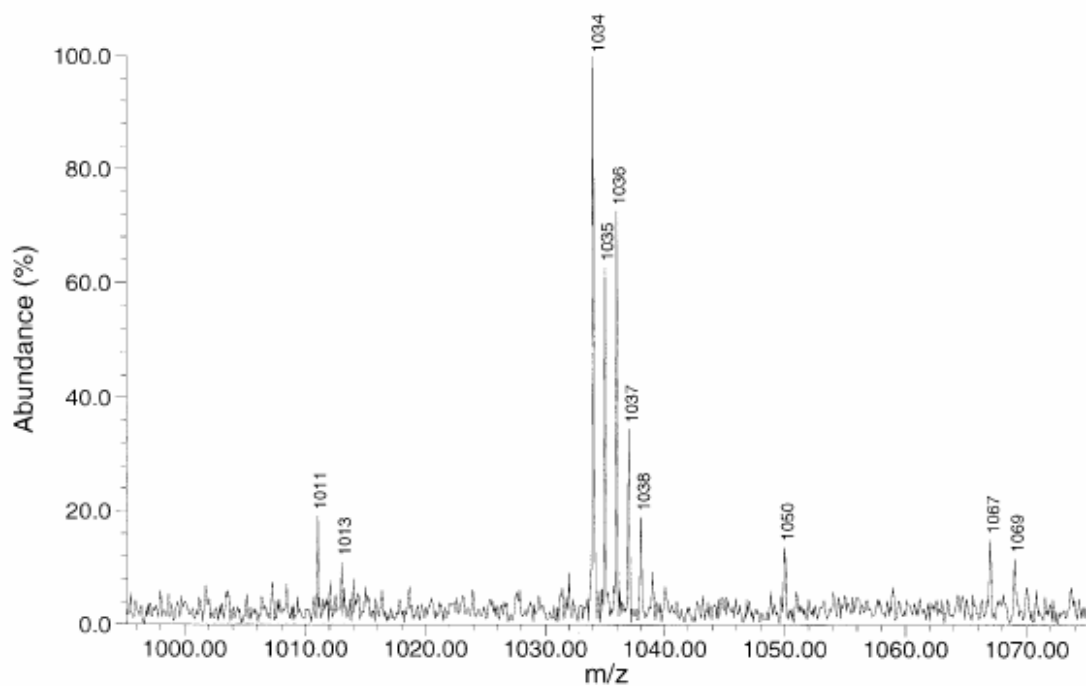
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SX-5-2.pro



## Diester radical 2-CO<sub>2</sub>Et without O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
No. of peaks: 10					
Height and Width: From Spectrum Points	1	1069.00764	11.695	0.19842	5388
Peak Fit Type: Lorentzian	2	1066.97563	15.025	0.19144	5574
Peak Threshold Set: Automatically	3	1049.99333	13.623	0.21163	4961
Min. Peak Width: 3	4	1038.00374	18.885	0.19597	5297
Search Start: 199.71001 m/z	5	1037.01090	34.468	0.16241	6385
Search Start: 1100.00000 m/z	6	1035.97883	72.591	0.15389	6732
Peak Thresh: 10.62 Relative (%)	7	1034.99812	62.687	0.14853	6968
Noise Thresh: 1.38 Relative (%)	8	1034.00046	100.000	0.16692	6195
Peak S/N: 5.00 (S/N)	9	1013.00398	10.961	0.13165	7695
	10	1011.00321	19.127	0.12644	7996

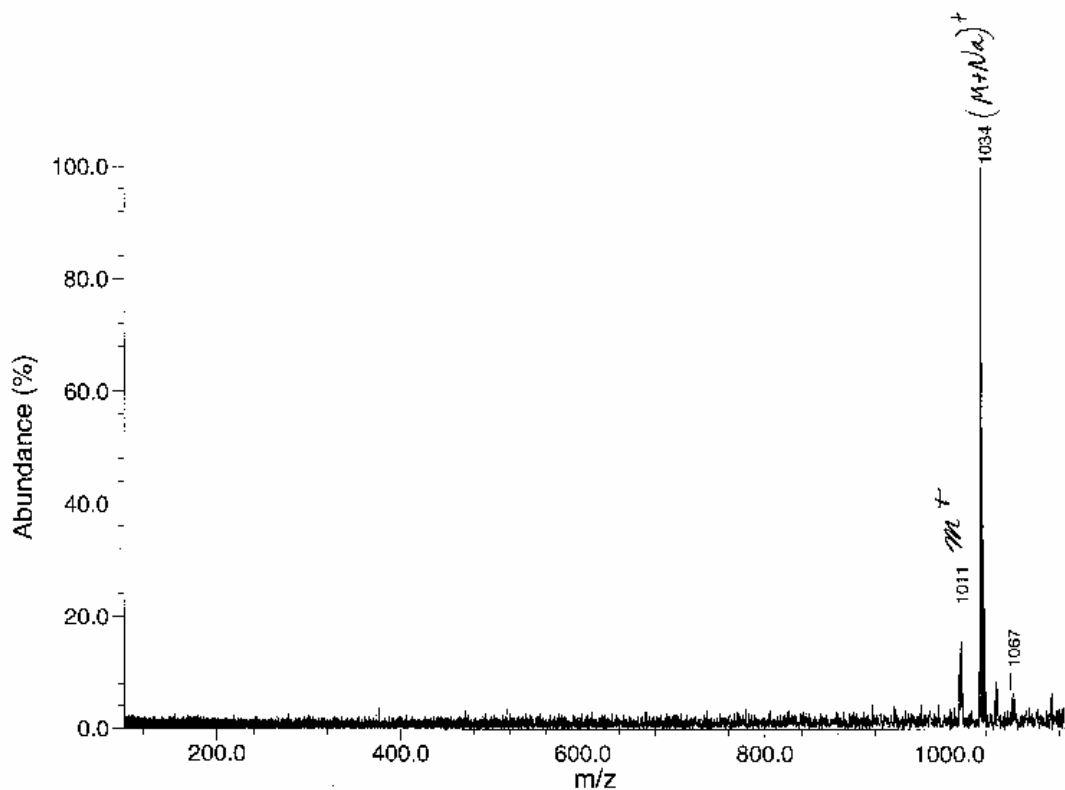


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SX-5-2.pro

## Diester radical 2-CO<sub>2</sub>Et with O<sub>2</sub> (ESI) spectrum

No. of peaks: 19		Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
Height and Width: From Spectrum Points		1	1068.96601	9.291	0.68280	1566
Peak Fit Type: 3-Point Quadratic		2	1067.97312	5.702	0.41345	2583
Peak Threshold Set: Automatically		3	1067.04653	10.157	0.47005	2270
Min. Peak Width: 3		4	1052.04130	7.218	0.54420	1933
Search Start: 99.86000 m/z		5	1050.99901	8.488	0.49665	2116
Search Start: 1100.00000 m/z		6	1049.98768	6.224	0.36504	2876
Peak Threshold: 5.58 Relative (%)		7	1039.97209	5.790	0.36711	2833
Noise Thresh: 0.73 Relative (%)		8	1039.02371	8.998	0.44988	2310
Peak S/N: 5.00 (S/N)		9	1037.99694	21.568	0.42164	2462
		10	1036.99514	32.380	0.45594	2274
		11	1035.99629	65.250	0.44099	2349
		12	1035.00988	53.732	0.44412	2330
		13	1033.99991	100.000	0.45607	2267
		14	1031.94814	10.353	0.46128	2237
		15	1014.99014	6.480	0.41071	2471
		16	1014.01690	6.420	1.68864	600
		17	1013.04252	15.886	0.51420	1970
		18	1011.98998	12.338	0.45271	2235
		19	1011.03032	21.373	0.46334	2162

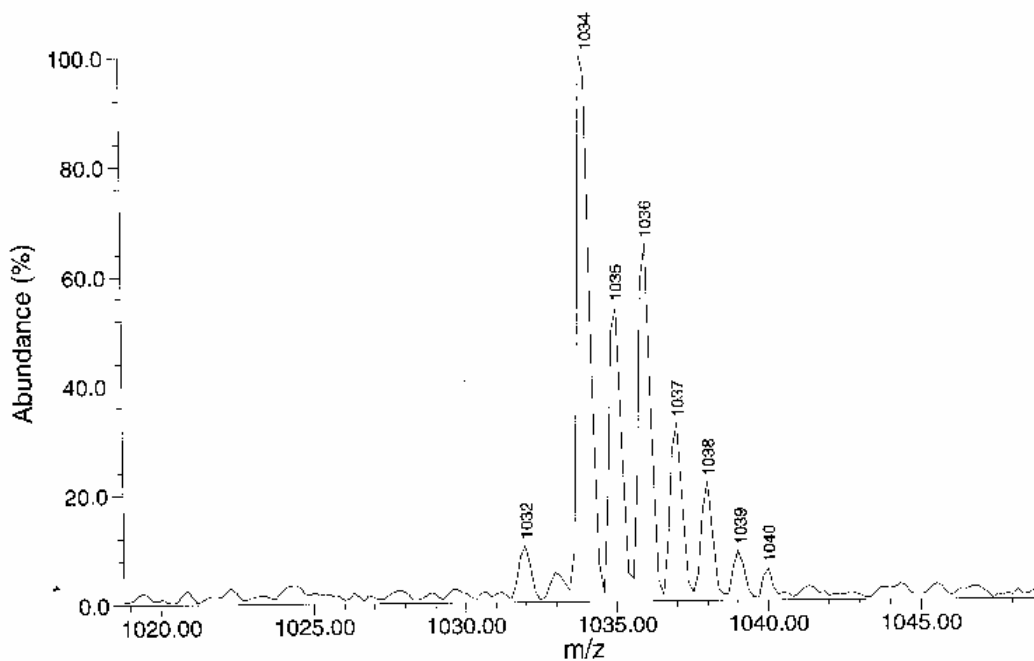


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sx-5-2-O2.pro

## Diester radical 2-CO<sub>2</sub>Et with O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
<b>No. of peaks:</b> 8	1	1039.97209	5.790	0.36711	2833
<b>Height and Width:</b> From Spectrum Points	2	1039.02371	8.998	0.44988	2310
<b>Peak Fit Type:</b> 3-Point Quadratic	3	1037.99694	21.568	0.42164	2462
<b>Peak Threshold Set:</b> Automatically	4	1036.99514	32.380	0.45594	2274
<b>Min. Peak Width:</b> 3	5	1035.99629	65.250	0.44099	2349
<b>Search Start:</b> 99.86000 m/z	6	1035.00988	53.732	0.44412	2330
<b>Search Start:</b> 1100.00000 m/z	7	1033.99991	100.000	0.45607	2267
<b>Peak Thresh:</b> 5.58 Relative (%)	8	1031.94814	10.353	0.46128	2237
<b>Noise Thresh:</b> 0.73 Relative (%)					
<b>Peak S/N:</b> 5.00 (S/N)					

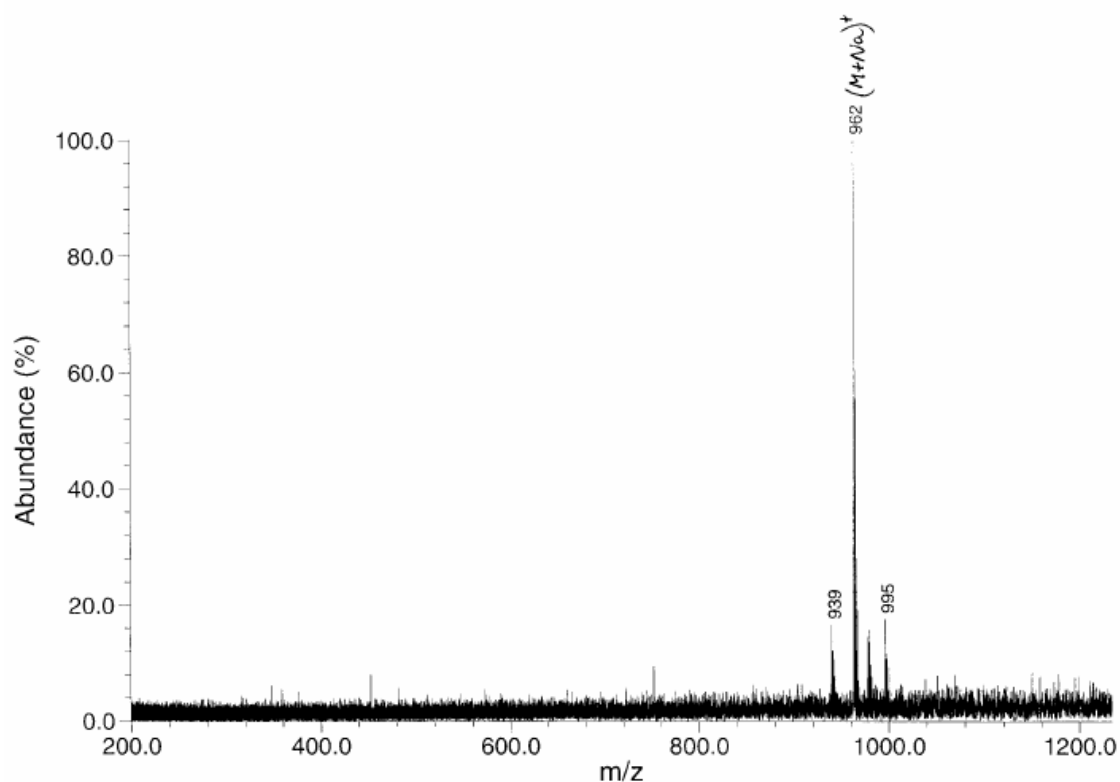


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sx-5-2-O2.pro

### Monoester radical 3-CO<sub>2</sub>Et without O<sub>2</sub> (ESI)

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
No. of peaks: 15					
Height and Width: From Spectrum Points	1	996.97647	11.700	0.17466	5708
Peak Fit Type: 3-Point Quadratic	2	995.96963	10.697	0.15246	6532
Peak Threshold Set: Automatically	3	994.97352	17.568	0.14211	7001
Min. Peak Width: 3	4	979.93454	9.695	0.17105	5729
Search Start: 199.71001 m/z	5	978.95570	15.738	0.16924	5784
Search Start: 1200.00000 m/z	6	977.96524	13.641	0.20439	4785
Peak Thresh: 9.36 Relative (%)	7	976.98240	14.582	0.19236	5079
Noise Thresh: 1.22 Relative (%)	8	965.95703	19.103	0.15831	6102
Peak S/N: 5.00 (S/N)	9	964.96642	28.046	0.14683	6572
	10	963.97185	60.566	0.12885	7481
	11	962.98079	55.748	0.11255	8556
	12	961.98135	100.000	0.13164	7308
	13	940.99693	10.622	0.16739	5622
	14	940.01085	12.165	0.13652	6886
	15	938.99476	16.569	0.14202	6612

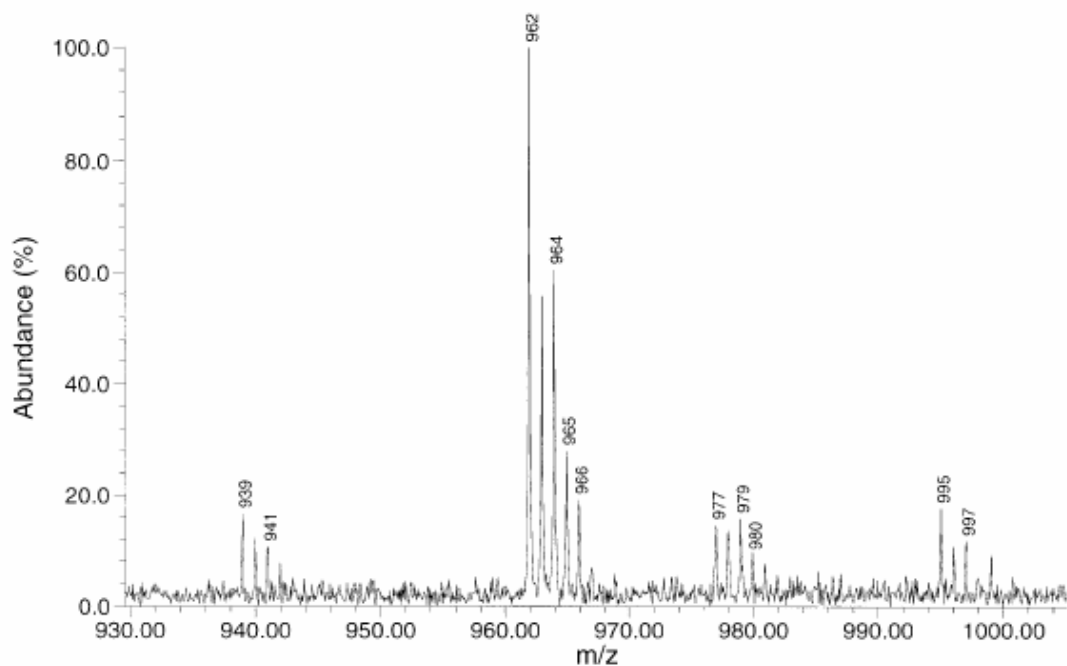


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SX-5-3.pro

### Monoester radical 3-CO<sub>2</sub>Et without O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
No. of peaks: 15					
Height and Width: From Spectrum Points	1	996.97647	11.700	0.17466	5708
Peak Fit Type: 3-Point Quadratic	2	995.96963	10.697	0.15246	6532
Peak Threshold Set: Automatically	3	994.97352	17.568	0.14211	7001
Min. Peak Width: 3	4	979.93454	9.695	0.17105	5729
Search Start: 199.71001 m/z	5	978.95570	15.738	0.16924	5784
Search Start: 1200.00000 m/z	6	977.96524	13.641	0.20439	4785
Peak Thresh: 9.36 Relative (%)	7	976.98240	14.582	0.19236	5079
Noise Thresh: 1.22 Relative (%)	8	965.95703	19.103	0.15831	6102
Peak S/N: 5.00 (S/N)	9	964.96642	28.046	0.14683	6572
	10	963.97185	60.566	0.12885	7481
	11	962.98079	55.748	0.11255	8556
	12	961.98135	100.000	0.13164	7308
	13	940.99693	10.622	0.16739	5622
	14	940.01085	12.165	0.13652	6886
	15	938.99476	16.569	0.14202	6612

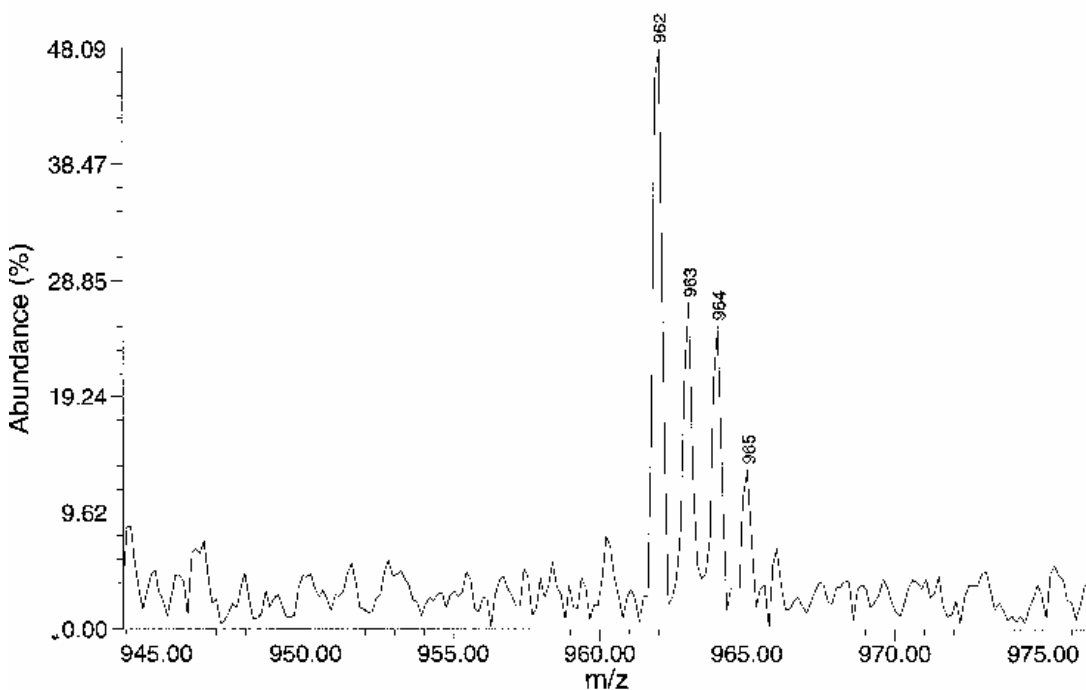


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SX-5-3.pro

### Monoester radical 3-CO<sub>2</sub>Et with O<sub>2</sub> (ESI) enlarged spectrum

	Peak Number	Mass (m/z)	Abundance (%)	FWHH (m/z)	Resolving Power
No. of peaks: 4					
Height and Width: From Spectrum Points	1	964.98815	13.141	0.38203	2526
Peak Fit Type: 3-Point Quadratic	2	963.99099	25.086	0.36827	2618
Peak Threshold Set: Automatically	3	963.00085	27.021	0.36026	2673
Min. Peak Width: 3	4	961.98294	48.090	0.36091	2665
Search Start: 99.86000 m/z					
Search Stop: 1050.00000 m/z					
Peak Thresh: 10.56 Relative (%)					
Noise Thresh: 1.36 Relative (%)					
Peak S/N: 5.00 (S/N)					

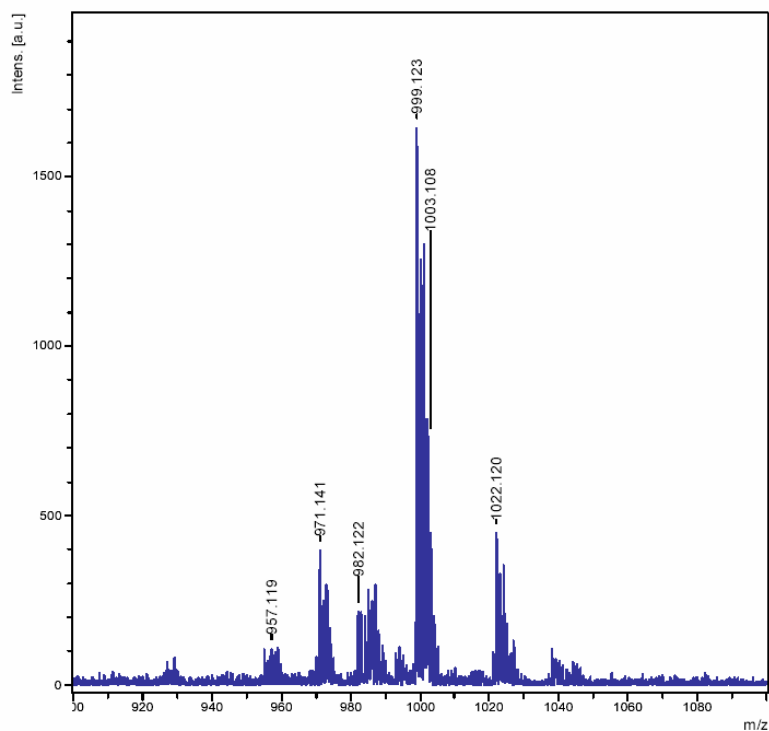


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sx-5-3-O2.pro

## Tri-salt radical 1-CO<sub>2</sub>Na without O<sub>2</sub> (MALDI) spectrum

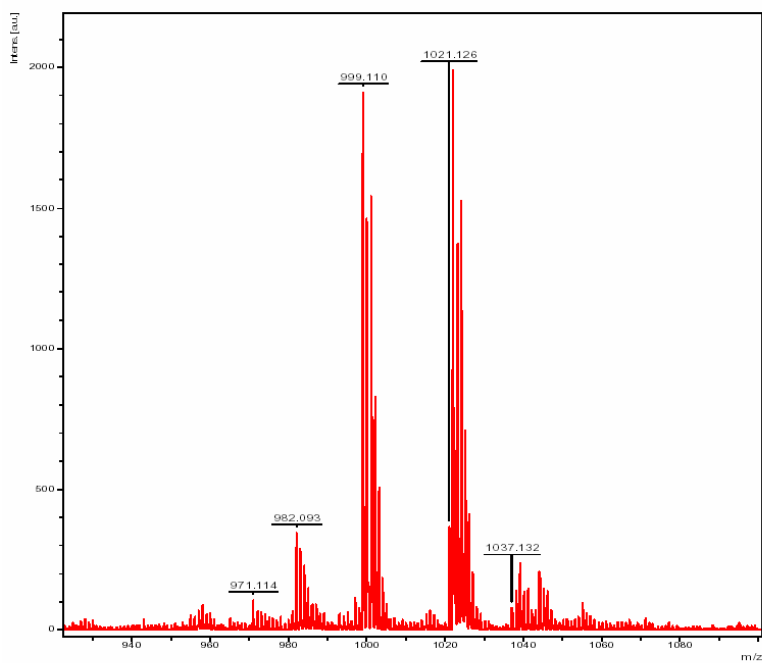
D:\DATA\MALDI\Oct 05\M111504 SX-6-1



m/z	SN	Quality Fac.	Res.	Intens.	Area
957.119	7.0	160	2014	83.13	94
971.141	34.5	2463	3594	409.26	200
973.150	16.8	1026	3339	198.78	101
982.122	19.0	220	4365	226.04	94
985.120	17.9	245	3627	210.93	136
987.096	9.2	447	1202	108.50	165
999.123	144.7	1514	3865	1699.17	835
1001.116	78.0	1407	3804	914.24	528
1003.108	14.6	175	5160	171.44	87
1022.120	24.9	543	4656	289.01	180
1023.660	8.2	125	2624	95.40	48
1024.135	16.2	293	5113	188.19	90

## Tri-salt radical 1-CO<sub>2</sub>Na with O<sub>2</sub> (MALDI) spectrum

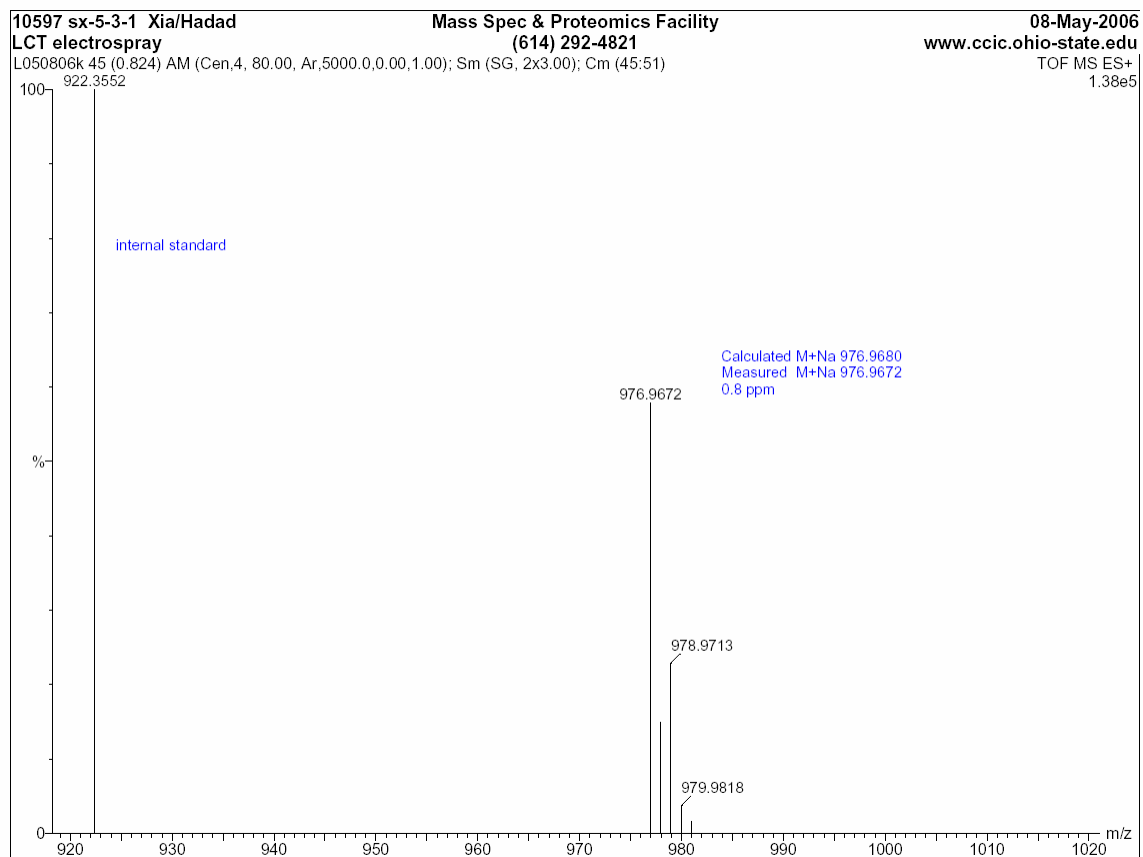
D:\DATA\MALDI\Oct 05\M101405\9477 SX-6-1-O2



m/z	SN	Quality Fac.	Res.	Intens.	Area
971.114	10.0	256	5503	100.73	35
982.093	33.6	723	5637	376.80	127
999.110	163.4	15809	4784	2092.17	888
1021.126	114.9	21405	5651	368.00	82
1037.132	24.0	4786	12475	77.00	12

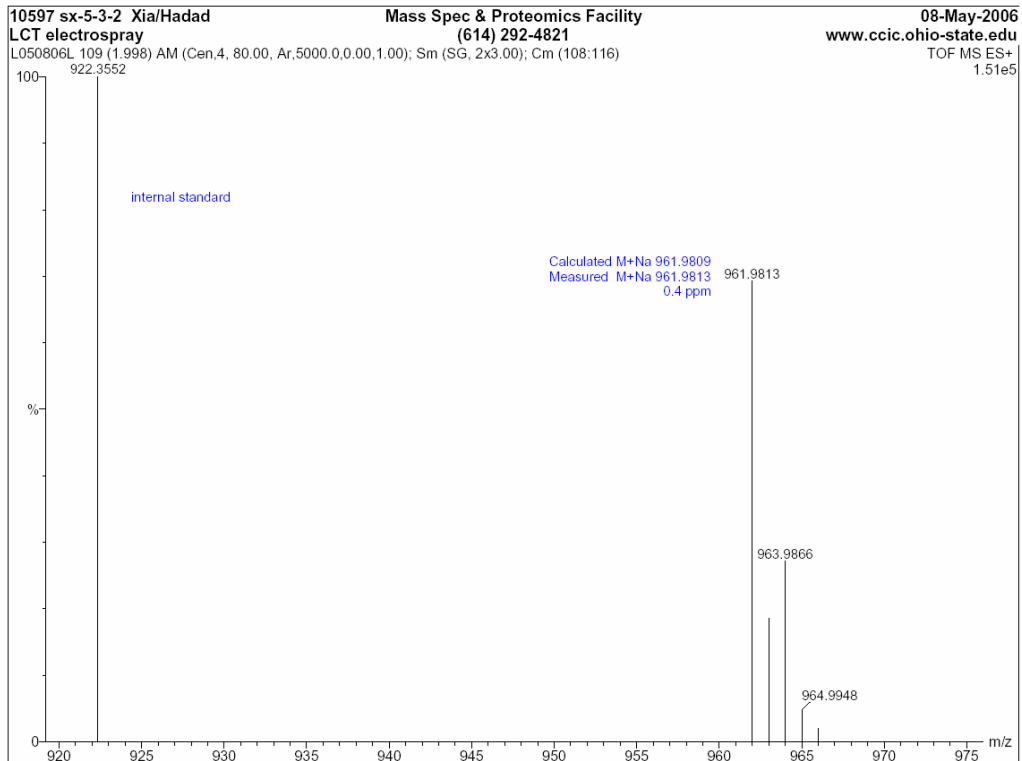
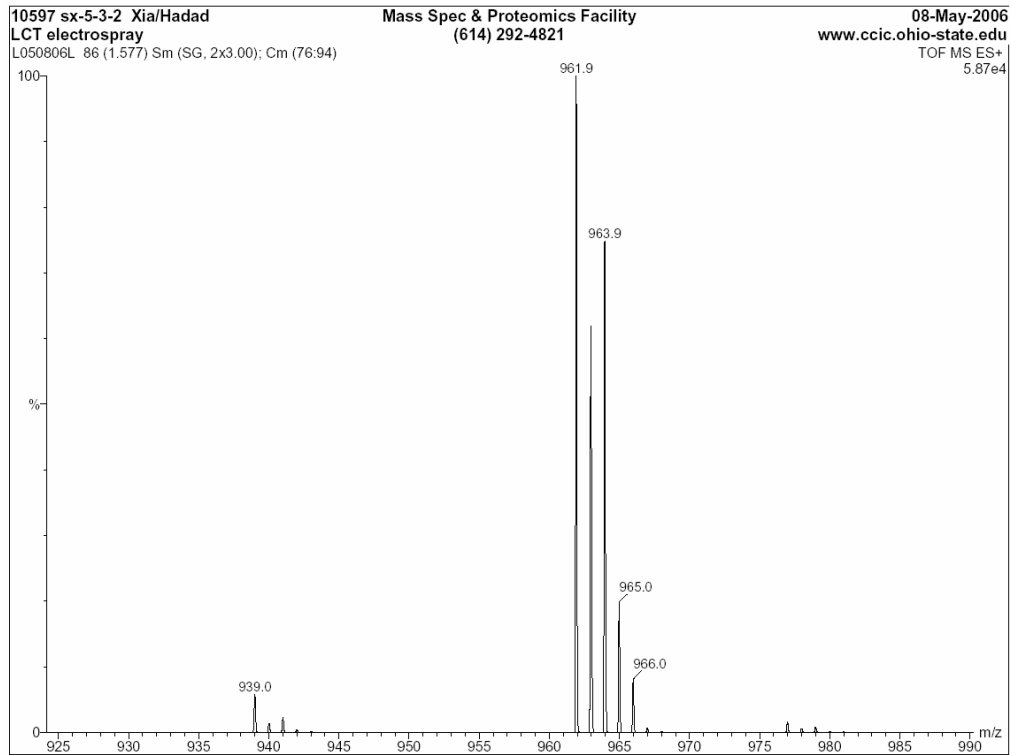
10/14/2005 09:26:27 AM

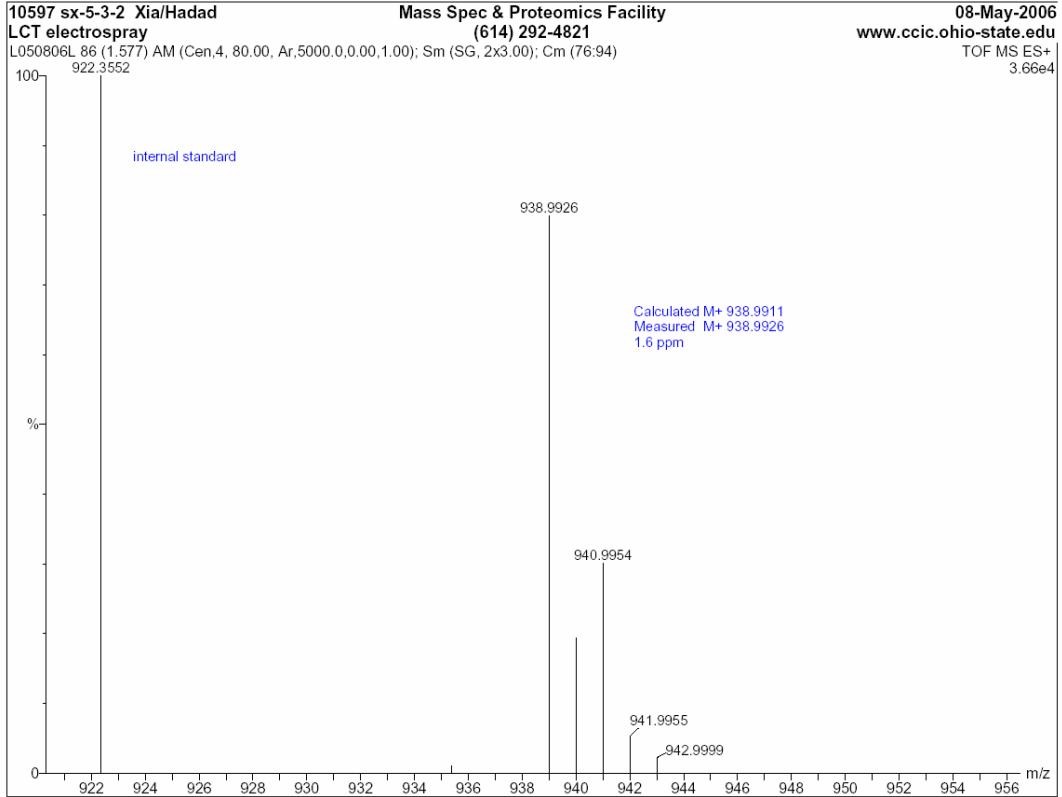
# (M+15) residue of monoester 3-CO<sub>2</sub>Et decomposition (ESI) spectrum



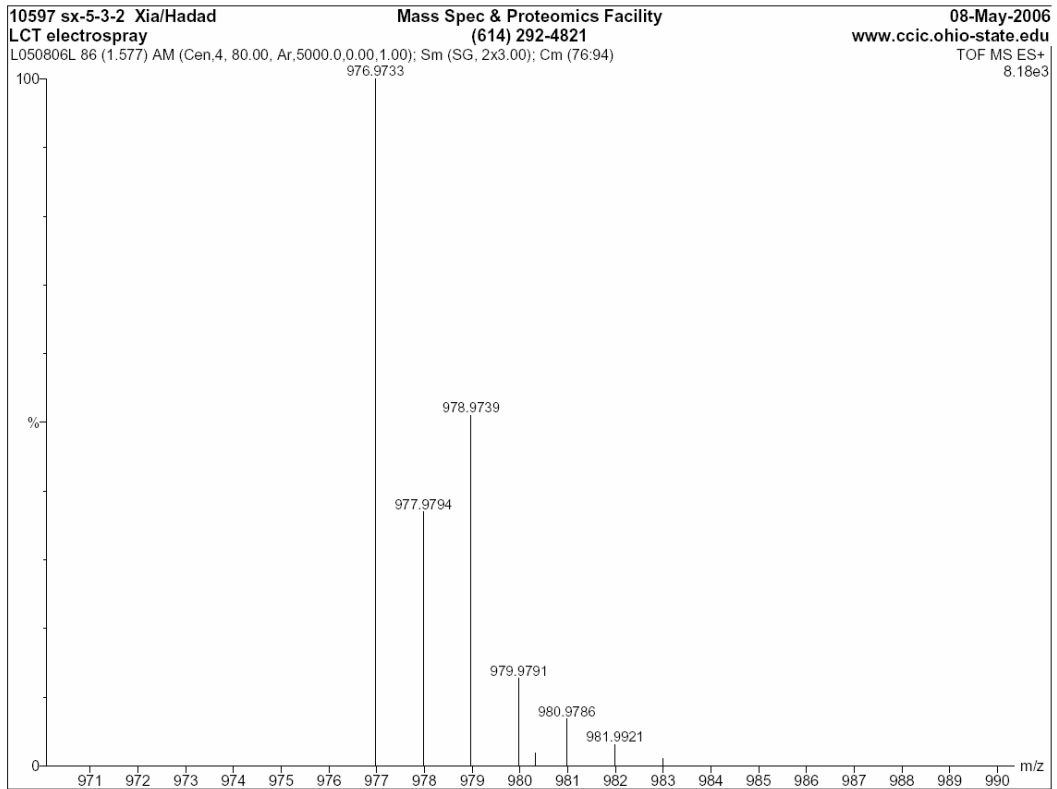


# M residue of monoester 3-CO<sub>2</sub>Et decomposition (ESI) spectrum

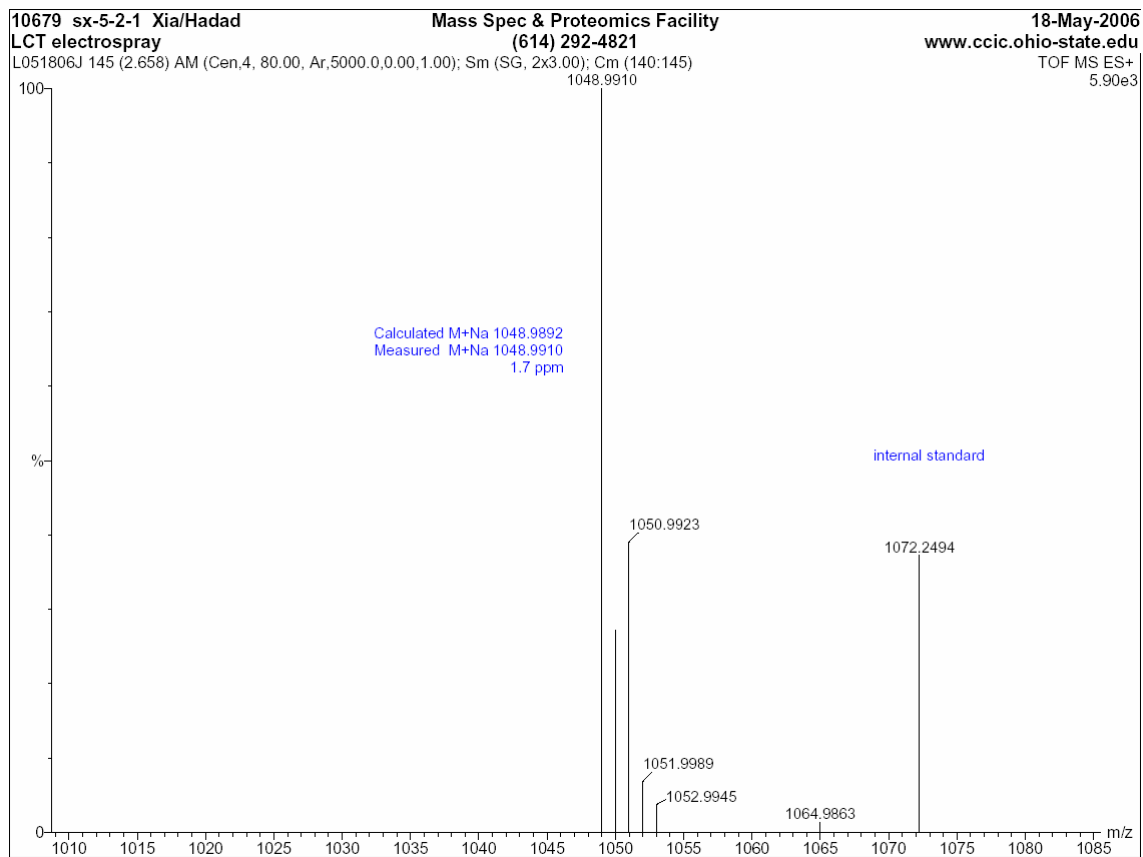




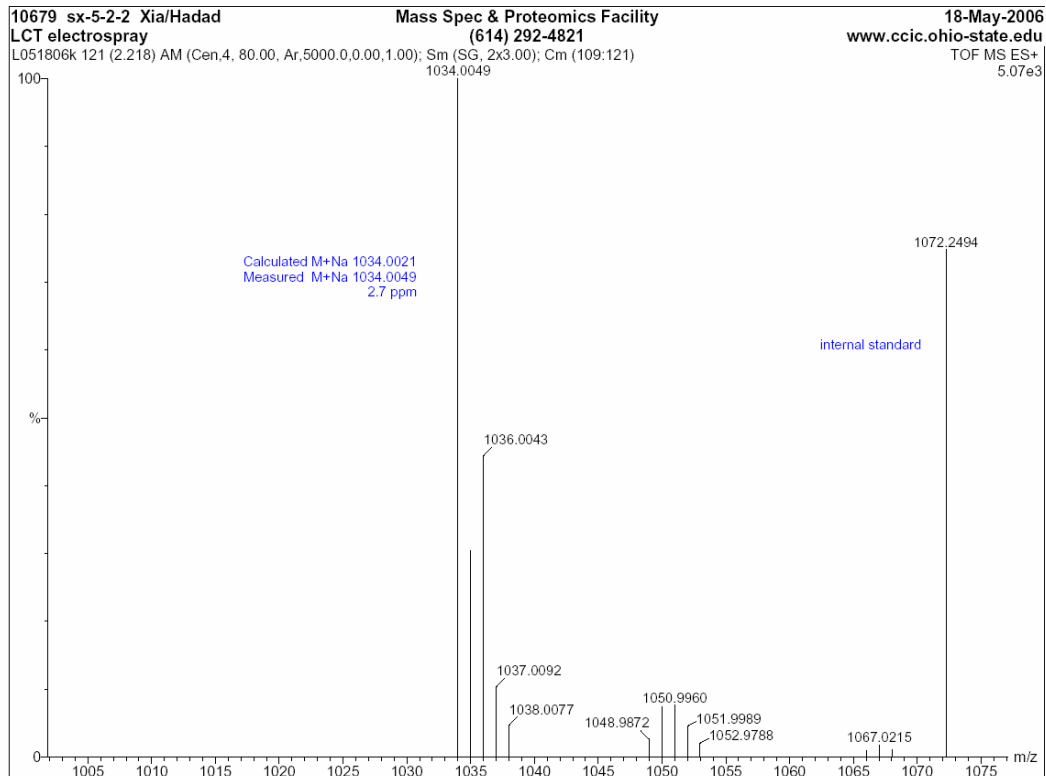
**(M+Na+15), (M+Na+16), (M+Na+17)**



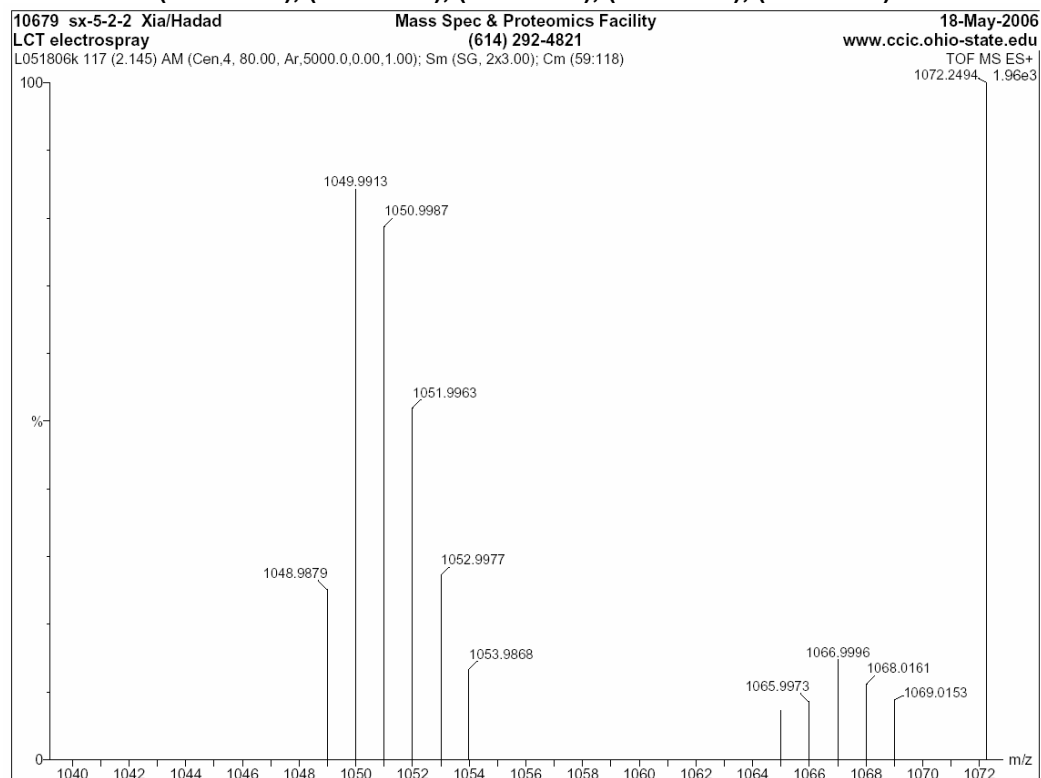
# (M+15) residue of monoester 2-CO<sub>2</sub>Et decomposition (ESI) spectrum



# M residue of monoester 2-CO<sub>2</sub>Et decomposition (ESI) spectrum

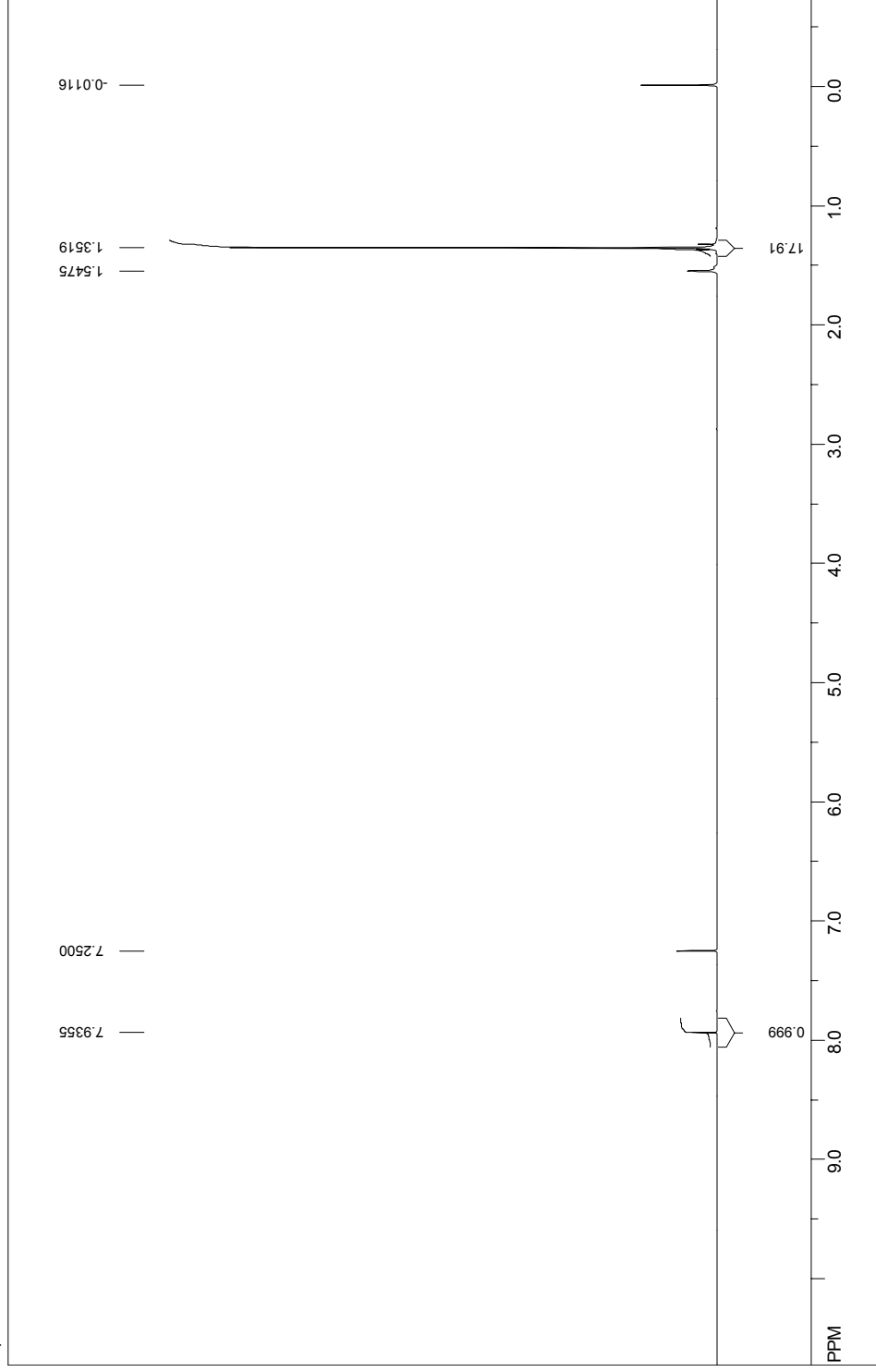


## (M+Na+15), (M+Na+16), (M+Na+17), (M+Na+32), (M+Na+33)



# NMR spectra Compound 5 <sup>1</sup>H NMR

SpinWorks 2.4:

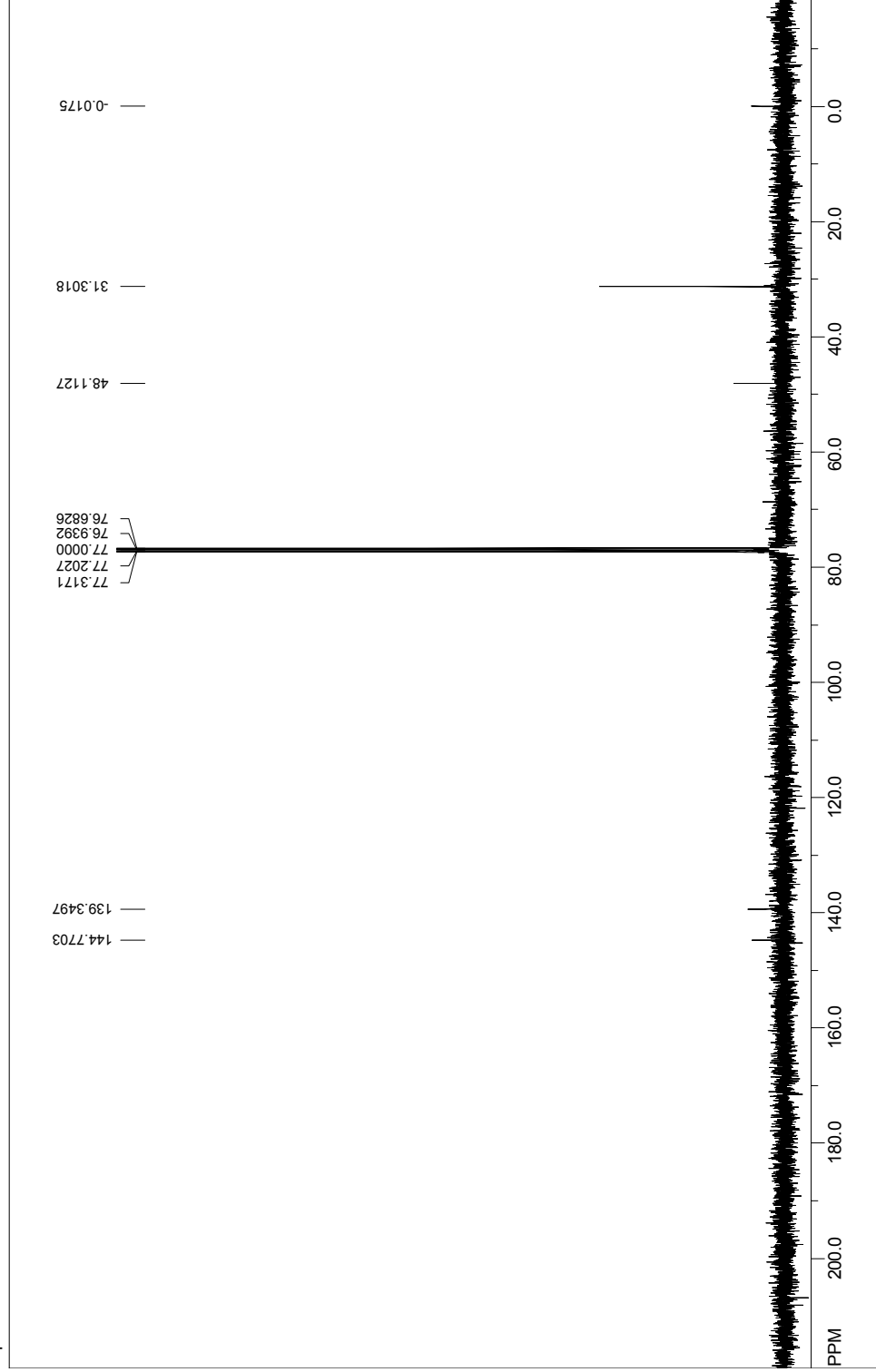


file: U:\research\paper\data\mm1-8-09-04\1\fid exp1 <zg30>  
transmitter freq: 400.132471 MHz  
time domain size: 32768 points  
width: 8278.15 Hz = 20.688513 ppm = 0.252629 Hz/pt  
number of scans: 16

freq. of 0 ppm: 400.130013 MHz  
processed size: 16384 complex points  
LB: 0.300 GB: 0.0000

# Compound 5 <sup>13</sup>C NMR

SpinWorks 2.4:

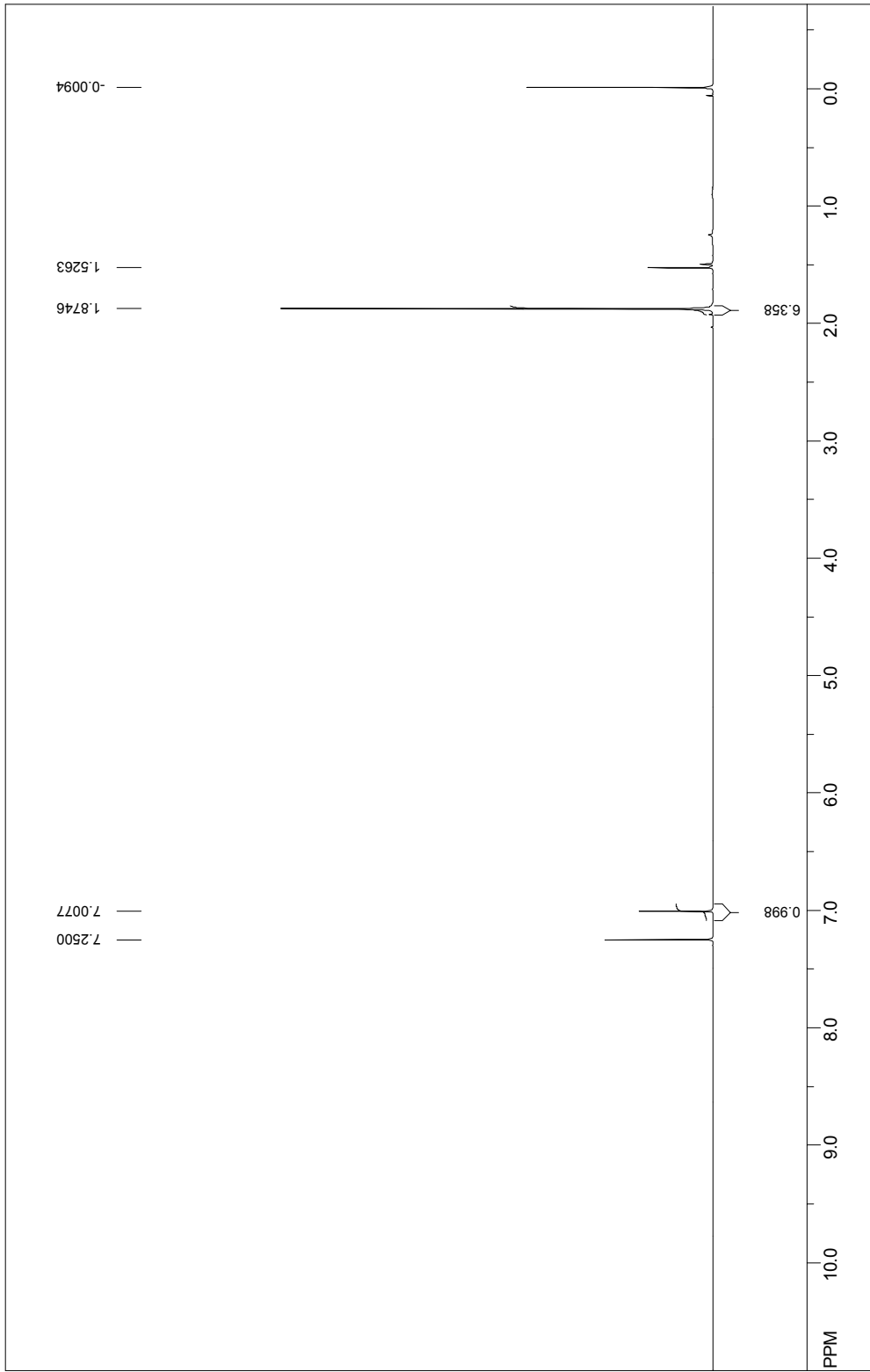


file: U:\research\paper\data\nmr\1-8-09-04\21fd exp: <2jg3Q>  
transmitter freq.: 100.622800 MHz  
time domain size: 65536 points  
width: 23880.82 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 100

freq. of 0 ppm: 100.612768 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 6 <sup>1</sup>H NMR

SpinWorks 2.4: proton-3

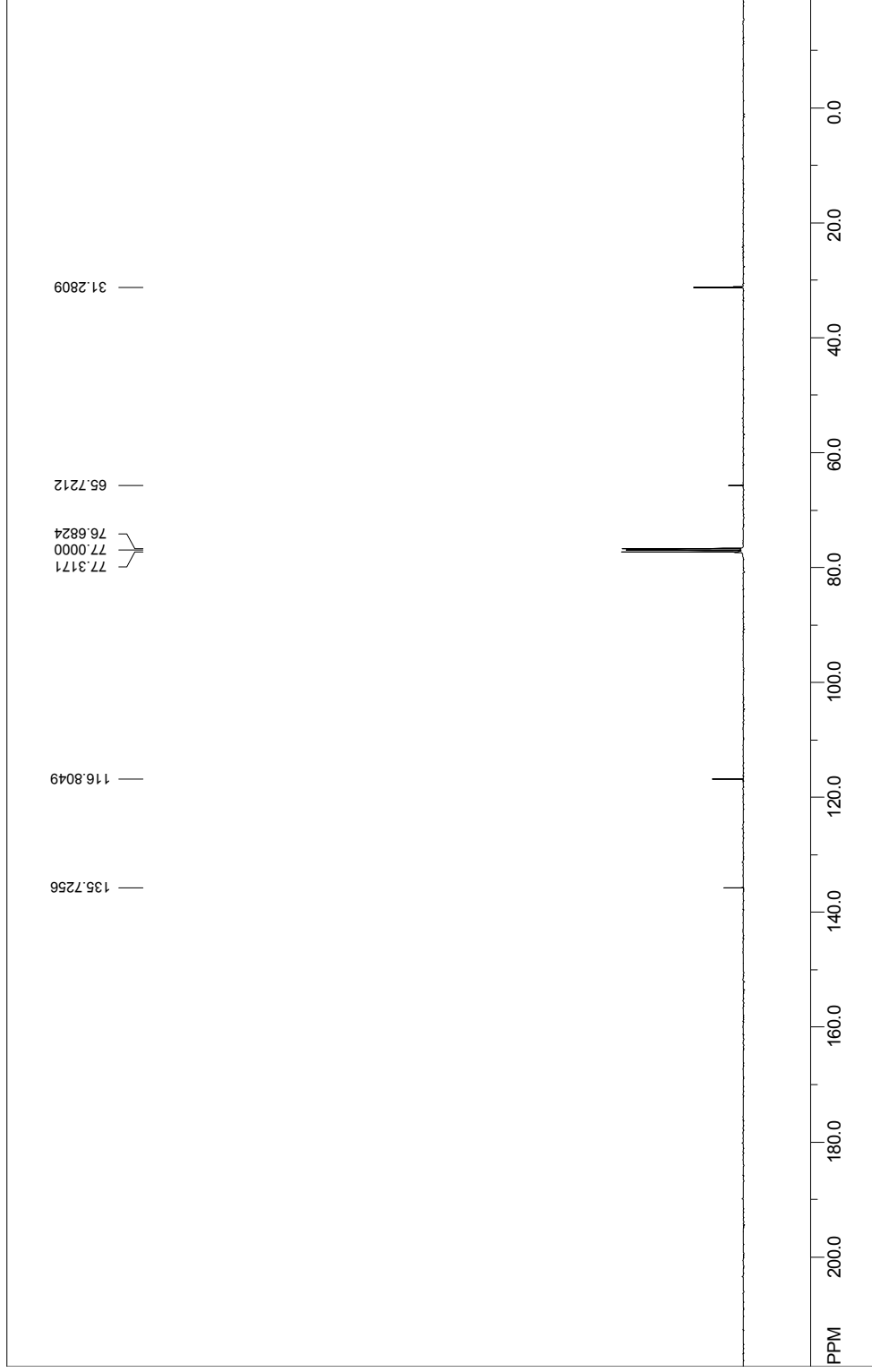


file: U:\research\paper\data\mri\Jun26-2004\1\fid exp1 ->g30->  
transmitter freq.: 400.132471 MHz  
time domain size: 32768 points  
width: 8278.15 Hz = 20.688513 ppm = 0.256659 Hz/pt  
number of scans: 16

freq. of 0 ppm: 400.130013 MHz  
processed size: 16384 complex points  
LB: 0.300 GB: 0.0000

# Compound 6 <sup>13</sup>C NMR

SpinWorks 2.4:



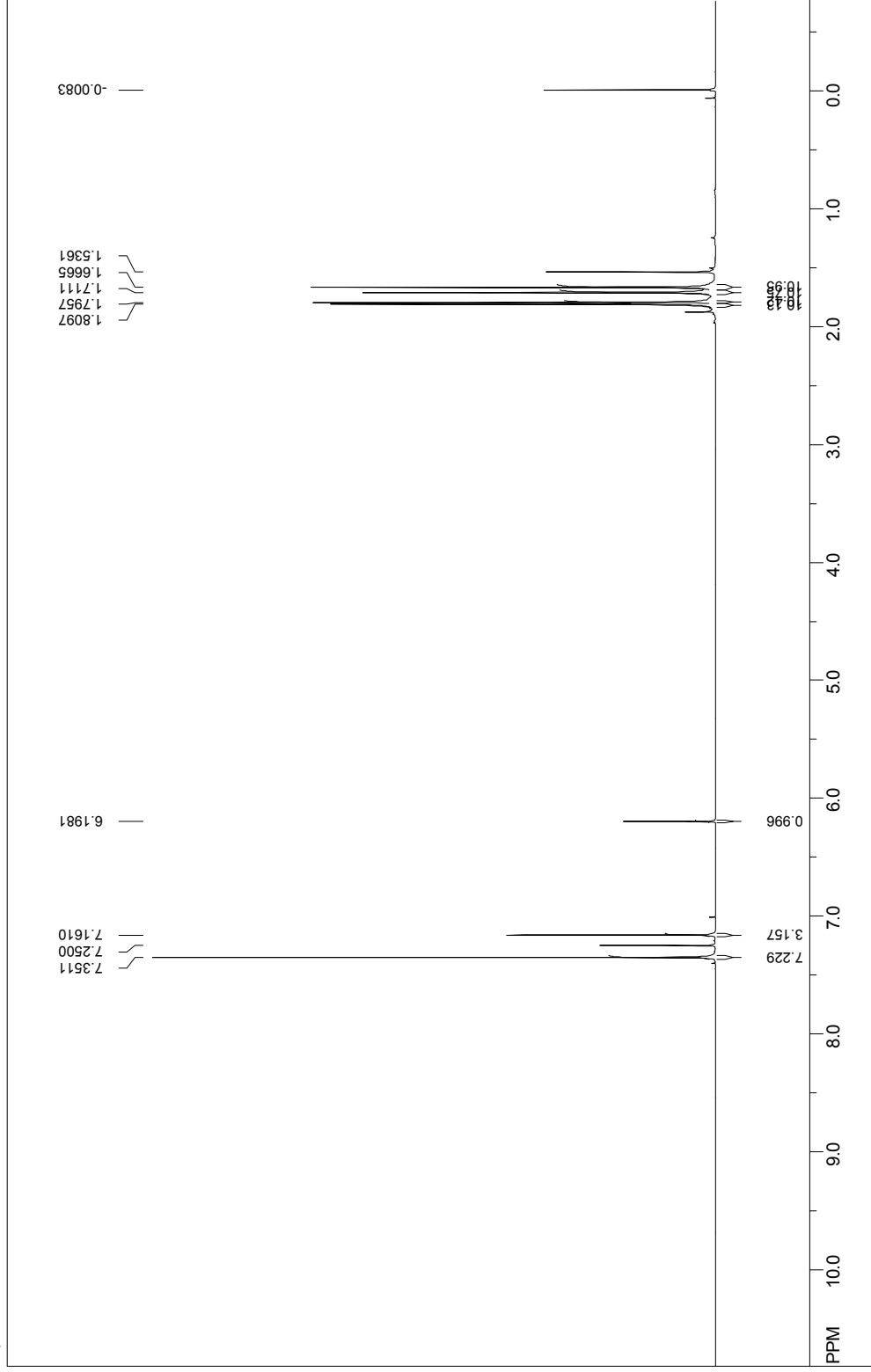
file: L:\research\paper\data\nmr\2-c\1\fid exp: <zipg90>  
transmitter freq.: 100.622830 MHz  
time domain size: 6556 points  
width: 23990.62 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 377

freq. of 0 ppm: 100.612769 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000



# Compound 7 <sup>1</sup>H NMR

SpinWorks 2.4:



file: U:\research\paper\data\mm3-h\1\fid exp1 -zg30-  
transmitter freq.: 400.132471 MHz  
time domain size: 32768 points  
width: 8278.15 Hz = 20.688513 ppm = 0.256659 Hz/pt  
number of scans: 16

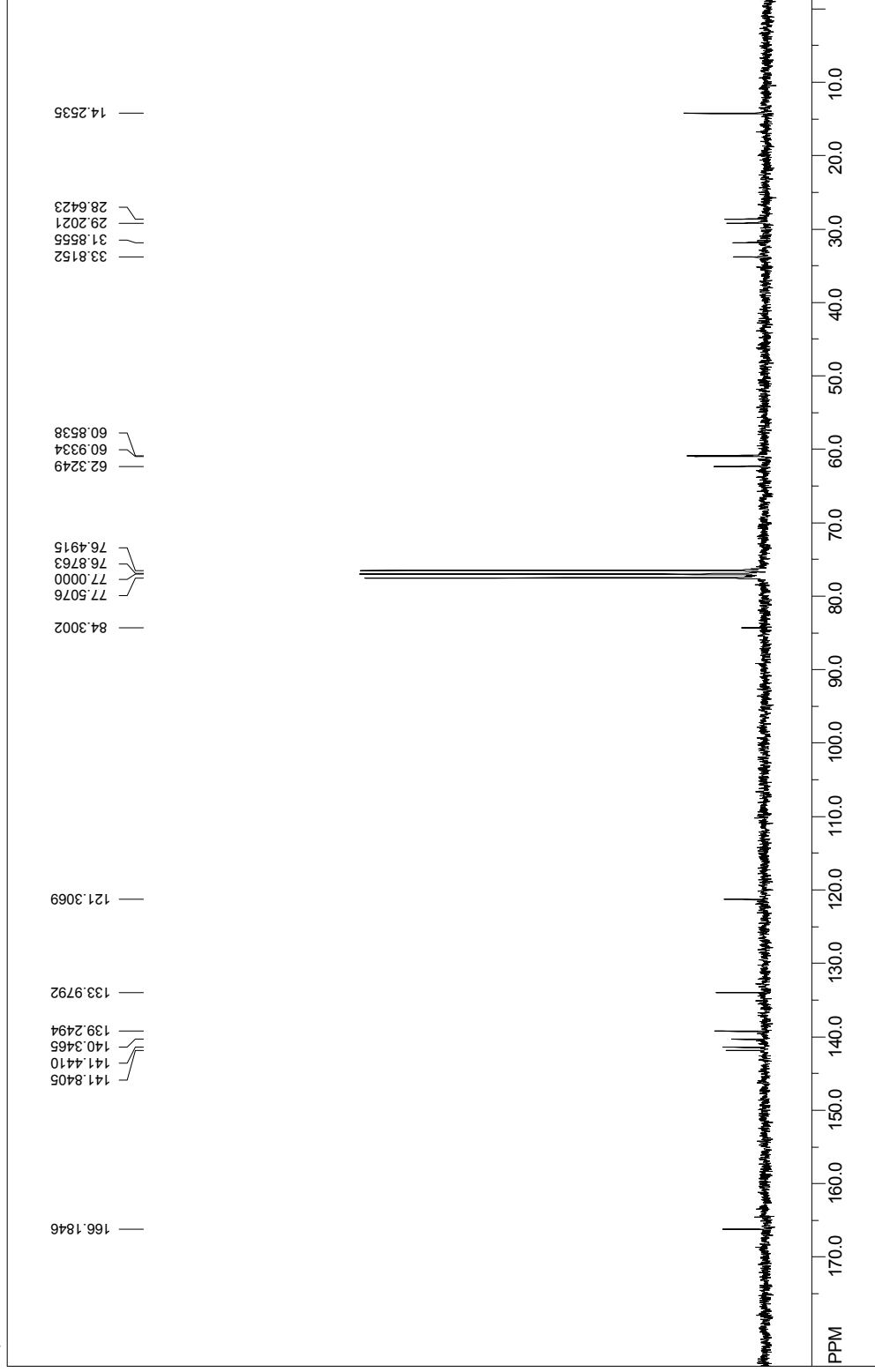
freq. of 0 ppm: 400.130013 MHz  
processed size: 16384 complex points  
LB: 0.300 GB: 0.0000





# Compound 8 <sup>13</sup>C NMR

SpinWorks 2.4:

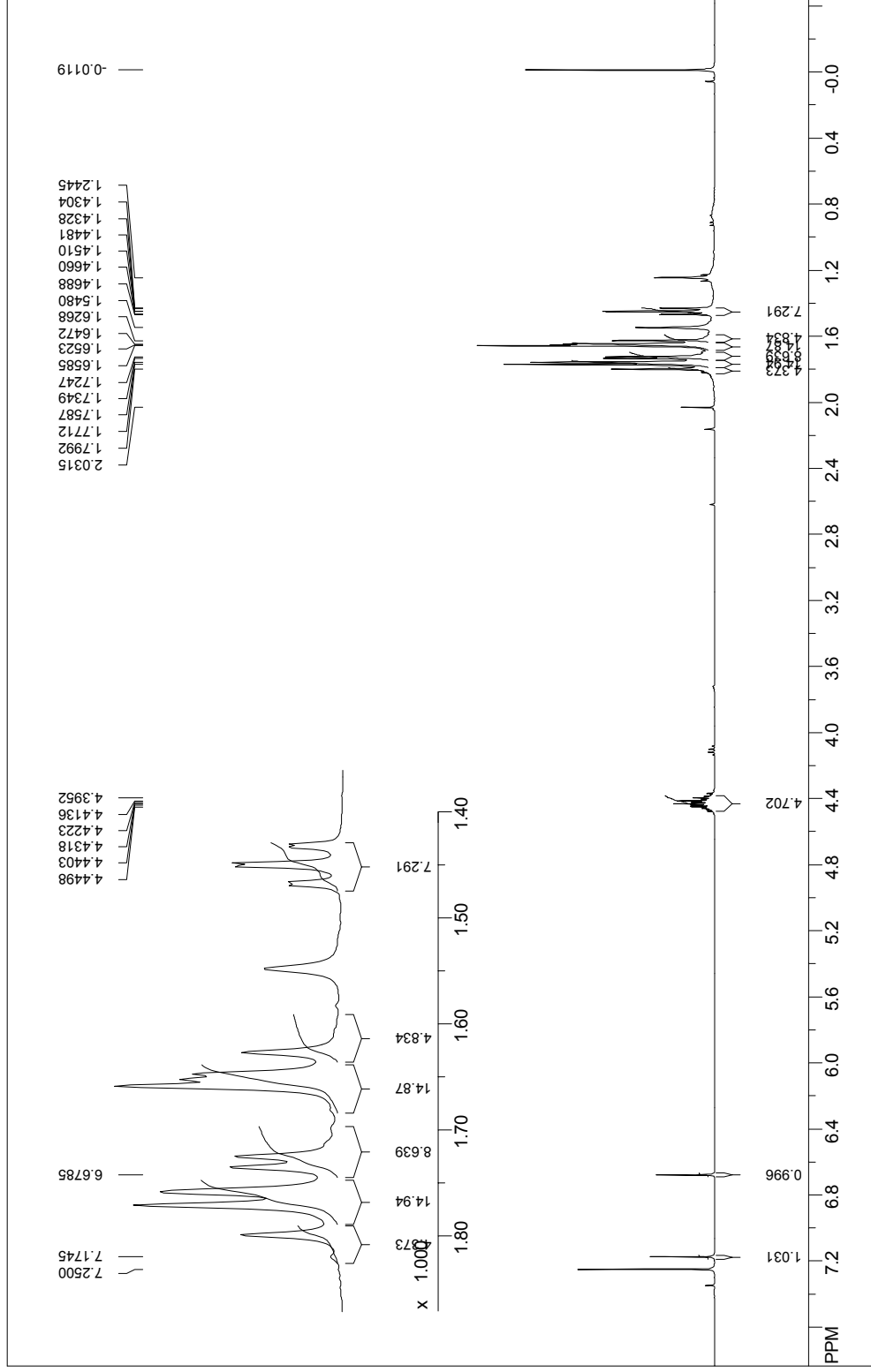


file: U:\nmr\sy-4-1-011\fid exp1 -<39930>  
transmitter freq: 62.901528 MHz  
time domain size: 65536 points  
width: 15060.24 Hz = 239.425677 ppm = 0.229801 Hz/pt  
number of scans: 326

freq. of 0 ppm: 62.895240 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 9 <sup>1</sup>H NMR

SpinWorks 2.4:

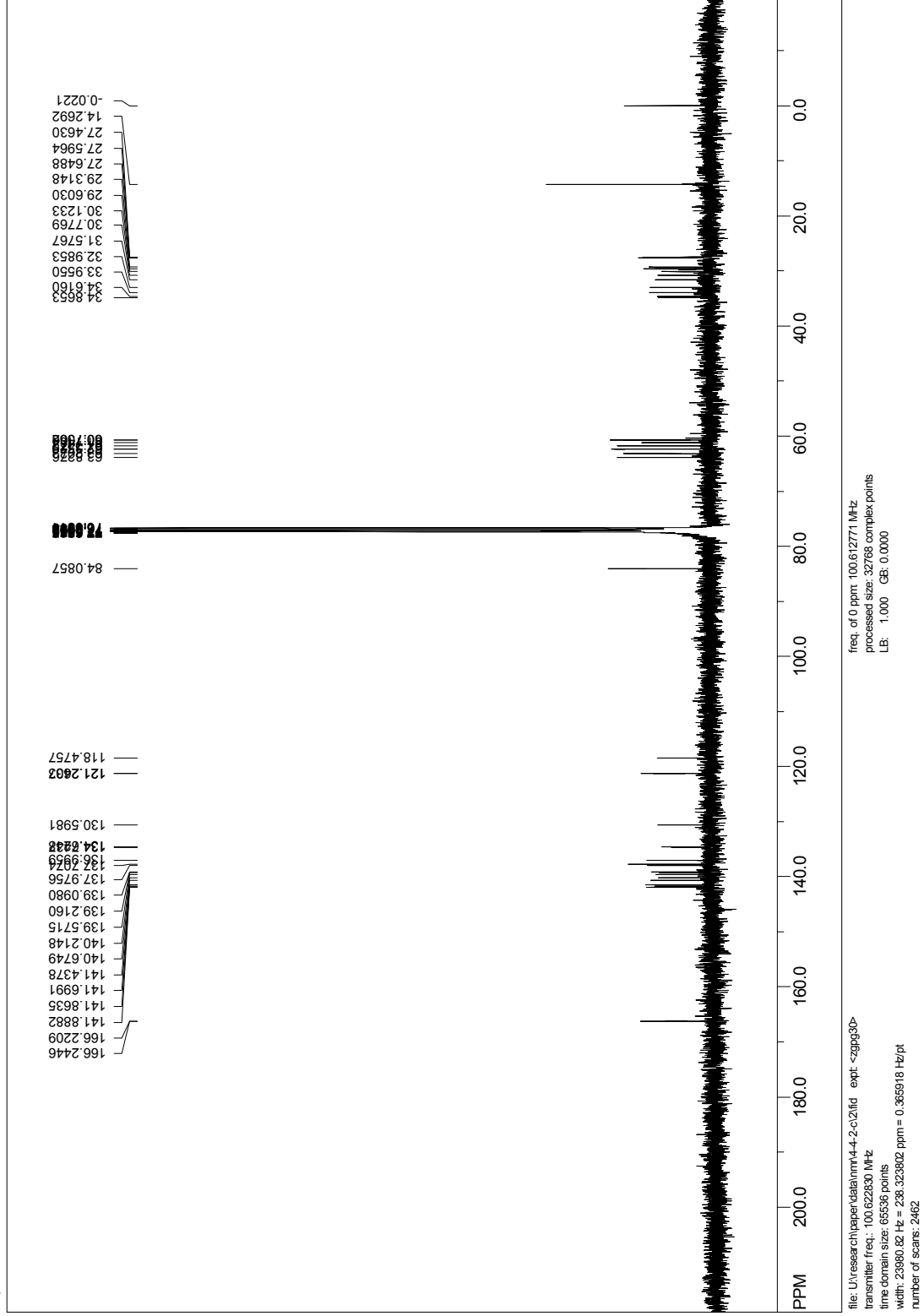


file: U:\research\paper\data\mrisk-4-4-2-h\1fid exp1 <cg30>  
 transmitter freq: 400.132471 MHz  
 time domain size: 32768 points  
 width: 8278.15 Hz = 20.688513 ppm = 0.252629 Hz/pt  
 number of scans: 16

freq. of 0 ppm: 400.130013 MHz  
 processed size: 16384 complex points  
 LB: 0.300 GE: 0.0000

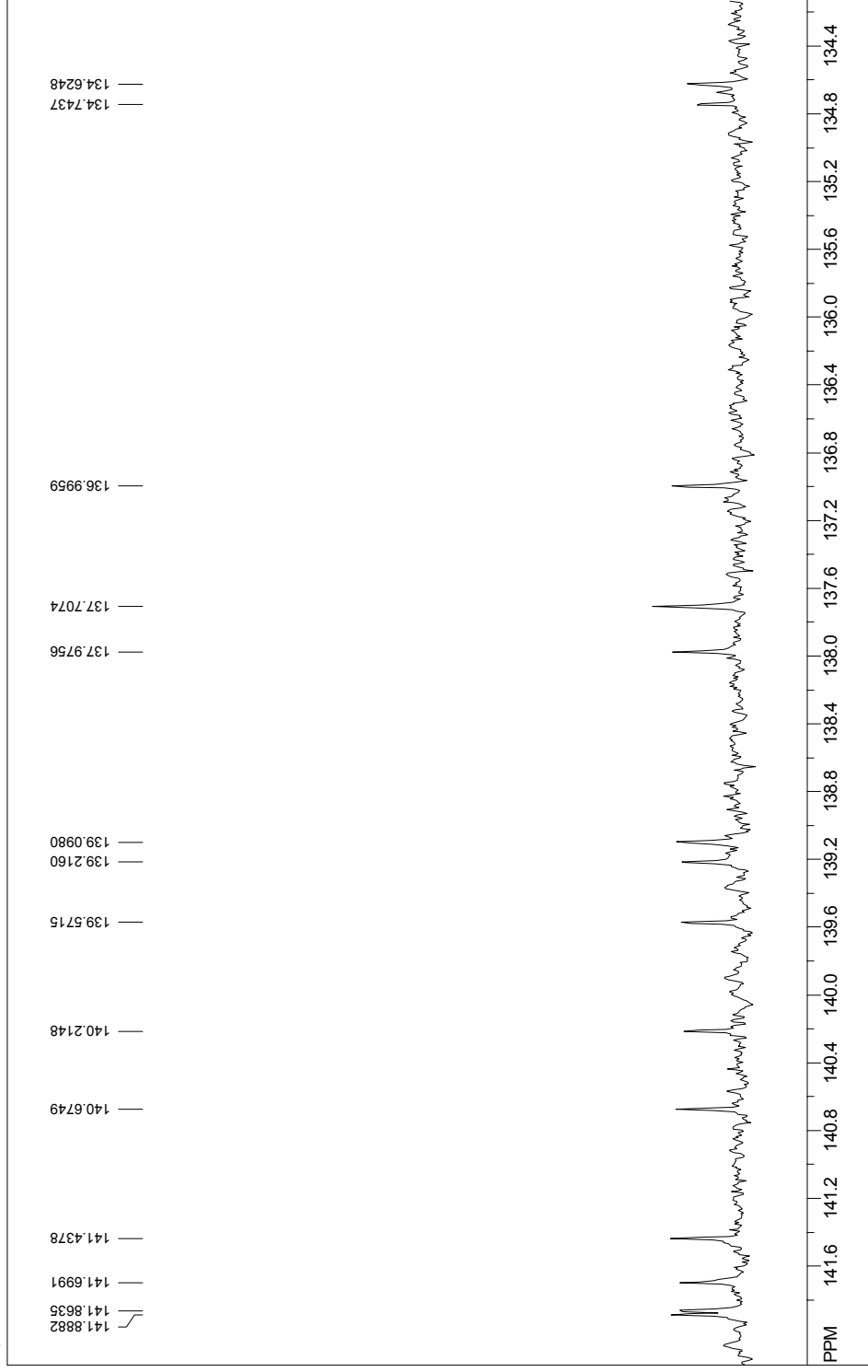
# Compound 9 <sup>13</sup>C NMR

SpinWorks 2.4:



# Compound 9 expanded <sup>13</sup>C NMR

SpinWorks 2.4:

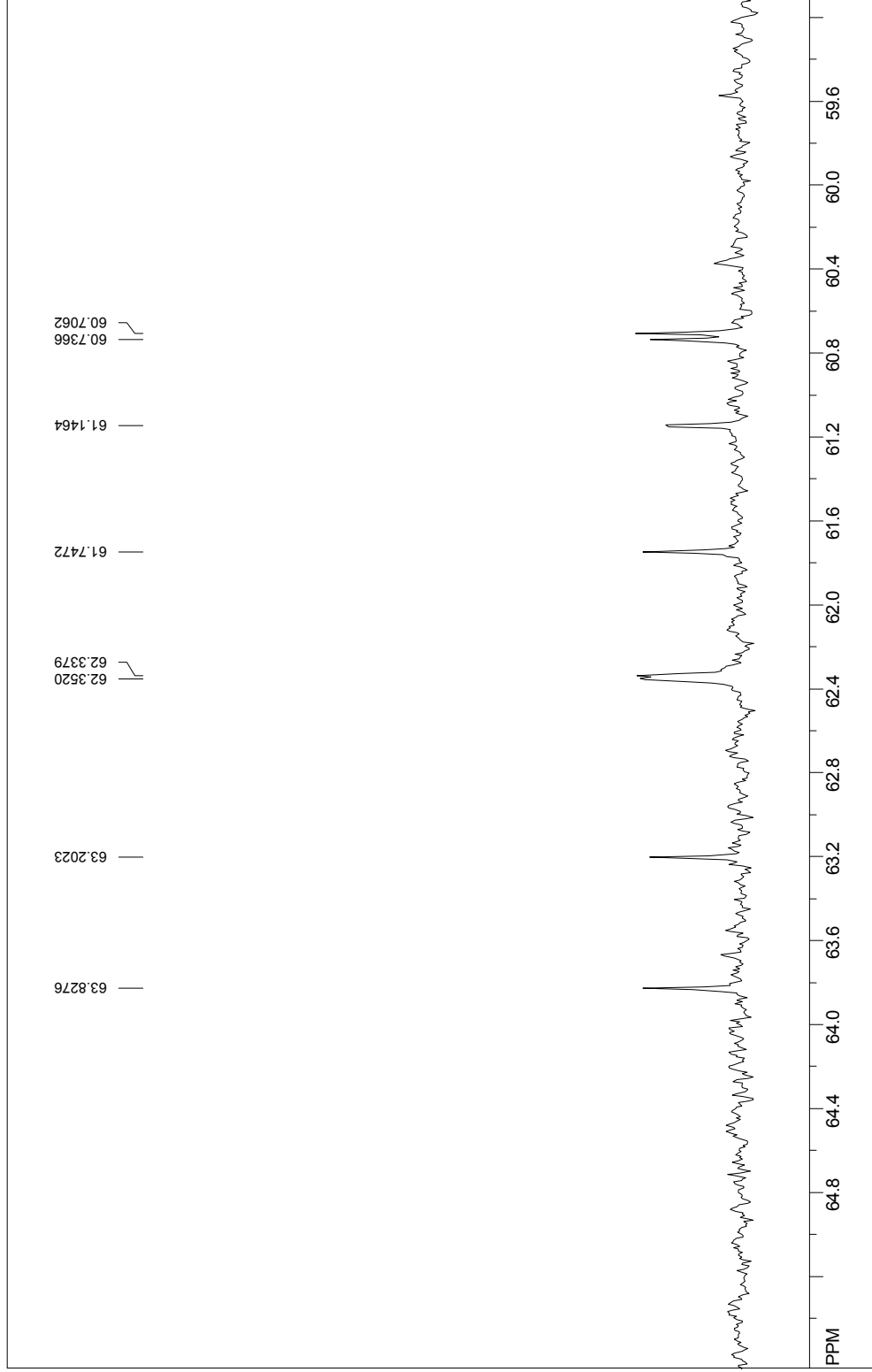


file: U:\research\paper\data\mm4-2-c12\fid exp1-zgpg30<  
transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 2380.02 Hz = 238.328002 ppm = 0.365918 Hz/pt  
number of scans: 2462

freq. of 0 ppm: 100.612771 MHz  
processed size: 32768 complex points  
LE: 1.000 GB 0.0000

# Compound 9 expanded <sup>13</sup>C NMR

SpinWorks 2.4:



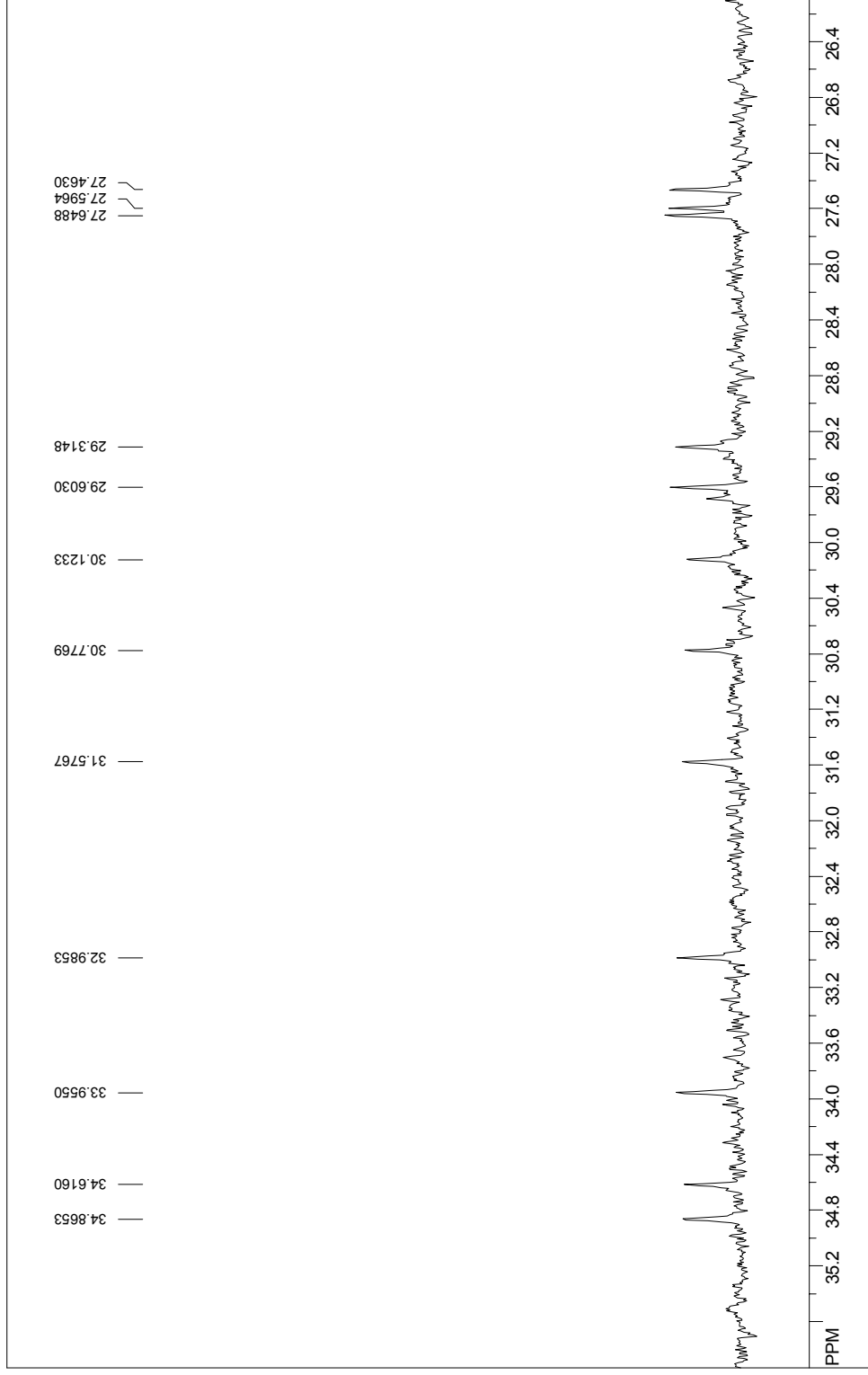
file: U:\research\paper\data\mr4-4-2-c\2\fid exp: <gg930>  
transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 23980.82 Hz = 238.32802 ppm = 0.365818 Hz/pt  
number of scans: 2462

freq. of 0 ppm: 100.612771 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000



# Compound 9 expanded <sup>13</sup>C NMR

SpinWorks 2.4:

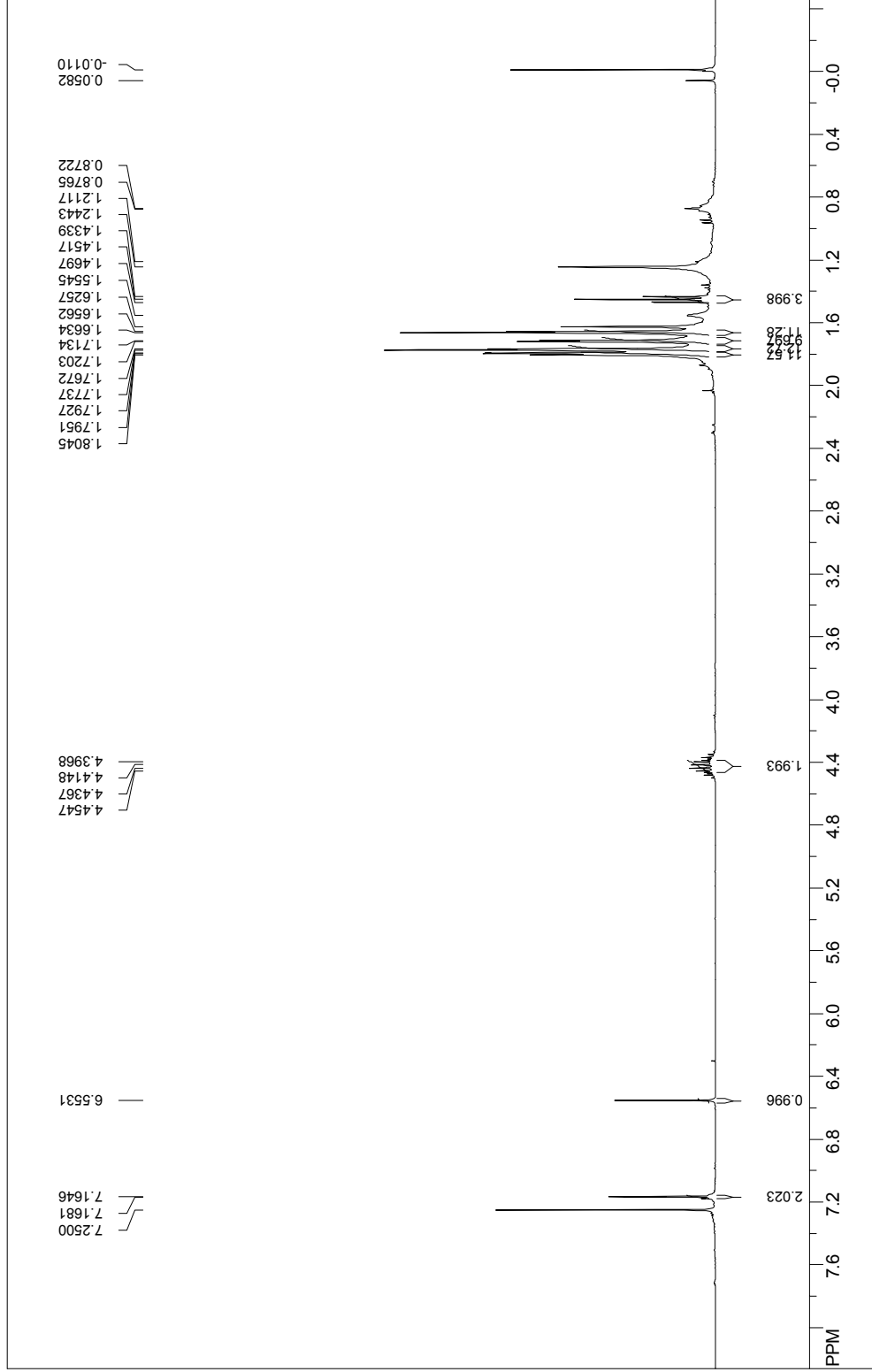


file: U:\research\paper\data\mnmv4-2-c2\fid exp1 <zgpg30>  
transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 23980.82 Hz = 238.322802 ppm = 0.365918 Hz/pt  
number of scans: 2462

freq. of 0 ppm: 100.612771 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 10 <sup>1</sup>H NMR

SpinWorks 2.4:

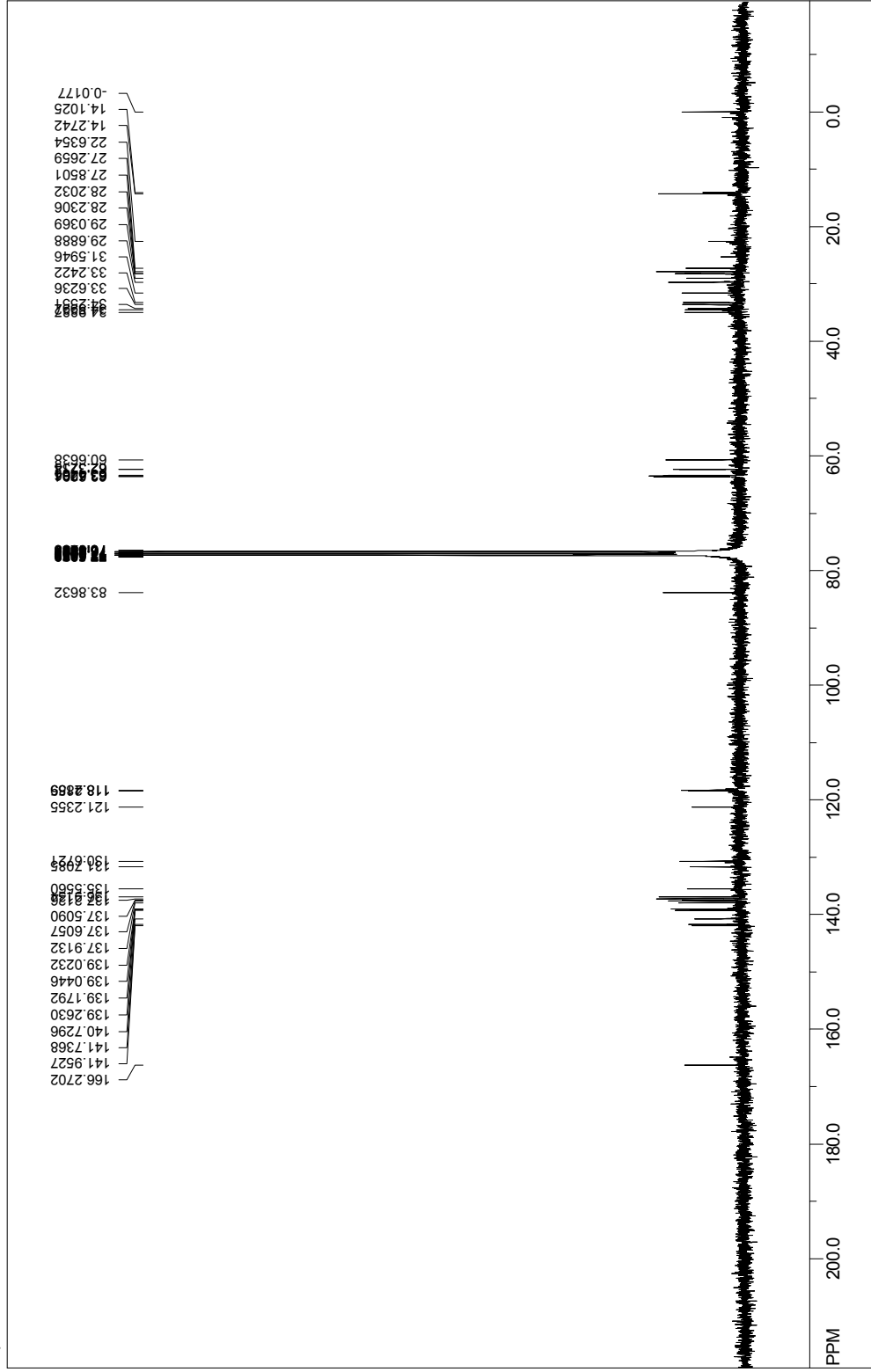


file: U:\research\paper\data\mr\4-4-3-h\1\fid exp: <zg30>  
transmitter freq: 400.132471 MHz  
time domain size: 32768 points  
width: 8278.15 Hz = 20.688513 ppm = 0.252629 Hz/pt  
number of scans: 16

freq. of 0 ppm: 400.130013 MHz  
processed size: 16384 complex points  
LE: 0.300 GE: 0.0000

# Compound 10 <sup>13</sup>C NMR

SpinWorks 2.4:

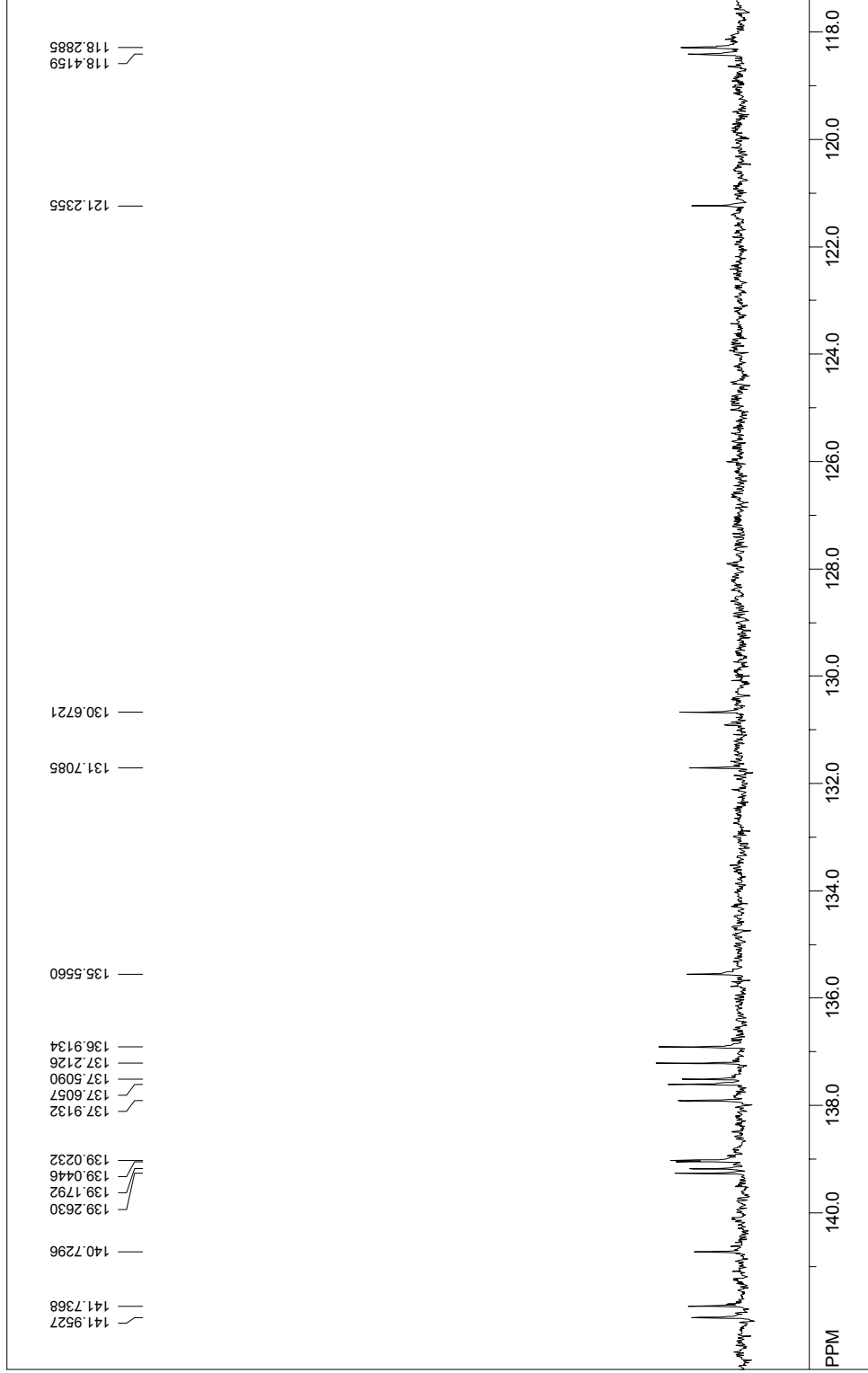


file: U:\research\paper\data\mm\4-4-3-c\11fid exp: <zigzag>  
transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 23960.82 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 4095

freq. of 0 ppm: 100.612770 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 10 expanded <sup>13</sup>C NMR

SpinWorks 2.4:

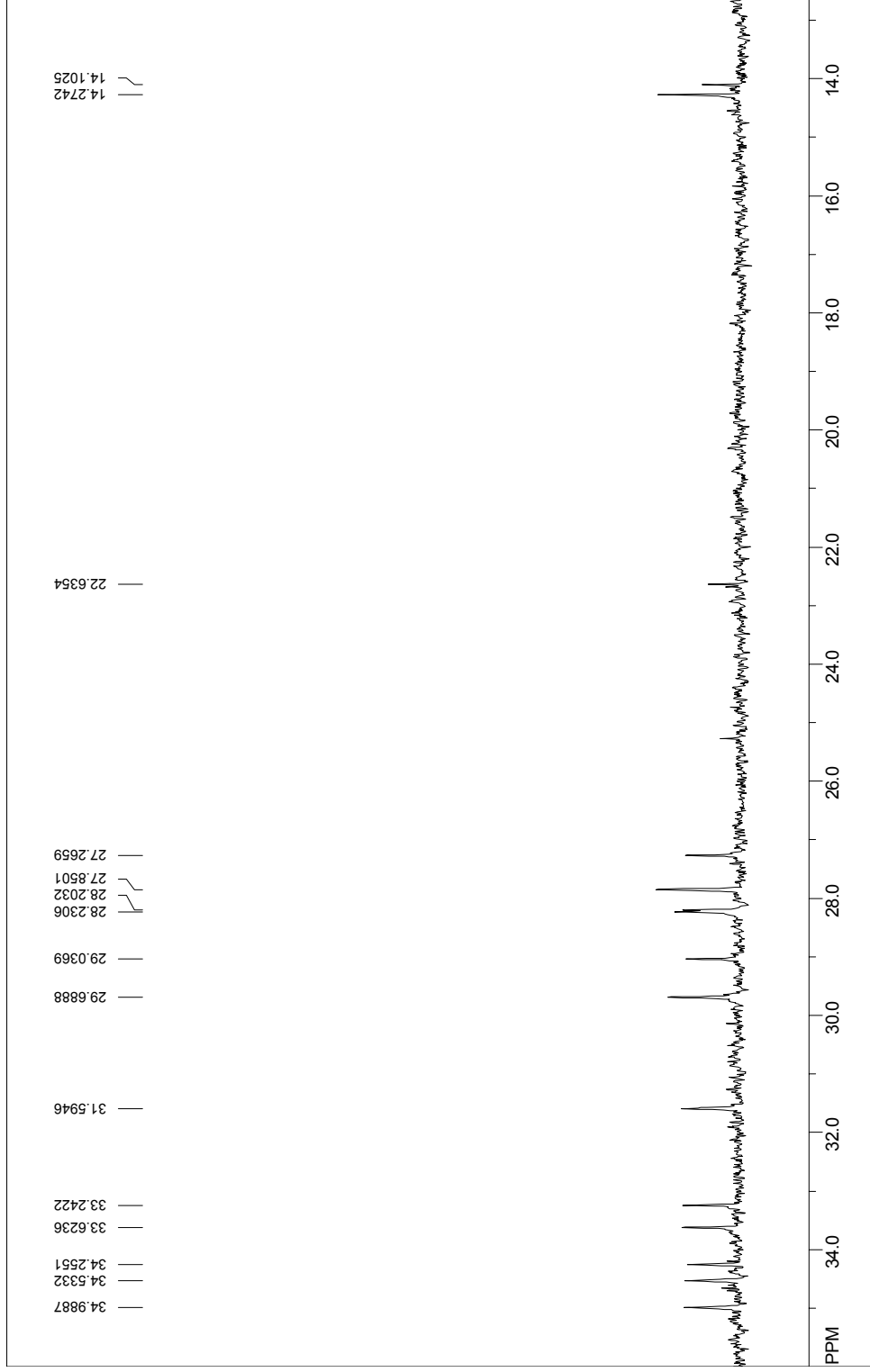


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transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 23980.82 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 4095

freq. of 0 ppm: 100.612770 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 10 expanded <sup>13</sup>C NMR

SpinWorks 2.4:

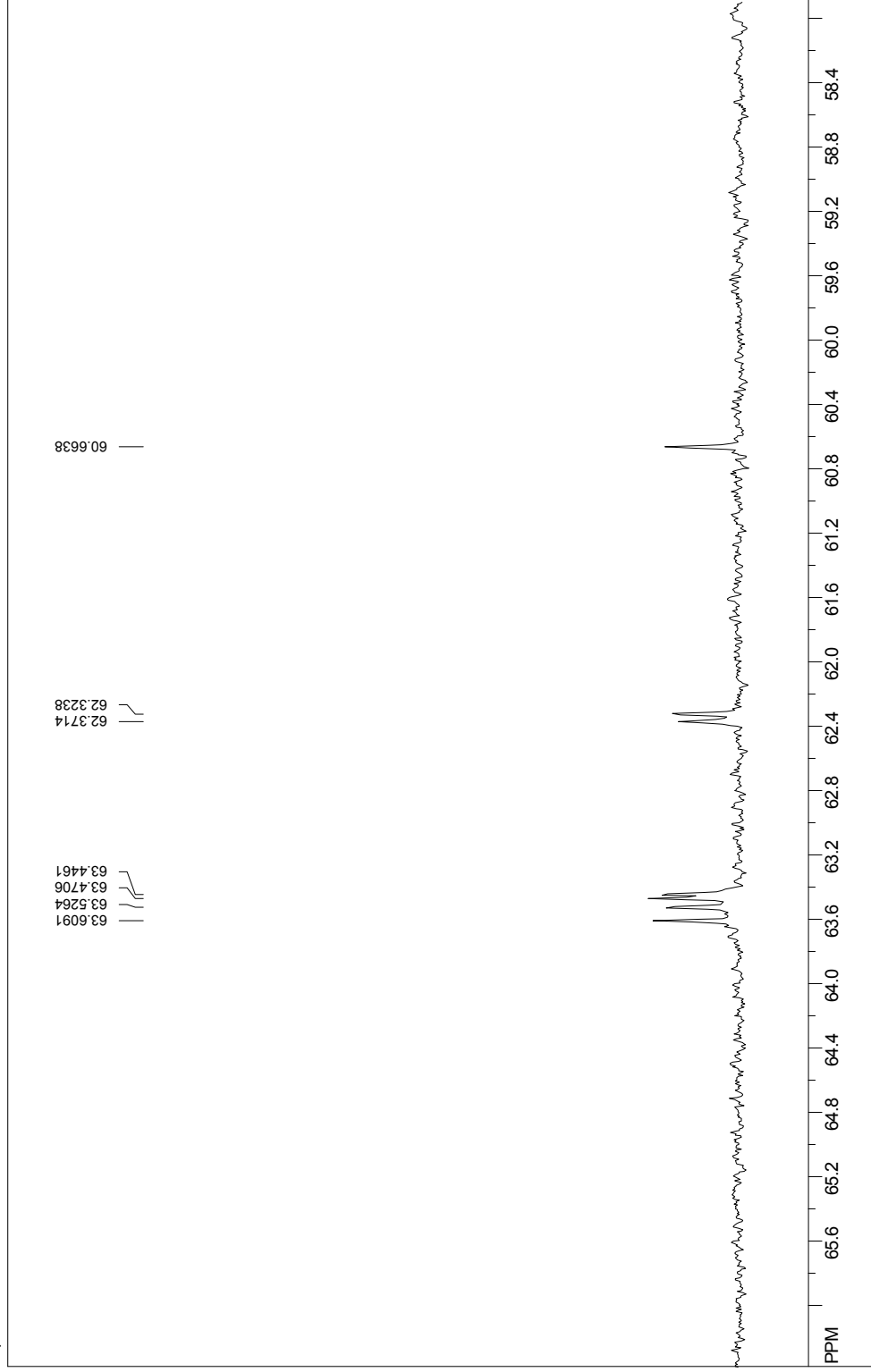


file: U:\research\paper\data\mm4-4-3-e1\fid exp1 ->zgpg50->  
transmitter freq.: 100.622830 MHz  
time domain size: 65536 points  
width: 23580.82 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 4095

freq. of 0 ppm: 100.612770 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

# Compound 10 expanded $^{13}\text{C}$ NMR

SpinWorks 2.4:

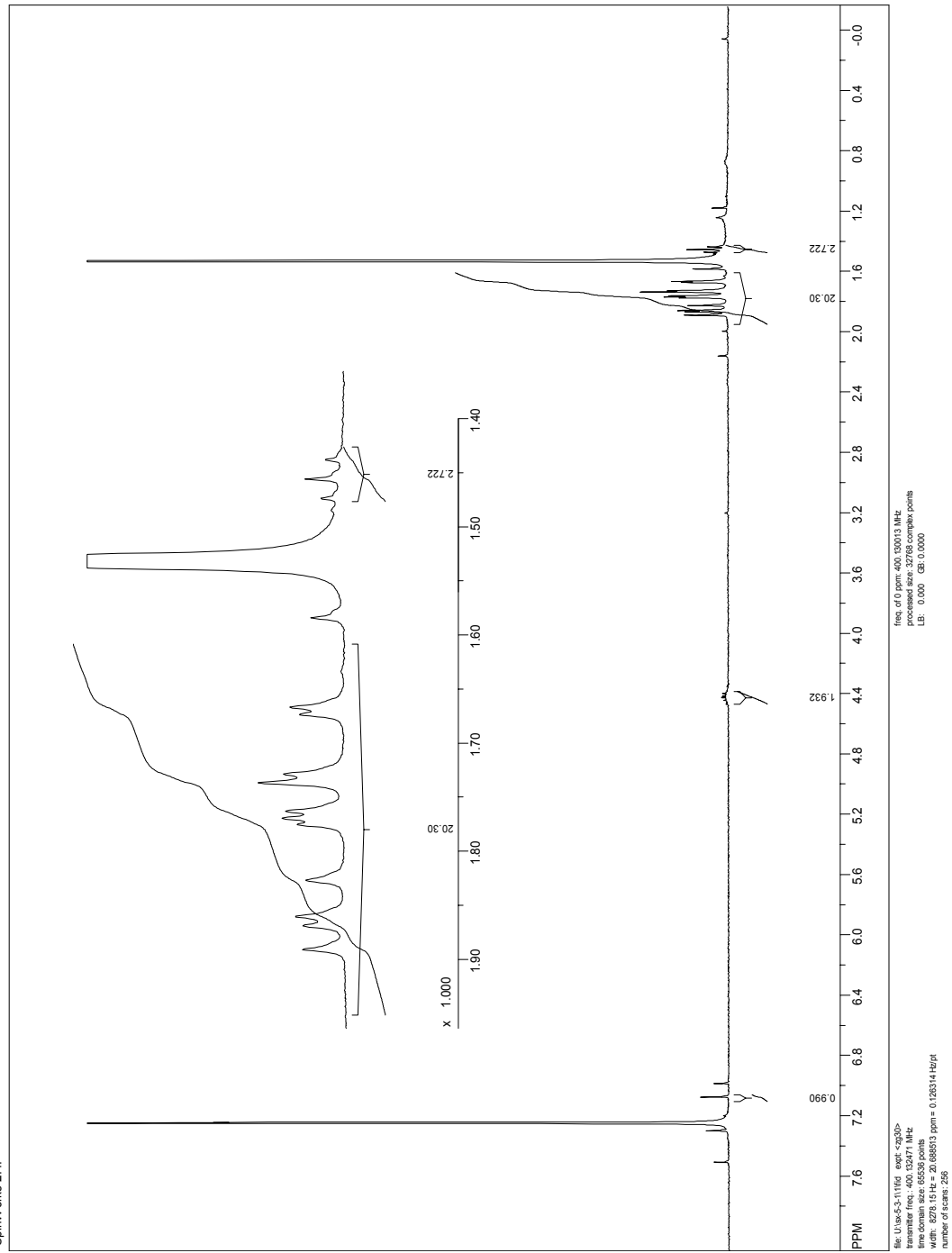


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transmitter freq.: 100.622830 MHz  
line domain size: 65536 points  
width: 23980.82 Hz = 238.323802 ppm = 0.365918 Hz/pt  
number of scans: 4095

freq. of 0 ppm: 100.612770 MHz  
processed size: 32768 complex points  
LB: 1.000 GB: 0.0000

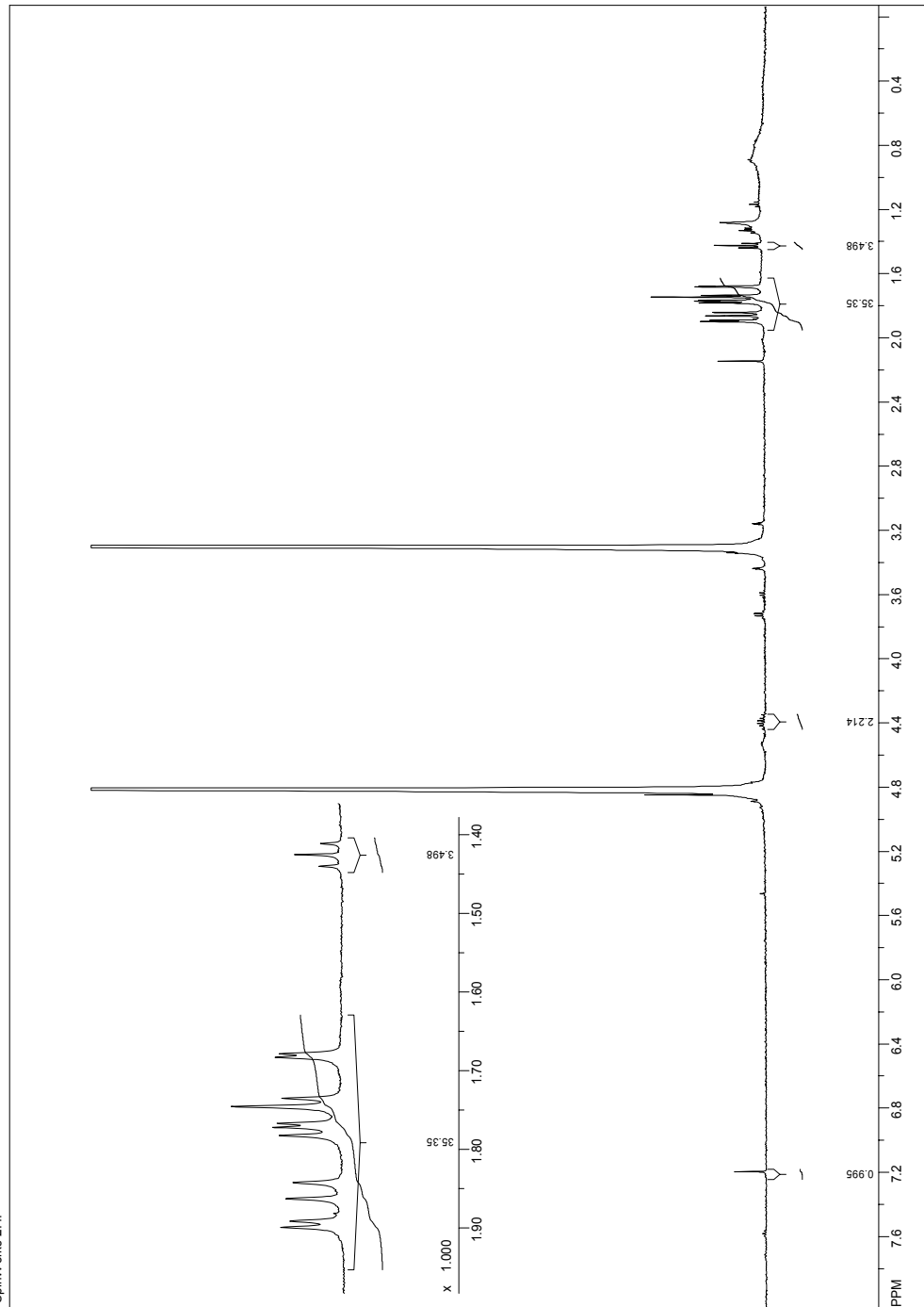
(M+15) residue of the decomposed monoester 3-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CDCl<sub>3</sub>

SpinWorks 2.4:



(M+15) residue of the decomposed monoester 3-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CD<sub>3</sub>OD

SpinWorks 2.4:



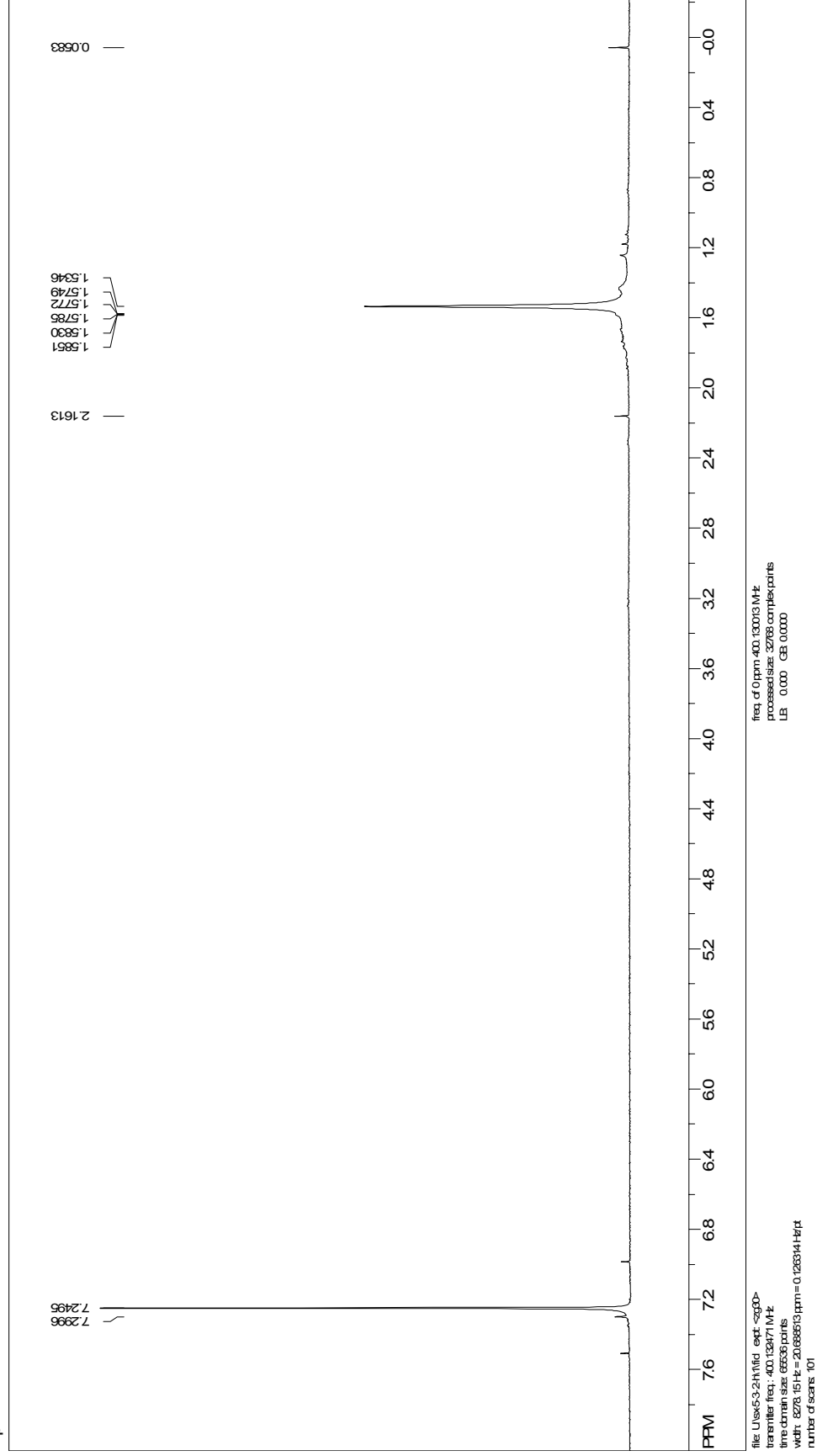
File: U:\nmr\mri\exp5-5-11\fid exp1. <exp5>  
Transmitter freq.: 500.023088 MHz  
Time domain size: 65536 points  
Number of scans: 2, 1600000  
Number of scans: 137

freq. of 0 ppm: 500.020014 MHz  
processed size: 32788 complex points  
LB: 0.000 GB: 0.0000



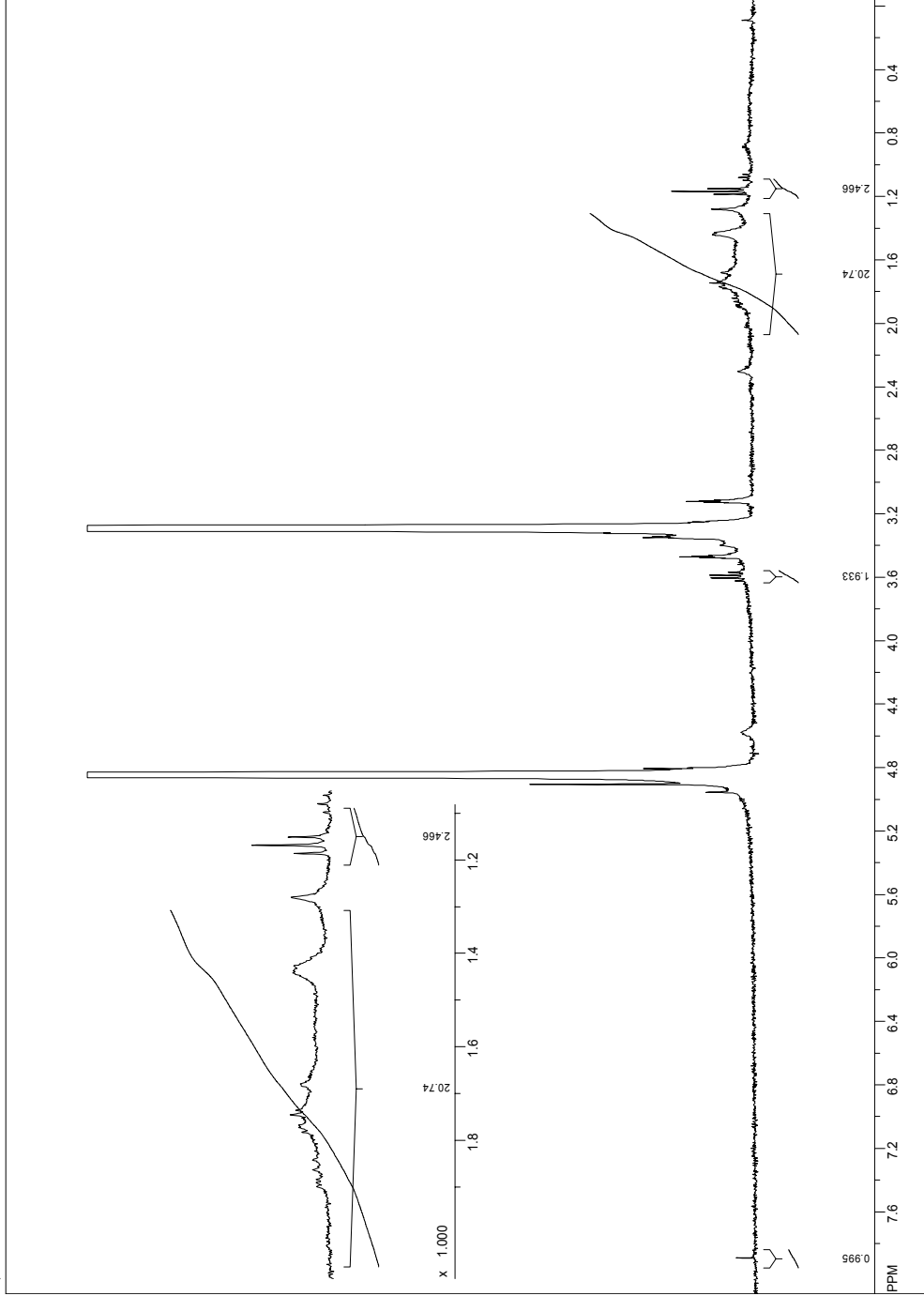
M residue of the decomposed monoester 3-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CDCl<sub>3</sub>

SpinWorks 2.4:



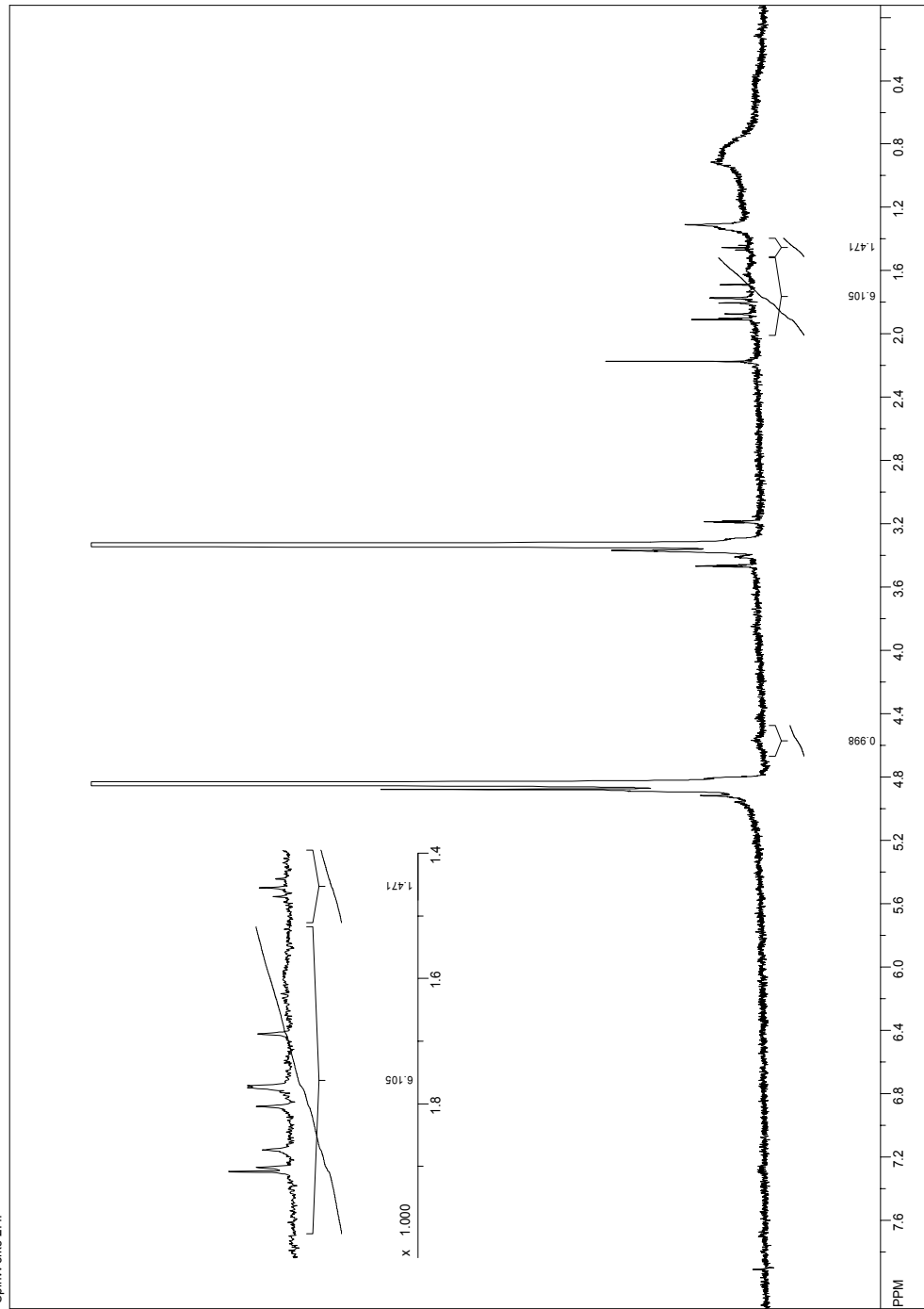
M residue of the decomposed monoester 3-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CD<sub>3</sub>OD

SpinWorks 2.4:



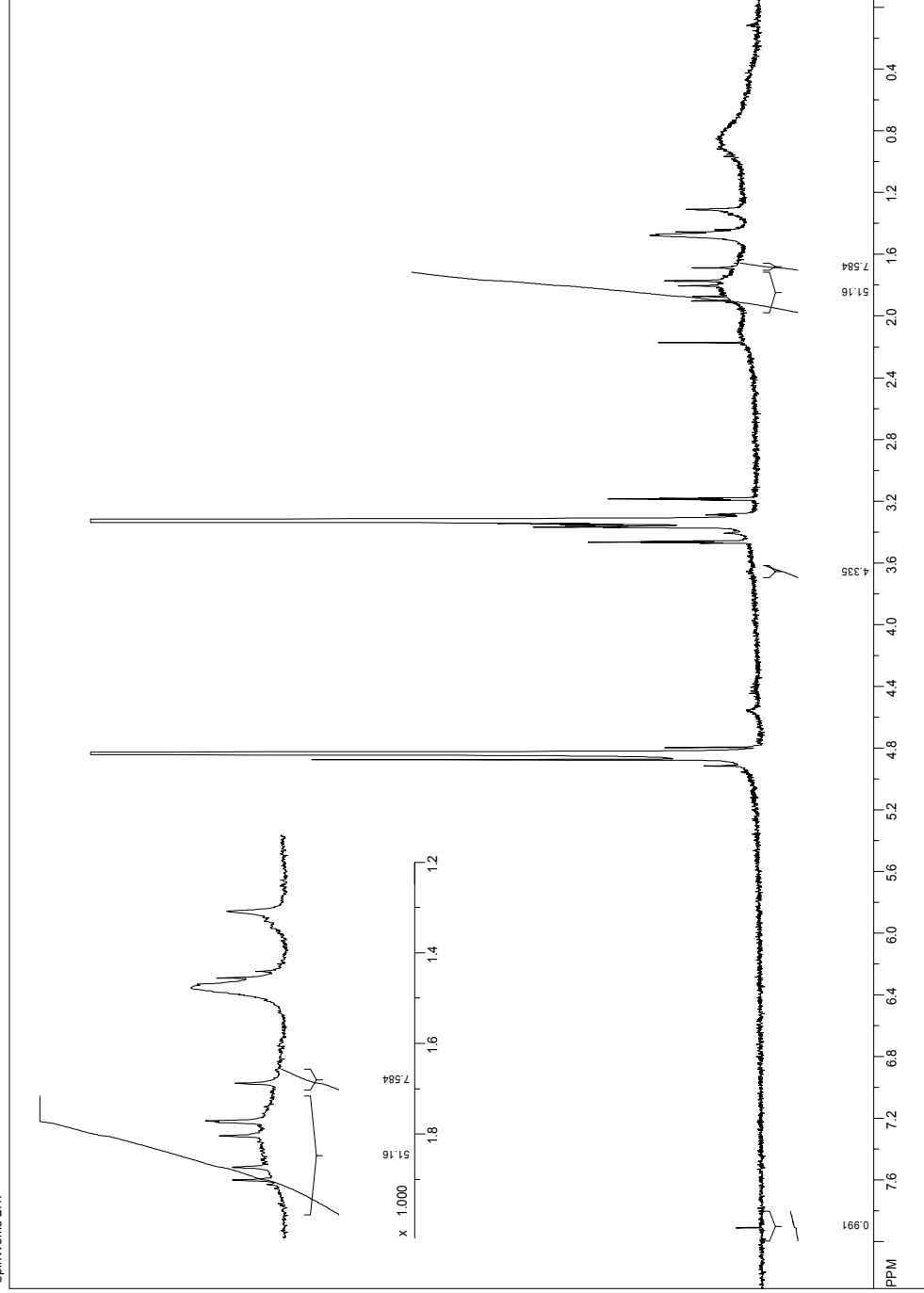
(M+15) residue of the decomposed monoester 2-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CD<sub>3</sub>OD

SpinWorks 2.4:

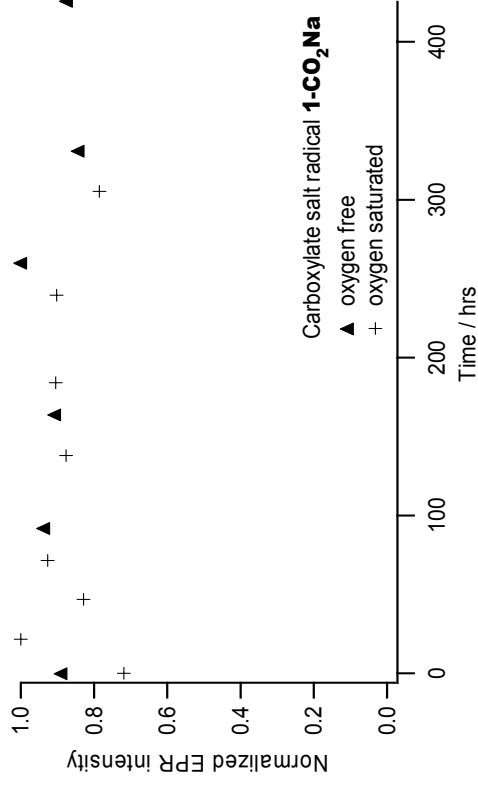
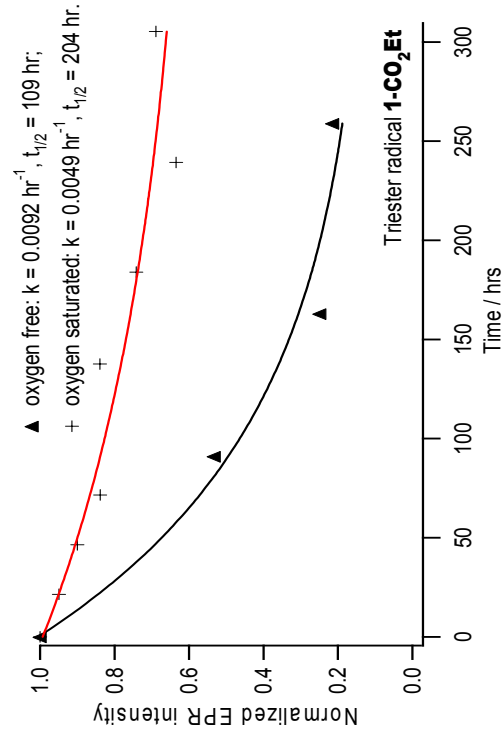
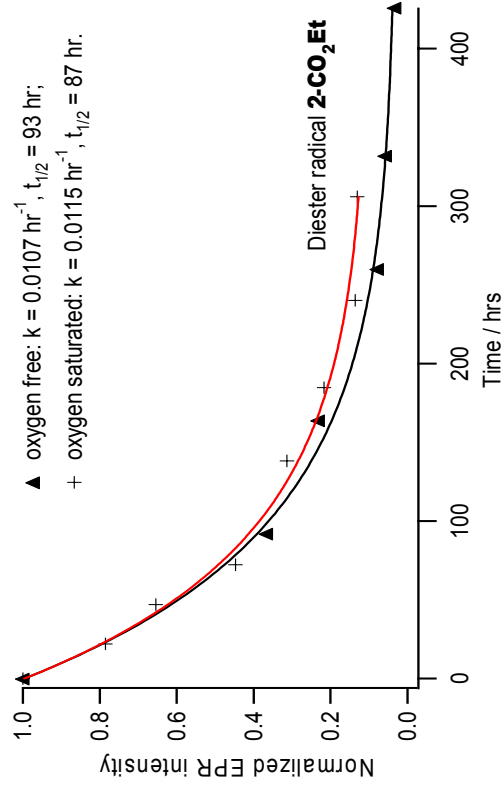
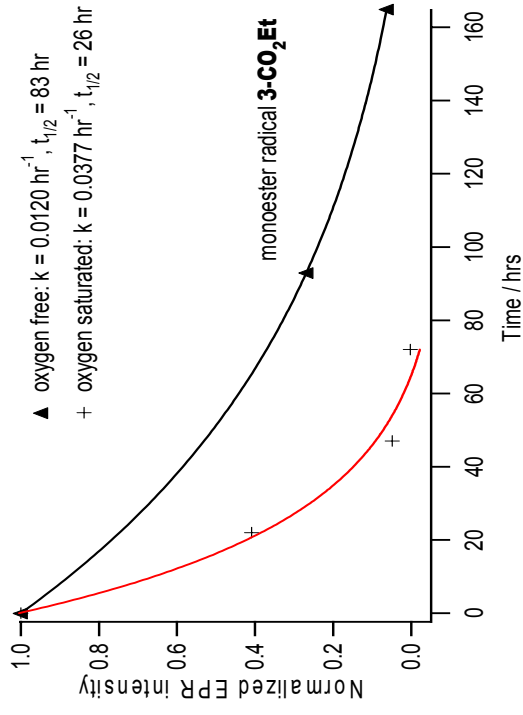


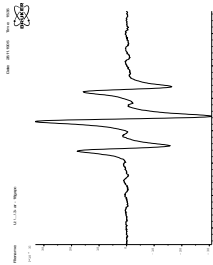
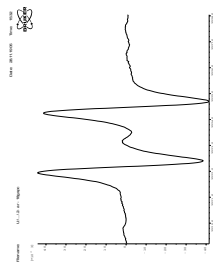
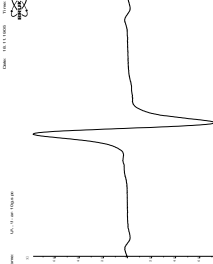
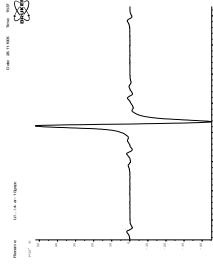
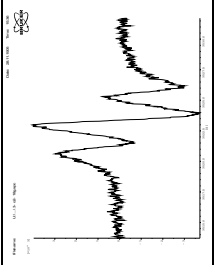
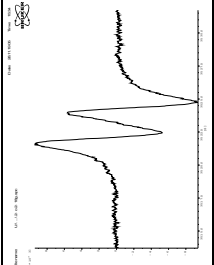
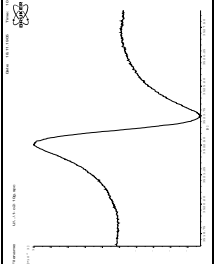
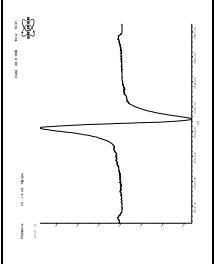
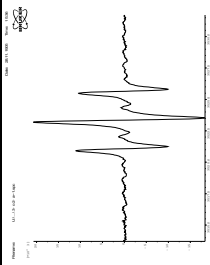
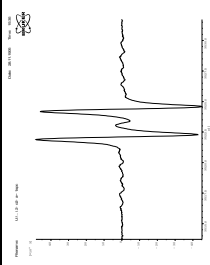
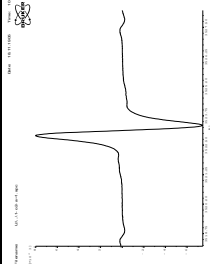
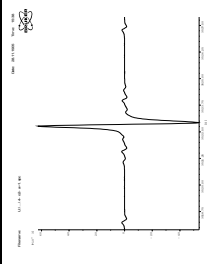
M residue of the decomposed monoester 2-CO<sub>2</sub>Et sample <sup>1</sup>H NMR  
Solvent CD<sub>3</sub>OD

SpinWorks 2.4:



## EPR result for synthesized trityl radicals



Trityl radicals		Monoester 3-CO <sub>2</sub> Et	Diester 2-CO <sub>2</sub> Et	Triester 1-CO <sub>2</sub> Et	Salt 1-CO <sub>2</sub> Na
O <sub>2</sub> free	ΔBpp, G	0.40	0.45	0.45	0.11
	Hfcc, G	2.29	2.30	-	-
	Integrated SI	1.159e+008	1.853e+008	3.365e+008	4.311e+007
	EPR spectra				
O <sub>2</sub> saturated	ΔBpp, G	1.25	1.27	1.22	0.36
	Hfcc, G	2.25	2.30	-	-
	Integrated SI	1.262e+008	1.762e+008	3.883e+008	5.055e+007
	EPR spectra				
O <sub>2</sub> saturated, then purge with Ar to make solution O <sub>2</sub> free	ΔBpp, G	0.37	0.41	0.45	0.11
	Hfcc, G	2.29	2.30	-	-
	Integrated SI	2.465e+007	1.375e+008	3.372e+008	4.420e+007
	EPR spectra				

No O<sub>2</sub>: Salt **1-CO<sub>2</sub>Na**

EPR parameter setting used:

HCF 3523.280000

HSW 2.000000

EMF 3522.575000

RCT 20.480000

RTC 20.480000

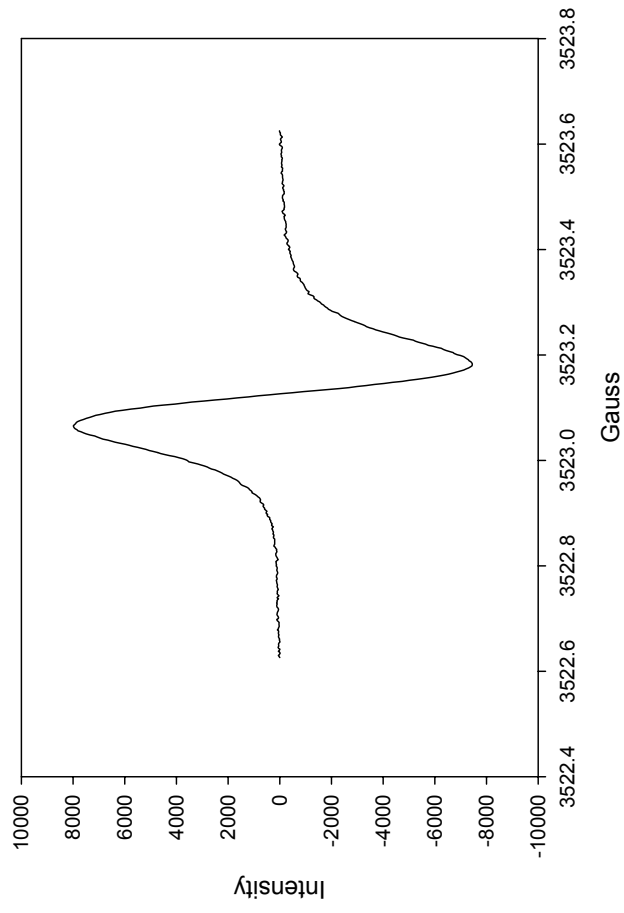
RRG 5.023773e+004

RMA 0.010000

MF 9.881777

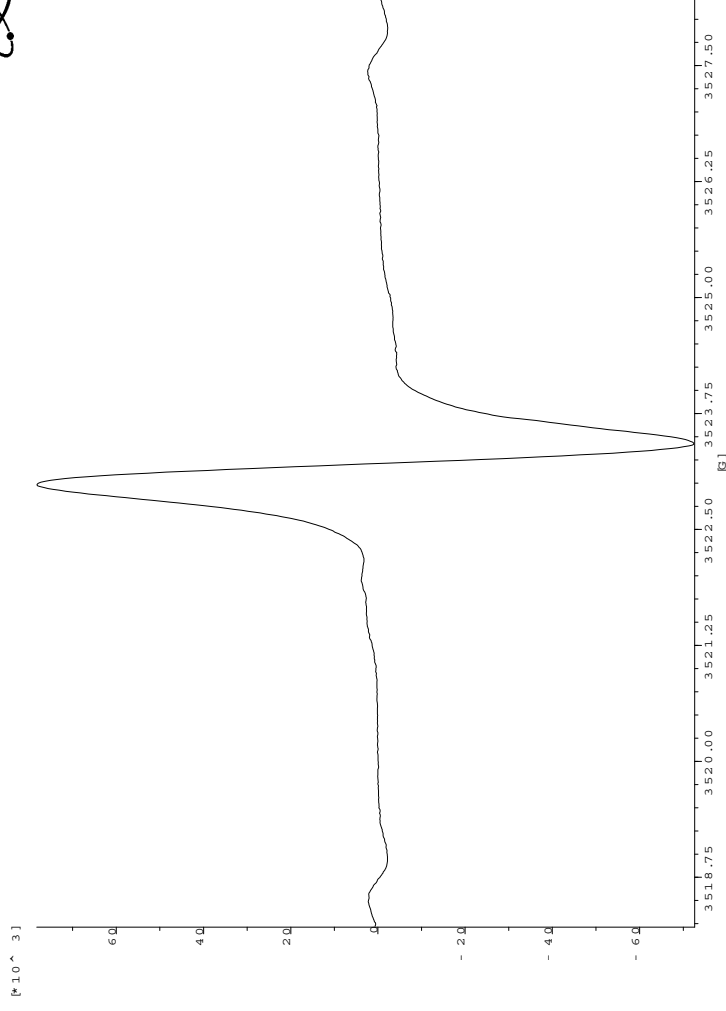
MP 5.002e-002

MPD 36.0



No O<sub>2</sub>: Triester 1-CO<sub>2</sub>Et  
EPR parameter setting used:  
HCF 3523.220000  
HSW 10.000000  
EMF 3522.727000  
RCT 40.960000  
RTC 81.920000  
RRG 4.477442e+004  
RMA 0.010000  
RMF 6.000000  
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Filename: U\...\11-ar-10g.spc  
Date: 18.11.1905  
Time: 10:10

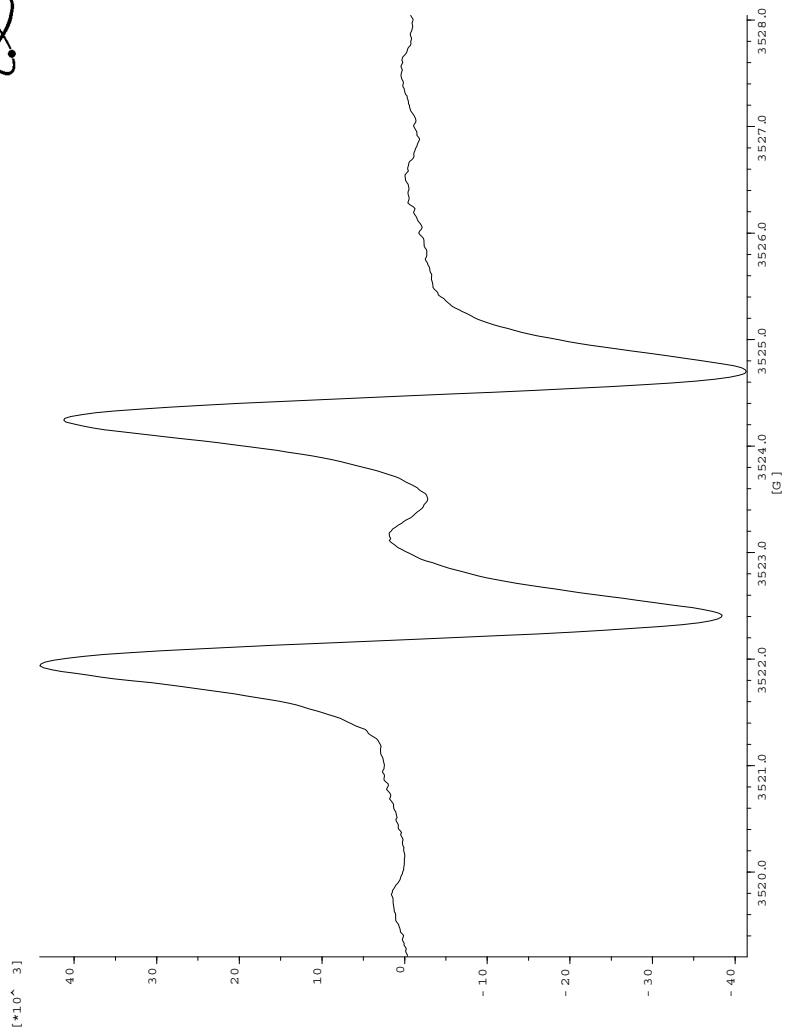





No O<sub>2</sub>: Triester 2-CO<sub>2</sub>Et  
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HSW 18.000000  
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Date: 28.11.1906  
Time: 15:32  

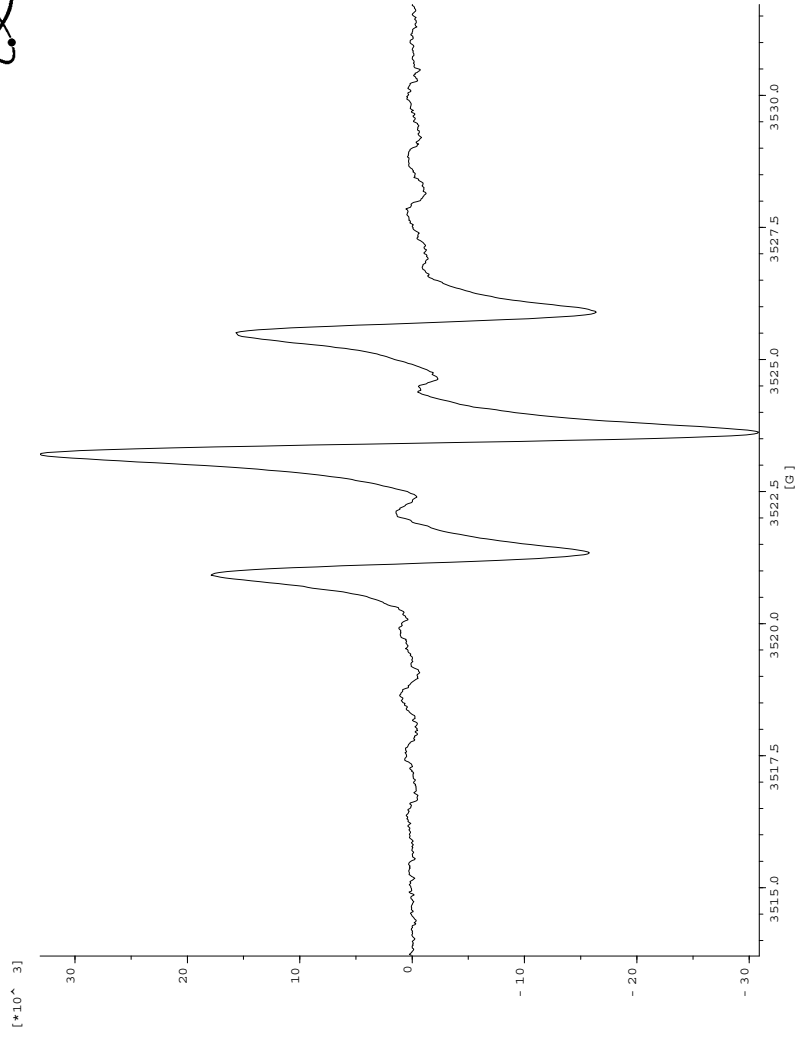

Filename: U:\...12-ar-18g.spc



No O<sub>2</sub>: Triester 3-CO<sub>2</sub>Et  
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MPD 10.0

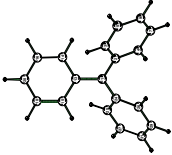
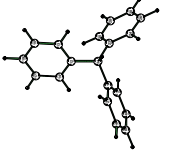
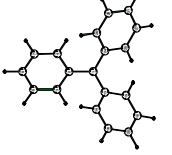
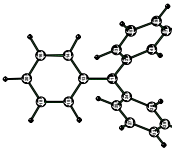
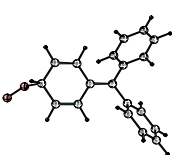
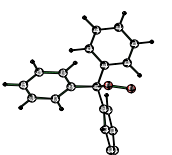
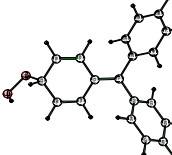
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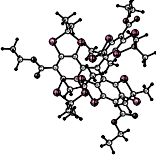
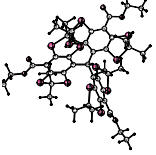
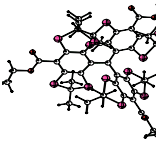
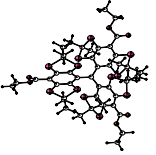
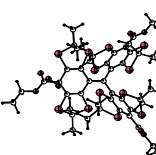
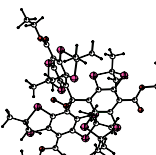
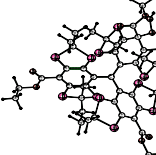
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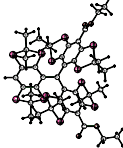
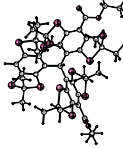
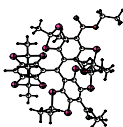
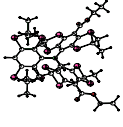
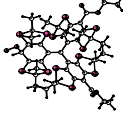
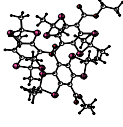
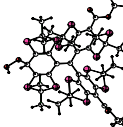
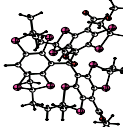
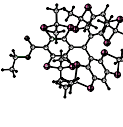
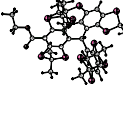
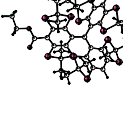
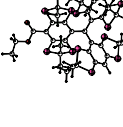
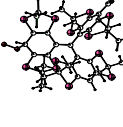
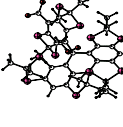
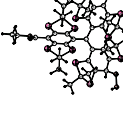
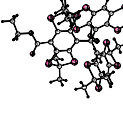
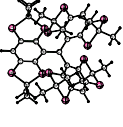
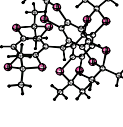
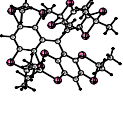
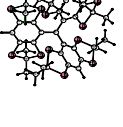
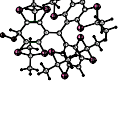
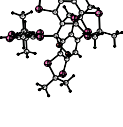
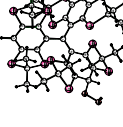
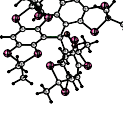


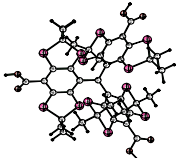
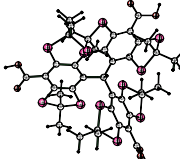
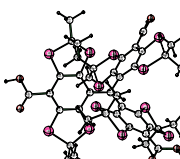
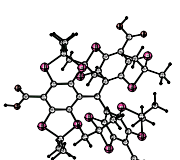
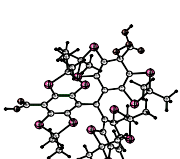
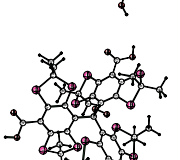
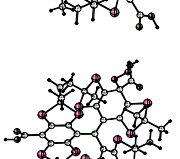
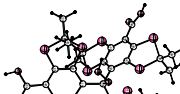
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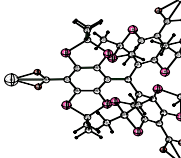
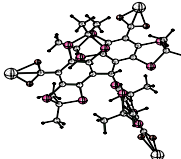
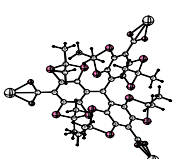
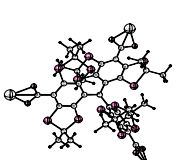
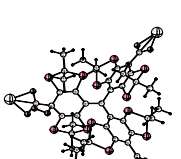
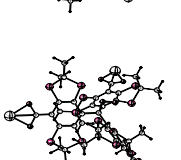
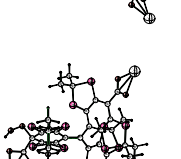
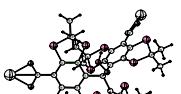
E: B3LYP/6-31G\*; E\*: B3LYP/6-311+G\*\*//B3LYP/6-31G\* tight, E\*-u: B3LYP/6-311+G\*\*//B3LYP/6-31G\* tight using radii=uff

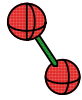
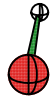
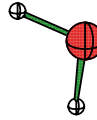
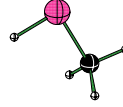
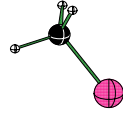
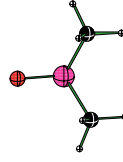
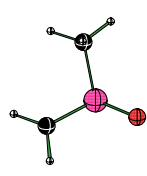
Compound							
<b>name</b>	CPh <sub>3</sub>	CPh <sub>3</sub> -H	CPh <sub>3</sub> <sup>+</sup>	CPh <sub>3</sub> -a-oo- radical	CPh <sub>3</sub> -b-oo- radical	CPh <sub>3</sub> -a-oo- radical	CPh <sub>3</sub> -b-oo- radical
<b>File name</b>	CPh3.log	cph3-h.log	CPh3+.log	CPh3-TOO.log	CPh3-OO_F.log	cph3-oo-h-b.log	cph3-oo-h-a.log
<b>E (gas phase)</b>	-733.0831877	-733.6608949	-732.8251123	-883.3903784	-883.4185288	-883.9625959	-883.9954135
<b>E* (gas phase)</b>	-733.2235689	-733.8537802	-733.0039531	-883.5737653	-883.6019292	-884.2113575	-884.2414497
<b>&lt;S<sup>2</sup>&gt;</b>	0.7764	0	0	0.7546	0.7542	0	0
<b>N Imag</b>	0	0	0	0	0	0	0

Compound							
<b>name</b>	1-CO <sub>2</sub> Et	1-CO <sub>2</sub> Et-H	1-CO <sub>2</sub> Et <sup>+</sup>	1-CO <sub>2</sub> Et-a-oo- radical	1-CO <sub>2</sub> Et-b-oo- radical	1-CO <sub>2</sub> Et-a-oo- radical.log	1-CO <sub>2</sub> Et-b-oo- radical
<b>File name</b>	SX-5-1-f1-2.log	SX-5-1-h.log	SX-5-1-+.log	SX-5-1-b-oo- radical.log	SX-5-1-a-oo- radical.log	SX-5-1-a-oo- radical.log	SX-5-1-b-oo- radical.log
<b>E (gas phase)</b>	-7013.281468	-7013.904545	-7013.067389	-7163.561696	-7163.567719	-7163.567719	-7164.196772
<b>E* (gas phase)</b>	-7014.209339	-7014.834534	-7013.98784	-7164.540079	-7164.543149	-7164.543149	-7165.181493
<b>&lt;S<sup>2</sup>&gt;</b>	0.7719	0	0	0.7542	0.7544	0	0
<b>N Imag</b>	0	0	0	0	0	0	0

							
<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>
<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>
2-CO <sub>2</sub> Et	2-CO <sub>2</sub> Et-H	2-CO <sub>2</sub> Et+	2-CO <sub>2</sub> Et-	2-CO <sub>2</sub> Et-a-oo-radical	2-CO <sub>2</sub> Et-b-oo-radical	2-CO <sub>2</sub> Et-a-ooH	2-CO <sub>2</sub> Et-b-ooH
SX-5-2-f-2.log	SX-5-2-h.log	SX-5-2-+.log	SX-5-2--.log	SX-5-2-a-oo-radical.log	SX-5-2-b-oo-radical.c.log	SX-5-2-a-ooH-c.log	SX-5-2-a-ooH-c.log
E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)
-6746.09068	-6746.71465	-6745.879136	-6746.171425	-6896.384017	-6896.378712	-6897.017616	-6897.007527
E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)
-6746.939456	-6747.565562	-6746.720849	-6747.031273	-6897.283236	-6897.275676	-6897.923516	-6897.910387
<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >
0.773	0	0	0	0.7539	0.7542	0	0
N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag
0	0	0	0	0	0	0	0
							
<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>
<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>
3-CO <sub>2</sub> Et	3-CO <sub>2</sub> Et-H	3-CO <sub>2</sub> Et+	3-CO <sub>2</sub> Et-	3-CO <sub>2</sub> Et-a-oo-radical	3-CO <sub>2</sub> Et-b-oo-radical	3-CO <sub>2</sub> Et-a-ooH	3-CO <sub>2</sub> Et-b-ooH
SX-5-3-f.log	SX-5-3-h.log	SX-5-3-+.c.log	SX-5-3--.log	SX-5-3-a-oo-radical.log	SX-5-3-b-oo-radical.c.log	3-CO <sub>2</sub> Et-a-ooH-c.log	3-CO <sub>2</sub> Et-b-ooH-c.log
E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)
-6478.898974	-6479.523084	-6478.689054	-6478.974261	-6629.192758	6629.18522972	-6629.82599714	-6629.81777728
E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)
-6479.668457	-6480.294718	-6479.451354	-6479.755129	-6630.0127243	-6630.0024265	-6630.6526992	-6630.6412365
<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >
0.7731	0	0	0	0.7542	0.7544	0	0
N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag
0	0	0	0	0	0	0	0
							
<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>	<b>Compound</b>
<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>	<b>name</b>
4-CO <sub>2</sub> Et	4-CO <sub>2</sub> Et-H	4-CO <sub>2</sub> Et+	4-CO <sub>2</sub> Et-	4-CO <sub>2</sub> Et-a-oo-radical	4-CO <sub>2</sub> Et-b-oo-radical	4-CO <sub>2</sub> Et-a-ooH	4-CO <sub>2</sub> Et-b-ooH
SX-5-4-c.log	SX-5-4-h.log	SX-5-4-+-2.log	SX-5-4--.log	SX-5-4-a-oo-radical.log	SX-5-4-b-oo-radical.log	SX-5-4-a-ooH-c.log	SX-5-4-a-ooH-c.log
E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)	E (gas phase)
-6211.70683	-6212.331249	-6211.499132	-6211.775167	-6362.000850	-6361.9996473	-6362.63412639	-6362.628942
E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)	E* (gas phase)
-6212.396936	-6213.023479	-6212.182128	-6212.477034	-6362.7415155	-6362.737487	-6363.3814991	-6363.3741495
<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >	<S <sup>2</sup> >
0.7734	0	0	0	0.7539	0.7541	0	0
N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag	N Imag
0	0	0	0	0	0	0	0

Compound								
<b>name</b>	1-CO <sub>2</sub> H	1-CO <sub>2</sub> H-H	1-CO <sub>2</sub> H+	1-CO <sub>2</sub> H-	1-CO <sub>2</sub> H-a-oo- radical	1-CO <sub>2</sub> H-b-oo- radical	1-CO <sub>2</sub> H-a-ooH	1-CO <sub>2</sub> H-b-ooH
<b>File name</b>	acid.log	trityl-co2h-h- c.log	acid+.log	acid-.log	acid-b-oo.log	acid-a-oo.log	acid-b-ooH.log	acid-a-ooH.log
<b>E (gas phase)</b>	-6777.402698	-6778.025775	-6777.182069	-6777.492922	-6927.681846	-6927.688792	-6928.31591	-6928.320597
<b>E* (gas phase)</b>	-6778.286348	-6778.911694	-6778.057249	-6778.38913	-6928.61579	-6928.61977	-6929.257599	-6929.25748
<b>E (PCM H<sub>2</sub>O)</b>	-6777.361818	-6777.986023	-6777.156511	-6777.484839	-6927.63876	-6927.657838	-6928.275093	-6928.291046
<b>E* (PCM H<sub>2</sub>O)</b>	-6778.248259	-6778.874543	-6778.052936	-6777.484839	-6928.575774	-6928.591662	-6929.219548	-6929.230682
<b>E*-u (PCM H<sub>2</sub>O)</b>	-6778.229152	-6778.855339	-6778.034482	-6778.379579				
<b>&lt;S2&gt;</b>	0.7718	0	0	0	0.7541	0.7544	0	0
<b>N Imag</b>	0	0	0	0	0	0	0	0

Compound								
<b>name</b>	1-CO <sub>2</sub> Na	1-CO <sub>2</sub> Na-H	1-CO <sub>2</sub> Na+	1-CO <sub>2</sub> Na-	1-CO <sub>2</sub> Na-a-oo- radical	1-CO <sub>2</sub> Na-b-oo- radical	1-CO <sub>2</sub> Na-a-ooH	1-CO <sub>2</sub> Na-b-ooH
<b>File name</b>	salt.log	salt-h.log	salt+.log	salt-.log	salt-b-oo.log	salt-a-oo.log	salt-b-ooH-4.log	salt-a-ooH.log
<b>E (gas phase)</b>	-7262.696867	-7263.319713	-7262.515716	-7262.748859	-7412.980617	-7412.985398	-7413.618236	-7413.616918
<b>E* (gas phase)</b>	-7263.582238	-7264.207191	-7263.394058	-7263.644019	-7413.915737	-7413.917954	-7414.560445	-7414.555404
<b>E (PCM H<sub>2</sub>O)</b>	-7262.772424	-7263.396405	-7262.604191	-7262.889913	-7413.053578	-7413.069955	-7413.689429	-7413.703468
<b>E* (PCM H<sub>2</sub>O)</b>	-7263.66177	-7264.287852	-7263.486813	-7263.788356	-7413.993318	-7414.006859	-7414.636084	-7414.646172
<b>&lt;S2&gt;</b>	0.7722	0	0	0	0.7545	0.7544	0	0
<b>N Imag</b>	0	0	0	0	0	0	0	0

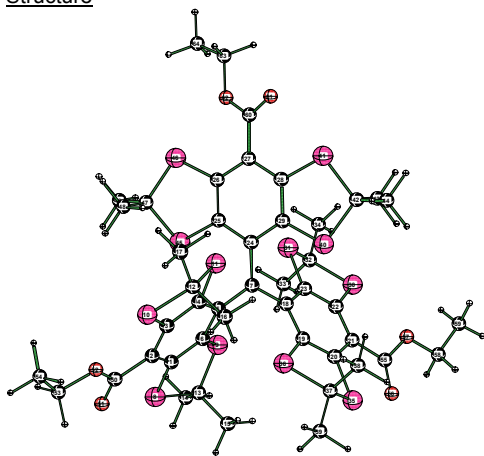


Compound

name	H radical	Molecular oxygen	Hydroxyl radical	Water	Methylthiol	CH <sub>3</sub> S radical	DMSO	CH <sub>2</sub> SOCH <sub>3</sub> radical
File name	H-radical.log	o2-triple.log	oh-1.log	h2o.log	ch3sh.log	ch3s.log	dmso.log	dmso-radical.log
E* (gas phase)	-0.5002728	-150.3200421	-75.7234548	-76.4089533	-438.6983484	-438.0597245	-553.1869359	-552.5149959
E* (gas phase)	-0.5021559	-150.3719978	-75.7630261	-76.4590669	-438.7441885	-438.1013432	-553.2699593	-552.5973948
E (PCM H <sub>2</sub> O)	-0.5003019	-150.3202085	-75.730291	-76.417569	-438.697705	-438.056683	-553.188212	-552.516801
E* (PCM H <sub>2</sub> O)	-0.5022133	-150.3723549	-75.771165	-76.469456	-438.7437	-438.098157	-553.274386	-552.602071
E*-u (PCM H <sub>2</sub> O)	-0.498319	-150.367882	-75.765523	-76.465217	-438.743619	-438.100625	-553.278113	-552.604491
<S <sup>2</sup> >	0.75	0	0.752	0	0	0.7525	0	0.7561
N Imag	0	0	0	0	0	0	0	0

## B3LYP/6-31G\* Optimized Geometries

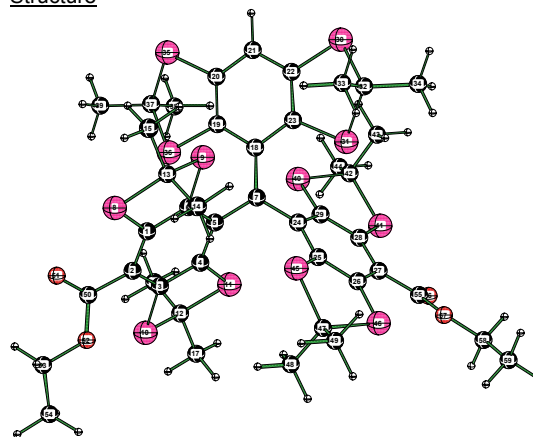
**1-CO<sub>2</sub>Et:**  
Structure



Coordinates

C	-2.566276	-2.612513	-1.255456
C	-3.666529	-2.359089	-0.404673
C	-3.540600	-1.359869	0.593796
C	-2.365777	-0.597005	0.688948
C	-1.251870	-0.834325	-0.163107
C	-1.389801	-1.847774	-1.144262
C	-0.007550	-0.051127	-0.034856
S	-2.597805	-3.829860	-2.547434
S	-0.188938	-2.092330	-2.426313
S	-4.802132	-0.976939	1.794912
S	-2.352527	0.665652	1.940585
C	-3.672742	-0.104010	2.977240
C	-0.771453	-3.778375	-2.901419
C	-0.552825	-3.981175	-4.405015
C	-0.045842	-4.851628	-2.079841
C	-3.068834	-1.099837	3.974848
C	-4.457015	0.999653	3.695288
C	1.298893	-0.730584	-0.015392
C	1.501666	-1.934520	0.709099
C	2.752213	-2.574821	0.728055
C	3.845163	-2.039971	0.014671
C	3.659809	-0.850190	-0.721526
C	2.412734	-0.204097	-0.723908
C	-0.075176	1.417334	0.108907
C	-0.857035	2.209466	-0.775655
C	-0.925709	3.607902	-0.650014
C	-0.211338	4.265628	0.375938
C	0.559690	3.494961	1.273335
C	0.630349	2.097338	1.137670
S	4.930526	-0.088317	-1.712149
S	2.321596	1.284939	-1.696006
C	3.757183	0.863731	-2.785138
C	3.303621	0.017131	-3.979700
C	4.435768	2.159435	-3.241053
S	2.865295	-4.065185	1.692487
S	0.228154	-2.727776	1.666008
C	1.394289	-3.670815	2.751474
C	1.810426	-2.825968	3.961364
C	0.726741	-4.979590	3.186002
S	1.499548	1.247044	2.429187
S	1.429200	4.199163	2.652431
C	2.501145	2.711995	2.951956
C	3.793818	2.802694	2.131927
C	2.796269	2.609199	4.452320
S	-1.661686	1.522070	-2.200177

**2-CO<sub>2</sub>Et:**  
Structure



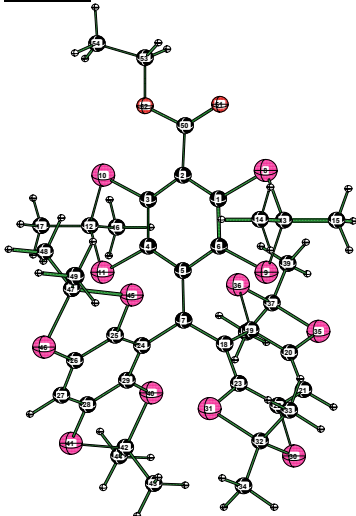
Coordinates

C	-3.528711	-0.271065	1.083609
C	-3.878633	-1.301289	0.185400
C	-2.929683	-1.723006	-0.771831
C	-1.654961	-1.134663	-0.813987
C	-1.291053	-0.082280	0.069865
C	-2.259931	0.330252	1.024286
C	0.033041	0.556214	0.001493
S	-4.632688	0.334685	2.338045
S	-1.952687	1.593486	2.237901
S	-3.244194	-2.977449	-1.998624
S	-0.551460	-1.773181	-2.054633
C	-1.889585	-2.439954	-3.144116
C	-3.288247	1.048736	3.398502
C	-2.756418	-0.005154	4.377362
C	-3.837667	2.272721	4.139121
C	-2.390153	-1.360079	-4.110260
C	-1.358318	-3.663358	-3.898319
C	0.138631	2.018539	0.082352
C	-0.770659	2.868558	-0.611361
C	-0.675964	4.265775	-0.506497
C	0.306073	4.861020	0.282116
C	1.214286	4.050263	0.960169
C	1.150806	2.651617	0.859414
C	1.250068	-0.266685	-0.144329
C	1.496073	-1.382555	0.699955
C	2.650910	-2.172220	0.563161
C	3.610462	-1.863507	-0.427273
C	3.380517	-0.761570	-1.280243
C	2.222079	0.022452	-1.137869
S	2.516848	4.729653	1.957879
S	2.398661	1.782078	1.782353
C	2.760376	3.180706	2.954128
C	1.797178	3.145923	4.145311
C	4.220488	3.087149	3.404370
S	-1.878895	5.225616	-1.391243
S	-2.064221	2.289434	-1.688068
C	-2.257273	3.887519	-2.621524
C	-1.279810	3.947461	-3.800157
C	-3.710808	4.017162	-3.085095
S	1.977367	1.263028	-2.381627
S	4.468559	-0.324347	-2.614153
C	3.761068	1.376718	-2.856885
C	4.490439	2.395545	-1.972827
C	3.862552	1.747231	-4.340434
S	0.458586	-1.768590	2.088738
S	2.809448	-3.510682	1.726838

S	-1.910662	4.443220	-1.875474	C	1.022602	-3.523278	2.225896
C	-2.839367	2.931284	-2.417544	C	0.207739	-4.431096	1.297091
C	-4.092726	2.730877	-1.558038	C	0.917203	-3.973816	3.686594
C	-3.191346	3.068072	-3.902445	C	-5.244340	-1.874811	0.286900
C	-4.920427	-3.106285	-0.670158	O	-6.190015	-1.294886	0.790399
O	-5.038682	-3.947403	-1.546405	O	-5.333386	-3.125178	-0.208763
O	-5.949476	-2.747292	0.120833	C	-6.649794	-3.727499	-0.183746
C	-7.203997	-3.429549	-0.115281	C	-6.524952	-5.124875	-0.759786
C	-8.220211	-2.873215	0.863520	C	4.846301	-2.657563	-0.644097
C	5.132497	-2.778723	0.058656	O	5.483688	-2.651852	-1.682920
O	5.225479	-3.968901	0.301561	O	5.217741	-3.374571	0.433917
O	6.202586	-1.991809	-0.168488	C	6.392287	-4.206087	0.272150
C	7.489658	-2.655389	-0.187365	C	6.638310	-4.913820	1.590640
C	8.550553	-1.590903	-0.391195	H	-1.952311	0.418394	4.990774
C	-0.248406	5.735849	0.584282	H	-2.358566	-0.872405	3.843091
O	0.022266	6.278640	1.641285	H	-3.562201	-0.344511	5.039243
O	-0.586393	6.423929	-0.522774	H	-3.055466	2.723155	4.761370
C	-0.681142	7.861664	-0.375385	H	-4.655867	1.972696	4.804284
C	-1.049016	8.438445	-1.728741	H	-4.210658	3.027301	3.442373
H	0.517436	-3.950004	-4.640612	H	-1.576037	-1.040722	-4.771120
H	-1.066409	-3.215276	-4.991325	H	-2.753938	-0.483612	-3.567356
H	-0.928219	-4.965294	-4.708621	H	-3.208485	-1.754416	-4.724609
H	1.030781	-4.826463	-2.285476	H	-2.147956	-4.090157	-4.527769
H	-0.429667	-5.845194	-2.341215	H	-1.002535	-4.434491	-3.210546
H	-0.192146	-4.694911	-1.007797	H	-0.532729	-3.370732	-4.557074
H	-2.391818	-0.579670	4.662535	H	0.365039	5.941807	0.364241
H	-2.500489	-1.877452	3.457889	H	1.929090	2.212733	4.705203
H	-3.864559	-1.578510	4.558280	H	0.757196	3.201261	3.812617
H	-5.268091	0.560863	4.288128	H	1.995696	3.991042	4.815008
H	-4.886526	1.711912	2.986602	H	4.383540	2.156074	3.959054
H	-3.799568	1.541842	4.384416	H	4.460613	3.919072	4.076459
H	2.592401	0.581763	-4.593583	H	4.904873	3.113815	2.552877
H	2.814446	-0.902328	-3.647185	H	-1.488848	3.132912	-4.503532
H	4.166939	-0.253078	-4.599644	H	-0.245667	3.849491	-3.459333
H	3.745310	2.751413	-3.852689	H	-1.383909	4.902969	-4.327745
H	5.310872	1.929220	-3.859921	H	-3.955869	3.209802	-3.784819
H	4.757557	2.763957	-2.389372	H	-3.853184	4.966660	-3.614000
H	0.934151	-2.580410	4.572791	H	-4.405037	3.974426	-2.242565
H	2.279854	-1.890486	3.644898	H	5.552949	2.432246	-2.242074
H	2.525728	-3.381484	4.579531	H	4.409108	2.131752	-0.914816
H	-0.160572	-4.770018	3.794753	H	4.058325	3.393814	-2.109613
H	1.418011	-5.566724	3.801717	H	4.914389	1.784797	-4.646669
H	0.427425	-5.582313	2.324955	H	3.433363	2.741120	-4.513082
H	4.359592	3.695991	2.422998	H	3.340382	1.022924	-4.970562
H	3.580912	2.860648	1.061070	H	0.579179	-5.461093	1.359506
H	4.417951	1.918873	2.308739	H	0.276008	-4.099293	0.257545
H	3.355974	3.490993	4.785085	H	-0.848633	-4.419587	1.589692
H	3.416361	1.728717	4.657196	H	1.281779	-5.002355	3.790469
H	1.876448	2.537539	5.038002	H	-0.130216	-3.961899	4.009511
H	-4.763020	3.592090	-1.666463	H	1.497604	-3.326932	4.349133
H	-3.834913	2.622382	-0.501178	H	-7.332086	-3.099019	-0.764863
H	-4.627442	1.828113	-1.874964	H	-7.006118	-3.736182	0.850821
H	-3.864267	3.920362	-4.052294	H	-5.828377	-5.729728	-0.170741
H	-3.714267	2.169463	-4.249169	H	-6.165161	-5.092329	-1.792683
H	-2.298094	3.213726	-4.514885	H	-7.504051	-5.616271	-0.748593
H	-7.045548	-4.504157	0.018236	H	7.231186	-3.565963	-0.017451
H	-7.498108	-3.264564	-1.156468	H	6.211213	-4.908318	-0.547663
H	-8.354638	-1.796704	0.718773	H	6.803892	-4.192542	2.397042
H	-7.904004	-3.045573	1.896872	H	7.527443	-5.548368	1.506617
H	-9.186257	-3.366508	0.709684	H	5.786453	-5.545129	1.861296
H	7.487100	-3.397299	-0.992320				
H	7.616149	-3.190830	0.758276				
H	9.541920	-2.057064	-0.402624				
H	8.524812	-0.854214	0.417875				
H	8.403537	-1.066347	-1.340197				
H	0.281549	8.235430	-0.013576				
H	-1.432740	8.084383	0.388526				
H	-0.291719	8.189663	-2.478764				
H	-1.118409	9.529414	-1.656354				
H	-2.013946	8.052036	-2.070918				



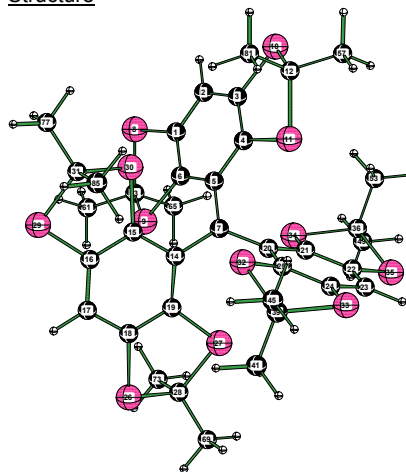
**3-CO<sub>2</sub>Et:**  
Structure



**Coordinates**

C	2.865442	-1.386634	0.969600
C	3.735250	-0.648357	0.138918
C	3.187083	0.312770	-0.739944
C	1.802083	0.539940	-0.766784
C	0.909604	-0.200757	0.055016
C	1.477507	-1.169376	0.925037
C	-0.542797	0.030536	0.009969
S	3.436487	-2.622944	2.111239
S	0.507276	-2.156235	2.041010
S	4.151724	1.283258	-1.882406
S	1.242951	1.784749	-1.908138
C	2.731543	1.688952	-3.002762
C	1.911579	-2.587359	3.168098
C	2.052213	-1.540137	4.279704
C	1.676404	-3.987133	3.746284
C	2.554512	0.599716	-4.067559
C	2.973769	3.060255	-3.641890
C	-1.464477	-1.112250	-0.024900
C	-1.212435	-2.245910	-0.849497
C	-2.098223	-3.335597	-0.869359
C	-3.243641	-3.343145	-0.076494
C	-3.513014	-2.242971	0.735643
C	-2.651368	-1.135449	0.761635
C	-1.071707	1.407077	0.005860
C	-0.612638	2.383453	0.934239
C	-1.124076	3.691590	0.921991
C	-2.096427	4.071564	-0.000908
C	-2.560619	3.134075	-0.921751
C	-2.064429	1.820269	-0.927246
S	-4.966053	-2.157406	1.753482
S	-3.154401	0.176515	1.852677
C	-4.259191	-0.884923	2.908534
C	-3.451932	-1.556386	4.024294
C	-5.390107	-0.020321	3.471259
S	-1.671139	-4.704453	-1.915751
S	0.185353	-2.400940	-1.940038
C	-0.574610	-3.703181	-3.030884
C	-1.393709	-3.055640	-4.152211
C	0.538903	-4.596094	-3.584991
S	-2.641982	0.810628	-2.270124
S	-3.714541	3.567308	-2.197412
C	-4.173382	1.811134	-2.601200
C	-5.328433	1.339196	-1.711478
C	-4.523776	1.706686	-4.088084
S	0.498344	2.030396	2.274933

**4-CO<sub>2</sub>Et:**  
Structure



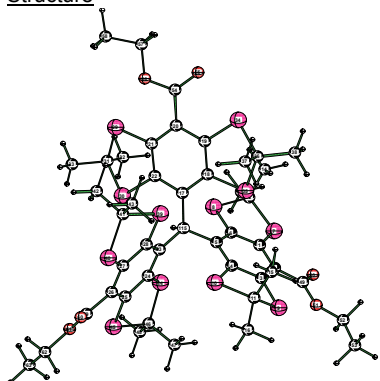
**Coordinates**

C	-2.710516	-2.570352	-0.732111
C	-3.722629	-2.187989	0.145628
C	-3.524203	-1.078500	0.965489
C	-2.326843	-0.347556	0.915896
C	-1.269960	-0.731139	0.043451
C	-1.498469	-1.863249	-0.789161
C	-0.000048	0.007038	-0.000140
S	-2.872341	-3.979723	-1.800193
S	-0.333580	-2.472615	-1.989396
S	-4.773210	-0.502516	2.089171
S	-2.251004	1.040985	2.025583
C	-3.579965	0.423782	3.171552
C	-1.587609	-3.396464	-3.007440
C	1.268799	-0.732940	-0.043853
C	1.495653	-1.865615	0.788459
C	2.706805	-2.574251	0.731455
C	3.719641	-2.192882	-0.145887
C	3.522825	-1.082902	-0.965475
C	2.326352	-0.350505	-0.916004
C	0.001035	1.481529	0.000059
C	-0.825102	2.226432	-0.887245
C	-0.815585	3.630845	-0.879281
C	0.003221	4.336603	0.000330
C	0.820930	3.629419	0.879831
C	0.828277	2.224999	0.887540
S	4.772876	-0.508066	-2.088590
S	2.252441	1.038339	-2.025442
C	3.581052	0.419855	-3.171154
S	2.866625	-3.984125	1.799185
S	0.329753	-2.473829	1.988308
C	1.582434	-3.399521	3.006362
S	1.802902	1.490366	2.178575
S	1.814025	4.447806	2.100840
S	-1.801024	1.493572	-2.178329
S	-1.807545	4.450965	-2.100065
C	-2.890194	2.977584	-2.439678
H	4.649581	-2.751136	-0.189237
H	0.004051	5.422252	0.000435
C	2.894253	2.972676	2.440579
H	-4.653248	-2.745105	0.189076
C	4.083169	2.941910	1.474137
H	4.702147	3.836384	1.612484
H	4.697701	2.054515	1.665036
H	3.747782	2.906297	0.434211
C	3.352890	3.003869	3.901021

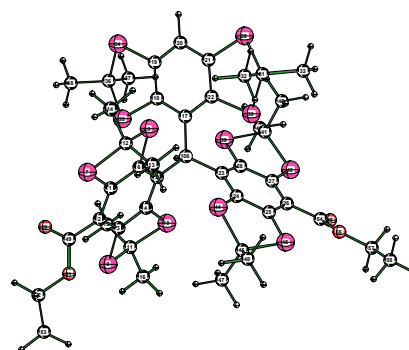
S	-0.549107	4.794704	2.186779
C	0.973000	3.801555	2.579499
C	2.133391	4.212558	1.666701
C	1.325528	3.976293	4.059125
C	5.187664	-0.942533	0.221558
O	5.647852	-1.986371	0.649818
O	5.961983	0.077027	-0.200715
C	7.389436	-0.164449	-0.197813
C	8.065118	1.076476	-0.748950
H	1.141476	-1.509102	4.889648
H	2.218723	-0.543369	3.862127
H	2.900713	-1.790686	4.927742
H	0.768637	-3.996950	4.360917
H	2.515218	-4.272164	4.392055
H	1.573470	-4.733402	2.954869
H	1.705978	0.843199	-4.717600
H	2.365338	-0.373985	-3.607495
H	3.459285	0.524922	-4.682767
H	2.127707	3.330849	-4.283948
H	3.870273	3.029295	-4.272089
H	3.102974	3.838139	-2.885305
H	-3.917780	-4.193819	-0.091790
H	-2.485633	5.085061	-0.004234
H	-3.010804	-0.794092	4.676964
H	-2.641778	-2.164305	3.612998
H	-4.103296	-2.202075	4.625159
H	-4.978302	0.757329	4.124597
H	-6.068696	-0.634508	4.074373
H	-5.964062	0.458555	2.674160
H	-0.742532	-2.443976	-4.787691
H	-2.177821	-2.411883	-3.744710
H	-1.864240	-3.828826	-4.771076
H	1.216379	-4.006803	-4.213610
H	0.110228	-5.386424	-4.212084
H	1.117947	-5.057606	-2.781638
H	-6.215859	1.958323	-1.889247
H	-5.064737	1.402693	-0.652366
H	-5.575356	0.295741	-1.939185
H	-5.409660	2.312988	-4.309182
H	-4.762416	0.668220	-4.344927
H	-3.698419	2.045674	-4.718806
H	2.384254	5.267271	1.830901
H	1.876820	4.075208	0.612816
H	3.017119	3.601773	1.884907
H	1.581319	5.022323	4.263280
H	2.201364	3.367386	4.310940
H	0.494886	3.684189	4.706196
H	7.594947	-1.052264	-0.803875
H	7.700455	-0.383798	0.828376
H	7.831660	1.953765	-0.137475
H	7.741171	1.275034	-1.775160
H	9.151474	0.934632	-0.749194

C	-3.349306	3.009790	-3.899945
H	-3.959876	2.126691	-4.120656
H	-3.972073	3.893928	-4.078301
H	-2.500357	3.032521	-4.587452
C	-4.078805	2.948486	-1.472807
H	-4.694681	2.061988	-1.663544
H	-3.743091	2.912312	-0.433007
H	-4.696532	3.843865	-1.610868
C	-4.288651	1.624097	3.804647
H	-5.092491	1.280588	4.466011
H	-3.581747	2.198740	4.413942
H	-4.715231	2.284434	3.045682
C	-0.907628	-4.607269	-3.652598
H	-1.637281	-5.184137	-4.232588
H	-0.125031	-4.274943	-4.344522
H	-0.457964	-5.260745	-2.901267
C	-2.214460	-2.473876	-4.058264
H	-1.440841	-2.101978	-4.740319
H	-2.965400	-3.020407	-4.641229
H	-2.698644	-1.613663	-3.588326
C	4.291330	1.619501	-3.803720
H	5.095014	1.275224	-4.464874
H	3.585298	2.195099	-4.413127
H	4.718398	2.279165	-3.044444
C	2.984548	-0.508057	-4.234783
H	2.472841	-1.357449	-3.774397
H	2.257467	0.040812	-4.844601
H	3.777195	-0.890519	-4.888724
C	0.900817	-4.609623	3.651101
H	1.629644	-5.187549	4.231079
H	0.118505	-4.276500	4.342963
H	0.450471	-5.262345	2.899522
C	-2.984182	-0.505041	4.234808
H	-2.256455	0.042949	4.844647
H	-3.777095	-0.886893	4.888785
H	-2.473373	-1.354802	3.774105
C	2.210271	-2.477955	4.057478
H	1.437042	-2.105317	4.739568
H	2.960530	-3.025506	4.640363
H	2.695488	-1.618187	3.587794

**1-CO<sub>2</sub>Et-H:**  
Structure



**2-CO<sub>2</sub>Et-H:**  
Structure



## Coordinates

H	3.977052	3.886942	4.079776
H	2.503729	3.027868	4.588222
C	-3.439813	-1.448921	0.605441
C	-2.276758	-0.649099	0.586058
C	-1.257068	-0.868162	-0.363093
C	-1.447082	-1.903940	-1.299807
S	-2.691600	-3.965361	-2.549433
S	-0.293603	-2.208338	-2.621363
S	-4.621054	-1.061706	1.882412
S	-2.221440	0.654847	1.797328
C	-3.447932	-0.105046	2.947245
C	-0.885108	-3.919608	-2.988166
C	-0.732919	-4.197318	-4.487775
C	-0.109445	-4.941076	-2.146639
H	3.961915	2.119717	4.121786
C	-2.752995	-1.034071	3.950389
C	-4.216843	1.011164	3.663655
C	1.352861	-0.710551	-0.194810
C	1.517797	-1.817352	0.659761
C	2.781952	-2.425636	0.819084
C	3.912031	-1.939334	0.131316
C	3.755708	-0.838890	-0.734409
C	2.492604	-0.243297	-0.884187
C	-0.097236	1.466863	-0.100007
C	-0.881529	2.300126	-0.931314
C	-1.020203	3.678064	-0.694787
C	-0.354250	4.270885	0.397433
C	0.428458	3.455873	1.239089
C	0.560116	2.070487	0.992343
S	5.067481	-0.132423	-1.710537
S	2.436866	1.167772	-1.972809
C	3.941521	0.688611	-2.936615
C	3.578358	-0.275118	-4.071746
C	4.620144	1.954726	-3.468485
S	2.859328	-3.834835	1.899263
S	0.197921	-2.587218	1.579367
C	1.297522	-3.428118	2.807544
C	1.587916	-2.509724	4.000638
C	0.630025	-4.732096	3.259018
S	1.492471	1.183802	2.219445
S	1.262698	4.091520	2.672910
C	2.424772	2.655701	2.833789
C	3.690630	2.886407	1.999501
C	2.759753	2.450739	4.315060
S	-1.701090	1.681300	-2.387126
S	-2.031825	4.567747	-1.858334
C	-2.914865	3.072398	-2.507241
C	-4.161084	2.771097	-1.666273
C	-3.272177	3.304165	-3.979103
C	-4.879840	-3.249814	-0.511554
O	-5.061803	-4.069003	-1.397692
O	-5.828980	-2.956637	0.396693
C	-7.080365	-3.672163	0.263695
C	-8.003843	-3.191155	1.366403
C	5.208833	-2.635530	0.331161
O	5.313518	-3.790470	0.703248
O	6.273981	-1.846605	0.085909
C	7.573552	-2.472772	0.213323
C	8.622150	-1.409963	-0.053091
C	-0.458538	5.716707	0.725096
O	-0.258381	6.180029	1.833696
O	-0.773759	6.480132	-0.339001
C	-0.936043	7.896123	-0.081682
C	-1.254679	8.568431	-1.403074
H	0.324747	-4.168916	-4.774772
H	-1.281769	-3.467444	-5.087877
H	-1.111149	-5.199192	-4.721889
H	0.957417	-4.909797	-2.397331
H	-0.486975	-5.951528	-2.344478

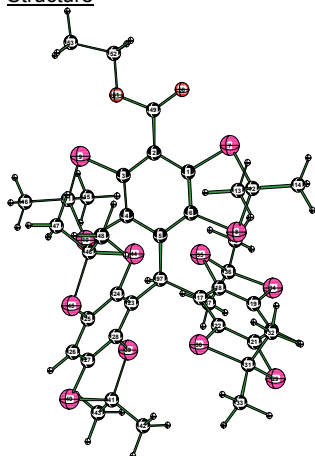
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C	-3.455708	-0.279446	1.133030
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C	-3.107809	-1.585518	-0.881815
C	-1.840967	-0.994204	-1.019790
C	-1.352143	-0.037576	-0.103643
C	-2.180204	0.306954	0.982923
S	-4.424473	0.265856	2.518577
S	-1.744581	1.495257	2.236826
S	-3.564754	-2.742352	-2.157180
S	-0.870881	-1.571272	-2.398777
C	-2.325986	-2.127717	-3.395898
C	-2.982621	0.913080	3.484169
C	-2.386771	-0.187528	4.369983
C	-3.442968	2.112669	4.320476
C	-2.905723	-0.965566	-4.210041
C	-1.903108	-3.290930	-4.298294
C	0.203734	2.054099	0.064930
C	-0.599982	3.053892	-0.528260
C	-0.459964	4.409704	-0.188662
C	0.488727	4.805273	0.748163
C	1.298340	3.836987	1.335887
C	1.171366	2.472977	1.003566
C	1.240827	-0.304433	-0.373018
C	1.402896	-1.418062	0.479354
C	2.548747	-2.241314	0.393461
C	3.570551	-1.955816	-0.534959
C	3.422836	-0.841267	-1.385594
C	2.271884	-0.040145	-1.301707
S	2.581691	4.277639	2.480114
S	2.331292	1.404956	1.835844
C	2.714903	2.582873	3.222866
C	1.714320	2.413892	4.371142
C	4.152776	2.340697	3.691059
S	-1.561750	5.556077	-0.976477
S	-1.881395	2.713226	-1.719733
C	-1.941662	4.438373	-2.413030
C	-0.899192	4.612029	-3.522322
C	-3.359002	4.722787	-2.916969
S	2.167200	1.275975	-2.496622
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C	3.983346	1.334835	-2.847487
C	4.682702	2.286702	-1.869407
C	4.201479	1.764306	-4.302026
S	0.280246	-1.837185	1.794666
S	2.606097	-3.614317	1.525789
C	0.792533	-3.607019	1.901278
C	0.022975	-4.463024	0.888370
C	0.578586	-4.103810	3.334853
C	-5.291614	-1.788219	0.409795
O	-6.164611	-1.239456	1.057840
O	-5.463609	-2.989903	-0.176947
C	-6.786554	-3.568076	-0.067345
C	-6.756509	-4.915422	-0.762825
C	4.794217	-2.783539	-0.694279
O	5.476213	-2.795814	-1.704016
O	5.100416	-3.504990	0.400586
C	6.258934	-4.367256	0.291708
C	6.436916	-5.067046	1.625309
H	-1.519176	0.195823	4.920036
H	-2.060142	-1.040989	3.770297
H	-3.135292	-0.536301	5.091711
H	-2.600834	2.525311	4.888316
H	-4.204787	1.797084	5.042956
H	-3.862071	2.901297	3.690945
H	-2.159997	-0.595915	-4.923439
H	-3.200212	-0.136788	-3.560481
H	-3.789217	-1.300615	-4.766392
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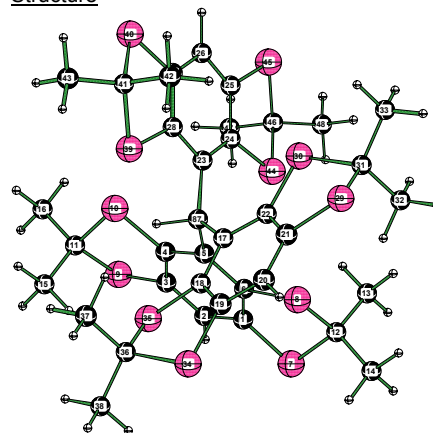
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H	-4.713048	1.675745	2.952311
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H	3.089189	-1.173328	-3.685276
H	4.483373	-0.578254	-4.611526
H	3.956961	2.470667	-4.172112
H	5.536166	1.691168	-4.009723
H	4.876589	2.642222	-2.658638
H	0.657076	-2.257430	4.521886
H	2.059432	-1.578722	3.675751
H	2.260784	-3.012196	4.705937
H	-0.310408	-4.517117	3.779761
H	1.282270	-5.263429	3.961871
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H	4.211399	3.785445	2.350434
H	3.449018	3.016575	0.941033
H	4.368233	2.029650	2.091662
H	3.284257	3.330389	4.705782
H	3.425522	1.588452	4.437559
H	1.858044	2.287726	4.910767
H	-4.856157	3.618186	-1.710799
H	-3.899026	2.591396	-0.620189
H	-4.669361	1.879656	-2.051301
H	-3.966940	4.147433	-4.067837
H	-3.772638	2.419543	-4.388991
H	-2.383807	3.516134	-4.579026
H	-6.875885	-4.744984	0.333388
H	-7.487729	-3.476348	-0.733061
H	-8.186848	-2.115347	1.282719
H	-7.574545	-3.392697	2.352651
H	-8.964733	-3.712390	1.293648
H	7.632628	-3.301224	-0.499774
H	7.656641	-2.893810	1.219736
H	9.621968	-1.847390	0.043124
H	8.535040	-0.587011	0.663257
H	8.518831	-1.000923	-1.062775
H	-0.010660	8.274101	0.363266
H	-1.736321	8.026923	0.653602
H	-0.447263	8.413109	-2.125504
H	-1.376497	9.645993	-1.247225
H	-2.181268	8.173423	-1.830691
C	0.017660	-0.013318	-0.528117
H	0.100098	0.081529	-1.621210

H	-1.149070	-2.954914	-5.019111
H	0.601935	5.851896	1.013067
H	1.778320	1.397220	4.776203
H	0.690202	2.581339	4.028378
H	1.937066	3.128532	5.172492
H	4.250731	1.325570	4.092417
H	4.409467	3.040732	4.494577
H	4.867113	2.465874	2.873802
H	-1.113007	3.925140	-4.349588
H	0.108049	4.401968	-3.152812
H	-0.922479	5.639929	-3.903004
H	-3.607893	4.046427	-3.742779
H	-3.421917	5.748033	-3.299397
H	-4.099031	4.596519	-2.123183
H	5.762376	2.292505	-2.061473
H	4.516075	1.982912	-0.832353
H	4.298416	3.306022	-1.992575
H	5.272980	1.771110	-4.533076
H	3.823990	2.781547	-4.458176
H	3.697224	1.089702	-4.998324
H	0.370936	-5.502105	0.933076
H	0.163574	-4.093342	-0.131029
H	-1.049514	-4.441029	1.113701
H	0.911817	-5.144097	3.426552
H	-0.487522	-4.076393	3.587994
H	1.128463	-3.493793	4.055920
H	-7.505737	-2.881410	-0.525120
H	-7.039174	-3.654999	0.993736
H	-6.023297	-5.580385	-0.295591
H	-6.497342	-4.805013	-1.820231
H	-7.743105	-5.386856	-0.694746
H	7.124012	-3.751322	0.028057
H	6.091275	-5.073579	-0.527478
H	6.590932	-4.341776	2.430433
H	7.311745	-5.725072	1.580938
H	5.559613	-5.673662	1.869965
C	0.003719	0.614810	-0.444384
H	-0.109773	0.769858	-1.528407

**3-CO<sub>2</sub>Et-H:**  
Structure



**4-CO<sub>2</sub>Et-H:**  
Structure



## Coordinates

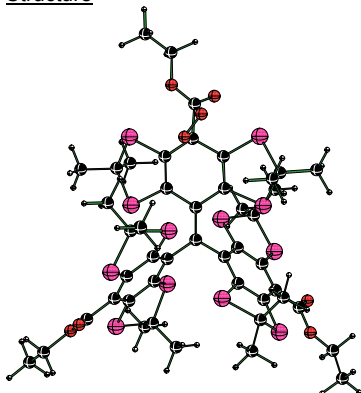
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C	-3.261595	-0.178552	-0.890890
C	-1.877817	-0.389424	-1.005970
C	-0.945069	0.251276	-0.160963
C	-1.449479	1.124321	0.823123
S	-3.351663	2.506703	2.191108
S	-0.435978	2.041920	1.966847
S	-4.278968	-1.055927	-2.060883
S	-1.382199	-1.561521	-2.254004
C	-2.910195	-1.361495	-3.276626
C	-1.790771	2.387140	3.180473
C	-1.893230	1.262991	4.218316
C	-1.522223	3.739615	3.850472
C	-2.770111	-0.179465	-4.242626
C	-3.189371	-2.668754	-4.024673
C	1.519621	1.118824	-0.073740
C	1.438339	2.312346	-0.825703
C	2.317078	3.385429	-0.603367
C	3.308129	3.291911	0.367928
C	3.414869	2.118376	1.109888
C	2.537813	1.034804	0.900921
C	1.038601	-1.444220	-0.193583
C	0.527901	-2.335724	0.776629
C	1.033296	-3.650180	0.874007
C	2.039999	-4.104056	0.028206
C	2.553853	-3.238270	-0.932412
C	2.056846	-1.930474	-1.047723
S	4.706544	1.897502	2.307658
S	2.864037	-0.383537	1.930545
C	3.840178	0.534493	3.219580
C	2.911946	1.107162	4.295881
C	4.877904	-0.417567	3.821645
S	2.072564	4.844022	-1.584169
S	0.213621	2.600591	-2.088495
C	1.153110	3.963016	-2.939244
C	2.131430	3.384520	-3.966628
C	0.154415	4.926633	-3.585556
S	2.758787	-0.980827	-2.383702
S	3.778822	-3.745429	-2.110804
C	4.295216	-2.015531	-2.552563
C	5.381453	-1.515085	-1.594371
C	4.763916	-1.981822	-4.009668
S	-0.677666	-1.929737	2.022755
S	0.385205	-4.677165	2.167820
C	-1.166282	-3.683447	2.389445
C	-2.255437	-4.156352	1.420394
C	-1.627196	-3.775118	3.846684
C	-5.201555	0.991361	0.267824
O	-5.635866	2.005654	0.783145
O	-5.998695	0.001232	-0.182000
C	-7.423784	0.240079	-0.086522
C	-8.132457	-1.002298	-0.590766
H	-0.957492	1.182248	4.783961
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H	-1.444771	4.542422	3.113334
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H	-4.113227	-2.578112	-4.607663
H	-3.290319	-3.510857	-3.335522
H	3.992656	4.116441	0.541122
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H	2.378156	0.293278	4.800405
H	2.171918	1.780941	3.857063

## Coordinates

C	2.784541	-2.349063	0.966399
C	3.822094	-2.089417	0.075650
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C	2.379128	-0.515868	-1.072666
C	1.313354	-0.762629	-0.178591
C	1.538206	-1.697934	0.854446
S	2.952358	-3.573460	2.239515
S	0.339651	-2.194757	2.079638
S	4.880495	-0.730040	-2.112216
S	2.294879	0.674240	-2.396550
C	3.691870	-0.063623	-3.378502
C	1.566628	-2.913906	3.279348
C	2.077686	-1.839890	4.245579
C	0.897602	-4.070219	4.029234
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C	4.375750	1.044346	-4.183354
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C	-1.632861	-1.960393	-0.678534
C	-2.802700	-2.674184	-0.369640
C	-3.663043	-2.216929	0.622667
C	-3.345921	-1.042233	1.299761
C	-2.174315	-0.316427	1.002788
C	-0.013622	1.485148	-0.285991
C	0.803723	2.215141	0.606380
C	0.730210	3.624371	0.649293
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C	-0.935709	3.627974	-1.073646
C	-0.873794	2.226886	-1.130457
S	-4.439937	-0.356340	2.518276
S	-1.977033	1.179998	1.951851
C	-3.141559	0.698653	3.319623
C	-2.403897	-0.084955	4.410418
C	-3.789276	1.967820	3.881311
S	-3.095061	-4.171544	-1.276291
S	-0.627938	-2.693017	-1.955481
C	-2.004349	-3.694973	-2.705398
C	-2.785889	-2.860717	-3.725416
C	-1.414133	-4.957966	-3.337358
S	-1.900078	1.486118	-2.386742
S	-2.002947	4.439871	-2.234599
C	-3.048717	2.938608	-2.561360
C	-4.186981	2.840060	-1.540114
C	-3.576630	2.989562	-3.997521
S	1.902796	1.510219	1.818415
S	1.722314	4.455945	1.862833
C	2.910523	3.048042	2.080804
C	4.043492	3.132963	1.052176
C	3.448187	3.049546	3.514556
H	1.243974	-1.432866	4.829611
H	2.549693	-1.015834	3.704981
H	2.812802	-2.272072	4.935110
H	0.047580	-3.698196	4.612941
H	1.606888	-4.523469	4.731458
H	0.540659	-4.840215	3.341275
H	2.464454	-0.792831	-5.009987
H	2.685875	-1.969700	-3.698872
H	4.019473	-1.643848	-4.826709
H	3.674588	1.468729	-4.910936
H	5.224575	0.633312	-4.741852
H	4.737067	1.845586	-3.534147
H	-4.572183	-2.760547	0.860247
H	-0.173040	5.415525	-0.137872
H	-1.613653	0.536597	4.847640
H	-1.942081	-0.986824	4.001272
H	-3.103385	-0.377330	5.202688
H	-3.022145	2.622317	4.310604
H	-4.490745	1.709052	4.682925
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H	-2.126939	-2.559780	-4.548279

H	3.495110	1.662694	5.039985
H	4.375303	-1.250335	4.326656
H	5.481399	0.108172	4.570658
H	5.542698	-0.822073	3.054586
H	1.582488	2.839283	-4.743325
H	2.835330	2.694316	-3.494051
H	2.701567	4.192685	-4.439758
H	-0.412565	4.411502	-4.369482
H	0.688380	5.759715	-4.056954
H	-0.546736	5.328531	-2.850277
H	6.273068	-2.148056	-1.676031
H	5.034419	-1.532885	-0.557832
H	5.657266	-0.484233	-1.845184
H	5.651965	-2.612500	-4.131958
H	5.043600	-0.960185	-4.291153
H	3.984948	-2.334721	-4.689763
H	-2.513757	-5.201960	1.626234
H	-1.923247	-4.078097	0.381697
H	-3.154807	-3.540933	1.538056
H	-1.894658	-4.809453	4.091470
H	-2.520907	-3.158789	3.997655
H	-0.847492	-3.440466	4.535254
H	-7.669170	1.126472	-0.680194
H	-7.667668	0.461288	0.956896
H	-7.860807	-1.877516	0.007793
H	-7.875228	-1.204948	-1.634902
H	-9.216637	-0.860190	-0.522557
C	0.544860	-0.008522	-0.459282
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**1-CO<sub>2</sub>Et-a-oo-radical**  
Structure

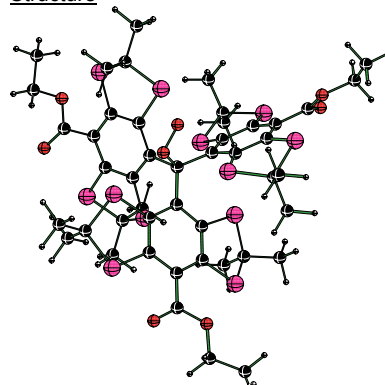


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C	-3.326141	-1.869531	0.768335
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C	-1.191334	-1.011929	-0.103483
C	-1.278690	-1.955764	-1.153423
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S	-2.386749	-3.921627	-2.660783
S	-0.116810	-1.992287	-2.498163
S	-4.516338	-1.734014	2.087960
S	-2.282859	0.201688	2.169023
C	-3.412381	-0.789668	3.241418
C	-0.608744	-3.654812	-3.137955
C	-0.503618	-3.653780	-4.668203
C	0.271014	-4.750540	-2.522020
C	-2.611335	-1.754408	4.124854
C	-4.269990	0.160067	4.084837
C	1.264915	-0.460756	-0.097901
C	1.713268	-1.754848	0.431195
C	3.032977	-2.089033	0.519735

H	-3.194400	-1.957503	-3.264322
H	-3.615918	-3.448004	-4.135520
H	-0.744698	-4.688323	-4.162275
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H	-0.853648	-5.546107	-2.606747
H	-4.846545	3.711589	-1.628716
H	-3.800078	2.797765	-0.518542
H	-4.775244	1.932962	-1.720830
H	-4.233710	3.857559	-4.124601
H	-4.169321	2.092994	-4.212308
H	-2.761440	3.055973	-4.722049
H	4.613601	4.058442	1.196268
H	3.652746	3.119957	0.031283
H	4.720775	2.278968	1.168438
H	4.038208	3.955755	3.693498
H	4.110199	2.189661	3.668776
H	2.637913	3.006345	4.246375
C	-0.016436	-0.044827	-0.474187
H	4.772624	-2.604574	0.173750
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**1-CO<sub>2</sub>Et-b-oo-radical**  
Structure



Coordinates

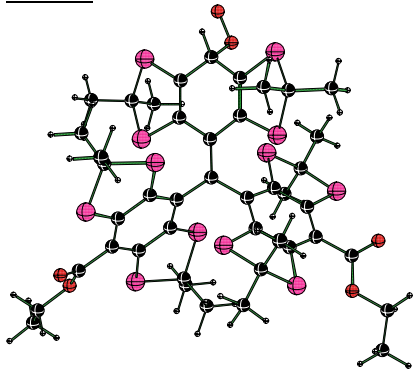
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C	-1.833801	-1.300283	0.521854
C	-0.766659	-1.223534	-0.410472
C	-0.509385	-2.362738	-1.217673
S	-0.859658	-4.914834	-2.115489
S	0.790878	-2.487201	-2.440141
S	-3.980902	-2.384426	1.788485
S	-2.227347	-0.028106	1.714127
C	-3.173540	-1.119431	2.862878
C	0.865303	-4.326726	-2.457664
C	1.274266	-4.783320	-3.864042
C	1.832981	-4.867249	-1.397480
C	-2.250644	-1.785820	3.889994
C	-4.255466	-0.280936	3.554185
C	1.581419	-0.087977	-0.185705
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C	3.418353	-1.378985	0.823924
C	4.382540	-0.613001	0.143846

C	4.132357	-1.123633	0.204111	C	3.949438	0.469820	-0.639649
C	3.650000	0.024636	-0.623128	C	2.571418	0.747172	-0.773572
C	2.334774	0.373146	-0.667195	C	-0.635672	1.372631	-0.229076
C	-0.390155	1.414360	0.008470	C	-1.807449	1.743206	-0.949014
C	-1.311969	2.043144	-0.862070	C	-2.464236	2.962472	-0.697190
C	-1.676725	3.392778	-0.699890	C	-1.987133	3.835492	0.297640
C	-1.115317	4.158387	0.344889	C	-0.881736	3.446046	1.074385
C	-0.194603	3.547568	1.223847	C	-0.199321	2.237497	0.806149
C	0.162961	2.196411	1.055701	S	5.068622	1.565334	-1.485294
S	4.808247	1.026627	-1.516380	S	2.236147	2.288852	-1.600105
S	1.975667	1.822651	-1.650090	C	3.781339	2.290917	-2.601588
C	3.528224	1.732298	-2.660209	C	3.611274	1.445238	-3.868718
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C	3.938725	3.146578	-3.078652	S	3.875422	-2.718158	1.900047
S	3.452695	-3.629696	1.276901	S	0.996719	-2.198134	1.646349
S	0.604194	-2.939345	1.181863	C	2.305047	-2.653966	2.870295
C	1.895664	-3.710528	2.273645	C	2.396473	-1.618642	3.997383
C	2.043303	-2.923422	3.578569	C	1.997521	-4.050923	3.420545
C	1.524975	-5.173110	2.530691	S	1.064379	1.842420	1.999794
S	1.219282	1.519568	2.313650	S	-0.336888	4.399758	2.470180
S	0.517513	4.384036	2.619194	C	1.304526	3.562246	2.633247
C	1.881295	3.149998	2.881052	C	2.377835	4.307163	1.831027
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C	2.194273	3.069101	4.379383	S	-2.560981	0.754064	-2.230390
S	-1.967557	1.233778	-2.296988	S	-3.911785	3.299581	-1.678101
S	-2.839708	4.020567	-1.893114	C	-4.231783	1.530330	-2.113974
C	-3.429598	2.352998	-2.454542	C	-5.096389	0.848374	-1.047959
C	-4.586417	1.864370	-1.574700	C	-4.894816	1.469901	-3.495209
C	-3.842311	2.439430	-3.927476	C	-3.398741	-4.671805	-0.420886
C	-4.602511	-3.649940	-0.550794	O	-3.186013	-5.656955	-1.106752
O	-4.717407	-4.388438	-1.515362	O	-4.554514	-4.502722	0.249487
O	-5.571535	-3.526174	0.375803	C	-5.519285	-5.576466	0.136898
C	-6.759337	-4.327315	0.167459	C	-6.747153	-5.177051	0.932535
C	-7.721724	-4.025808	1.300145	C	5.812146	-1.002796	0.290033
C	5.381358	-1.815025	-0.383945	O	6.180054	-2.131886	0.557755
O	5.334867	-2.884130	-0.948652	O	6.664601	0.025161	0.124186
O	6.478976	-1.072834	-0.229128	C	8.075532	-0.295761	0.209068
C	7.702026	-1.617286	-0.790147	C	8.850270	0.999313	0.060967
C	8.831514	-0.682832	-0.404777	C	-2.637071	5.140452	0.602618
C	-1.467898	5.580256	0.594303	O	-2.608936	5.677163	1.694918
O	-1.308414	6.141308	1.663992	O	-3.234411	5.690272	-0.470269
O	-1.962352	6.206278	-0.490634	C	-3.925097	6.944003	-0.244522
C	-2.367676	7.583827	-0.300097	C	-4.465822	7.415732	-1.580393
C	-2.902296	8.093163	-1.624662	H	2.286588	-4.432120	-4.096034
H	0.536647	-3.497036	-4.976913	H	0.586904	-4.404140	-4.624279
H	-1.124688	-2.871899	-5.111814	H	1.285910	-5.878334	-3.915072
H	-0.822342	-4.624014	-5.066985	H	2.852540	-4.519156	-1.601100
H	1.319122	-4.602783	-2.807910	H	1.829810	-5.964072	-1.409877
H	-0.054036	-5.735394	-2.879112	H	1.553136	-4.530516	-0.396124
H	0.210264	-4.738571	-1.430958	H	-1.752545	-1.022888	4.499839
H	-1.953191	-1.190347	4.796198	H	-1.482478	-2.385160	3.395848
H	-1.992180	-2.420623	3.517938	H	-2.832821	-2.440201	4.549994
H	-3.291504	-2.365767	4.730004	H	-4.851295	-0.913244	4.222811
H	-4.964888	-0.413549	4.709320	H	-4.923694	0.189366	2.828761
H	-4.845167	0.843812	3.455820	H	-3.793291	0.503005	4.164830
H	-3.633295	0.749508	4.754343	H	2.822600	1.867115	-4.501125
H	2.542056	1.213918	-4.516644	H	3.333366	0.417158	-3.622429
H	3.049626	-0.193217	-3.562403	H	4.550117	1.427136	-4.434717
H	4.263009	0.752724	-4.452136	H	3.389865	4.194071	-3.563623
H	3.170407	3.583062	-3.726858	H	5.102505	3.759912	-3.491173
H	4.873767	3.114664	-3.649736	H	4.277473	4.339378	-2.026505
H	4.077433	3.797585	-2.212026	H	1.449927	-1.573801	4.548453
H	1.097084	-2.935827	4.132447	H	2.607798	-0.621097	3.602985
H	2.316103	-1.882906	3.383957	H	3.196841	-1.892893	4.694953
H	2.824180	-3.373471	4.202788	H	1.048445	-4.043449	3.968924
H	0.576990	-5.230854	3.077892	H	2.781544	-4.357134	4.122778
H	2.292917	-5.651577	3.149328	H	1.934846	-4.792900	2.620673
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H	3.502683	4.509465	2.404065	H	2.130116	4.336506	0.767266
H	2.898510	3.596421	1.003723	H	3.348845	3.810178	1.940543



H	3.912834	2.784243	2.209376
H	2.559729	4.038279	4.738362
H	2.983864	2.330882	4.560800
H	1.310611	2.791507	4.959374
H	-5.434745	2.554900	-1.652900
H	-4.287911	1.801315	-0.524674
H	-4.911952	0.869319	-1.899258
H	-4.686379	3.129447	-4.041486
H	-4.169199	1.456213	-4.284668
H	-3.017892	2.786092	-4.555498
H	-6.466806	-5.381604	0.142608
H	-7.179446	-4.076586	-0.811497
H	-7.996663	-2.966502	1.309719
H	-7.277715	-4.275967	2.268559
H	-8.634138	-4.618888	1.173624
H	7.576444	-1.695265	-1.874610
H	7.841267	-2.625901	-0.390967
H	9.776946	-1.064515	-0.805524
H	8.920762	-0.609384	0.683370
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H	-1.499068	8.154194	0.042930
H	-3.121954	7.618050	0.492163
H	-2.137014	8.033460	-2.404849
H	-3.207033	9.140198	-1.519127
H	-3.770754	7.510659	-1.946984
O	4.538252	-0.475751	1.544845
O	5.310730	-1.256379	2.268085

**2-CO<sub>2</sub>Et-a-oo-radical**  
Structure

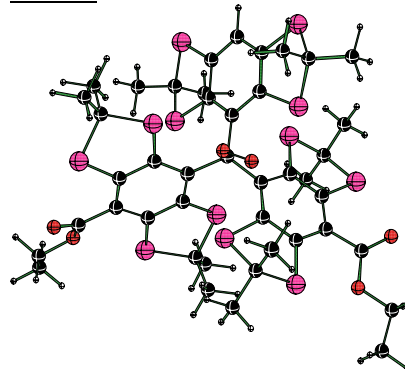


Coordinates

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C	2.776375	-2.049425	0.740119
C	1.557222	-1.357402	0.839180
C	1.265647	-0.250093	0.004726
C	2.232535	0.111965	-0.967223
C	-0.030824	0.480887	0.060686
S	4.581565	-0.007580	-2.321834
S	2.001038	1.444421	-2.120041
S	3.002717	-3.384297	1.899555
S	0.431493	-1.951403	2.079697
C	1.731327	-2.777198	3.103897
C	3.293384	0.881007	-3.320126
C	2.686504	-0.057725	-4.369841
C	3.934061	2.110390	-3.974257
C	2.353925	-1.786003	4.094139
C	1.112405	-3.977961	3.826829
C	-0.066285	1.868370	0.096527
C	1.014049	2.666964	0.704334
C	1.002460	4.025604	0.705574
C	-1.156458	4.015241	-0.505609
C	-1.184460	2.655042	-0.450291
C	-1.283254	-0.331565	0.076199

H	1.792865	4.497671	4.526984
H	2.635314	2.969223	4.244159
H	0.913393	2.961487	4.697667
H	-6.069751	1.349015	-0.978315
H	-4.614899	0.880101	-0.067513
H	-5.260874	-0.202735	-1.311964
H	-5.873142	1.963503	-3.463607
H	-5.060918	0.426773	-3.787543
H	-4.279431	1.954715	-4.256991
H	-5.061886	-6.496090	0.514847
H	-5.744045	-5.729143	-0.923130
H	-7.177136	-4.246903	0.547992
H	-6.501293	-5.032896	1.989055
H	-7.504538	-5.965101	0.857723
H	8.315465	-1.015659	-0.579773
H	8.260277	-0.781938	1.171512
H	9.924152	0.794442	0.131493
H	8.581690	1.707774	0.850828
H	8.650761	1.469105	-0.906979
H	-3.215605	7.654317	0.190198
H	-4.720148	6.775280	0.488794
H	-3.654546	7.563925	-2.299931
H	-4.989298	8.369054	-1.448505
H	-5.169400	6.689363	-1.998346
C	0.085440	0.068283	-0.614876
O	0.225480	0.038442	-2.142665
O	0.123751	1.186626	-2.795544

**2-CO<sub>2</sub>Et-b-oo-radical**  
Structure



Coordinates

C	-3.480814	-0.260456	0.970420
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C	-2.978009	-1.840396	-0.798578
C	-1.714110	-1.241324	-0.961520
C	-1.334043	-0.100725	-0.209471
C	-2.214091	0.341311	0.807755
S	-4.527556	0.403995	2.246009
S	-1.840842	1.602731	2.020534
S	-3.324663	-3.244636	-1.836098
S	-0.628175	-2.103328	-2.085439
C	-1.978262	-2.897857	-3.061648
C	-3.128579	1.081265	3.244019
C	-2.574653	0.020429	4.202664
C	-3.610798	2.321722	4.004990
C	-2.483565	-1.970959	-4.172978
C	-1.464346	-4.225465	-3.628688
C	0.119039	2.080331	-0.046486
C	-0.757164	3.096499	-0.535542
C	-0.535797	4.451879	-0.214106
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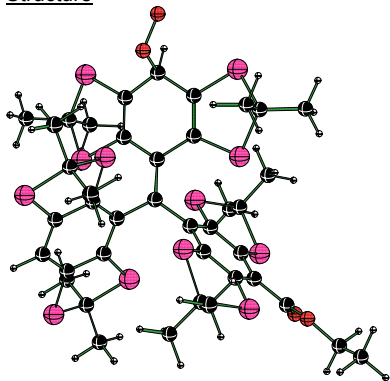
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H	-7.183016	-3.759016	-0.134849
H	-6.099579	-5.125812	0.150574
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### 3-CO<sub>2</sub>Et-a-oo-radical

Structure



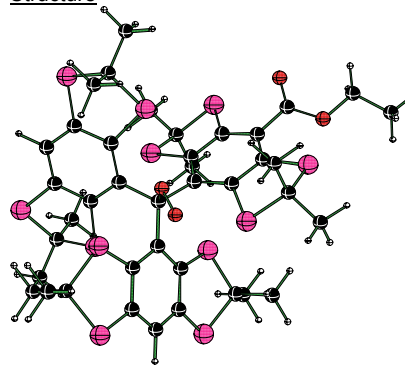
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C	-0.430842	0.113148	0.060878
S	-3.632206	3.453484	-2.365095
S	-2.646215	0.672799	-2.130426
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S	0.916294	2.396360	1.926030
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C	-1.330006	-0.941985	0.136924
C	-2.671051	-0.785911	0.729812
C	-3.591154	-1.785418	0.723213
C	-3.392837	-3.060149	-0.010182
C	-1.977991	-3.270850	-0.415532
C	-1.026356	-2.298838	-0.350103
C	1.043319	-0.114723	0.090951
C	1.906638	0.378132	-0.912892
C	3.302336	0.234400	-0.820038
C	3.873357	-0.409288	0.299240
C	3.024840	-0.902539	1.314316
C	1.628302	-0.769343	1.202376
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S	0.551634	-2.766072	-1.047271
C	-0.116007	-4.157838	-2.083442
S	-5.105276	-1.558972	1.598357
S	-3.139650	0.649223	1.691535
C	-4.431922	-0.225859	2.705320
S	0.678910	-1.336382	2.593892
S	3.629726	-1.645178	2.808320
S	1.296236	1.072804	-2.425546
S	4.233321	0.888514	-2.188827

H	-0.510032	-3.725280	3.793205
H	1.101378	-3.079109	4.189153
H	-7.390718	-3.136119	-0.539018
H	-7.046532	-3.634488	1.121330
H	-5.931944	-5.738113	0.259434
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H	-7.616749	-5.638106	-0.293599
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H	6.038030	-5.066117	-0.139737
H	6.581482	-4.078541	2.735089
H	7.262082	-5.551414	2.012844
H	5.514011	-5.430659	2.305754
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### 3-CO<sub>2</sub>Et-b-oo-radical

Structure

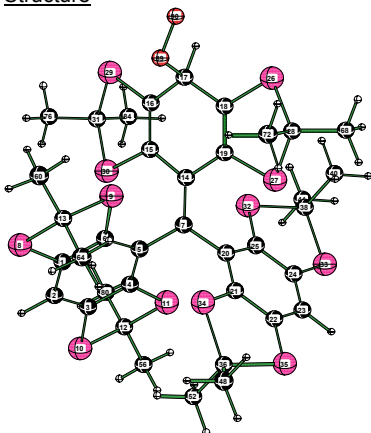


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C	-1.002107	0.034727	-0.166088
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C	2.412950	-1.672907	-1.070147
S	4.592560	2.180519	2.002690
S	2.911578	-0.220632	1.704887
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C	1.903364	-3.839917	2.729143	S	3.199685	-0.588723	-2.251662
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H	0.948797	-4.292135	3.023376	C	4.864880	-1.408825	-2.216747
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C	1.905025	-2.415608	4.822284	C	5.509291	-1.253412	-3.598441
H	0.951107	-2.855135	5.136382	S	-0.543935	-2.162699	1.779375
H	2.706811	-3.025378	5.254885	S	0.959591	-4.688726	2.024705
H	1.977430	-1.403201	5.226855	C	-0.733619	-3.960870	2.202316
C	2.999636	2.085996	-4.352752	C	-1.722605	-4.647144	1.254472
H	2.187329	2.701378	-4.756393	C	-1.186806	-4.071132	3.661964
H	3.944526	2.578722	-4.609466	C	-5.235351	0.877793	0.400676
H	2.972671	1.105897	-4.835492	O	-5.605937	1.957743	0.822451
C	2.898555	3.340983	-2.152405	O	-6.087498	-0.114515	0.082434
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H	2.798143	3.249137	-1.067658	C	-8.274407	-1.057944	-0.156775
H	3.847697	3.844645	-2.371363	H	-0.924548	0.854283	4.752865
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H	1.595643	5.441194	4.010380	H	-2.669093	1.171761	4.929350
H	2.205737	3.792376	4.205553	H	-0.506254	3.374231	4.508477
H	2.567933	4.698316	2.718439	H	-2.238632	3.687462	4.670164
C	-4.531135	1.411780	-4.012508	H	-1.359038	4.297238	3.248649
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H	-1.363463	-2.872204	-3.323359	H	5.603703	0.444374	4.223567
H	0.255063	-3.185824	-3.982123	H	5.661132	-0.469188	2.697601
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C	-5.545130	0.765127	3.055315	H	1.814588	3.362699	-3.647169
H	-6.331321	0.262086	3.630232	H	1.394845	4.965317	-4.290280
H	-5.145789	1.572944	3.679402	H	-1.652370	4.865349	-3.564331
H	-5.988331	1.202010	2.157375	H	-0.594852	6.254830	-3.286238
C	-0.552883	3.689663	3.917262	H	-1.509930	5.553180	-1.929420
H	-0.179677	2.965247	4.650490	H	6.719338	-1.341762	-1.096136
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C	-3.807975	-0.846086	3.958928	H	6.481703	-1.758919	-3.617237
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H	-3.814513	-3.923248	0.511662	H	-1.402724	-4.556182	0.213839
O	-4.248154	-2.974696	-1.268304	H	-2.713194	-4.186590	1.346171
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C	5.338430	-0.576146	0.482801	H	-2.172756	-3.608639	3.786138
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C	7.466700	-0.659451	-0.562060	H	-7.693254	0.524837	1.225656
H	7.840154	0.165185	0.053278	H	-8.015311	-1.883090	0.514035
H	7.692331	-1.593553	-0.038915	H	-8.065829	-1.369914	-1.184644
C	8.039865	-0.634594	-1.965782	H	-9.348530	-0.862759	-0.065356
H	9.129323	-0.739979	-1.919138	C	0.497195	-0.056713	-0.589899
H	7.638905	-1.457140	-2.566264	O	0.399348	0.154879	-2.117139
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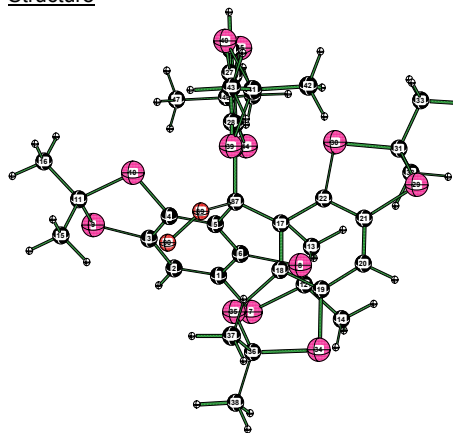
**4-CO<sub>2</sub>Et-a-oo-radical**  
Structure



Coordinates

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C	-2.241215	-3.748673	-0.003101
C	-2.704959	-2.691717	0.779048
C	-2.034805	-1.457962	0.796490
C	-0.848461	-1.265046	0.042622
C	-0.408814	-2.344392	-0.770195
C	-0.113655	0.026943	0.013062
S	-0.430734	-4.866896	-1.786491
S	1.009507	-2.278081	-1.841851
S	-4.185211	-2.819314	1.751418
S	-2.785717	-0.213891	1.820560
C	-3.747594	-1.405896	2.875501
C	0.515679	-3.724655	-2.904899
C	1.266208	0.065792	0.158858
C	2.000911	-0.942499	0.945293
C	3.355886	-0.943055	1.044459
C	4.227396	-0.034014	0.259233
C	3.468879	1.069396	-0.386754
C	2.108916	1.118116	-0.434425
C	-0.914580	1.269818	-0.174467
C	-1.819795	1.437646	-1.248956
C	-2.628584	2.583114	-1.340819
C	-2.563956	3.579719	-0.369381
C	-1.678829	3.435083	0.697275
C	-0.853557	2.301640	0.799159
S	4.398128	2.317385	-1.220756
S	1.453236	2.470394	-1.402222
C	3.012785	2.776601	-2.367369
S	4.132384	-2.084967	2.143104
S	1.179322	-2.122393	2.012287
C	2.611456	-2.338979	3.180637
S	0.128303	2.213588	2.280644
S	-1.619041	4.600161	2.032698
S	-1.927335	0.328336	-2.629197
S	-3.663985	2.719419	-2.774563
C	-3.610105	0.902812	-3.175273
H	-3.200269	4.456713	-0.439292
C	0.026105	4.027688	2.682943
H	-2.768829	-4.697480	-0.012063
C	1.168156	4.794787	2.008197
H	1.079445	5.866363	2.223351
H	2.133414	4.438743	2.387184
H	1.154847	4.651708	0.924980
C	0.054074	4.199632	4.204926
H	1.005140	3.831903	4.607079
H	-0.024581	5.261544	4.465120
H	-0.764328	3.657679	4.684684
C	-3.737632	0.712749	-4.688913

**4-CO<sub>2</sub>Et-b-oo-radical**  
Structure



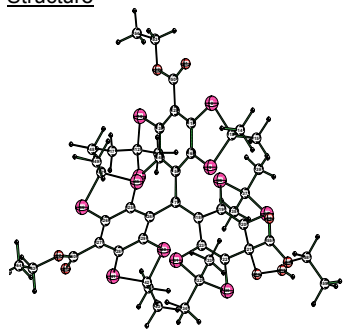
Coordinates

C	2.311790	-2.799370	0.869331
C	3.474851	-2.583928	0.140958
C	3.536414	-1.504838	-0.733307
C	2.429006	-0.658307	-0.909815
C	1.204855	-0.910300	-0.233580
C	1.178635	-1.974098	0.704716
S	2.190601	-4.148376	2.016382
S	-0.160587	-2.379892	1.824385
S	5.033283	-1.095230	-1.592039
S	2.776982	0.770556	-1.922302
C	4.200291	0.007159	-2.834129
C	0.870949	-3.345948	3.034365
C	1.482569	-2.420509	4.091354
C	-0.012381	-4.422611	3.672137
C	3.707701	-0.807684	-4.034499
C	5.165001	1.117006	-3.260750
C	-1.393074	-0.622858	-0.140877
C	-1.882131	-1.816097	-0.753270
C	-3.193191	-2.269778	-0.497572
C	-4.026984	-1.592719	0.380553
C	-3.547302	-0.462709	1.030428
C	-2.250508	0.032391	0.783173
C	0.168616	1.466606	-0.299246
C	1.058820	1.977274	0.686316
C	1.207251	3.369209	0.858863
C	0.503617	4.272328	0.073634
C	-0.386312	3.793089	-0.879254
C	-0.569359	2.410419	-1.074886
S	-4.573404	0.428400	2.170715
S	-1.856163	1.480034	1.757686
C	-3.147473	1.199685	3.062987
C	-2.618814	0.268350	4.159245
C	-3.567651	2.557831	3.632045
S	-3.715342	-3.786114	-1.251735
S	-0.942384	-2.951412	-1.761755
C	-2.403361	-3.760793	-2.561386
C	-2.869414	-2.957350	-3.780593
C	-2.024185	-5.195685	-2.938965
S	-1.775023	2.033885	-2.344141
S	-1.317616	4.904682	-1.899643
C	-2.649786	3.670848	-2.273574
C	-3.729562	3.686726	-1.187049
C	-3.239769	3.962083	-3.657144
S	1.934552	1.023042	1.916826
S	2.227073	3.945534	2.189894
C	3.137169	2.348789	2.407597
C	4.385418	2.310288	1.519093
C	3.494501	2.159785	3.885733

H	-3.677453	-0.352375	-4.940356
H	-4.712253	1.077645	-5.032597
H	-2.951724	1.247116	-5.228182
C	-4.708367	0.153081	-2.413712
H	-4.647208	-0.920440	-2.626766
H	-4.609499	0.292964	-1.333858
H	-5.695033	0.517690	-2.723034
C	-5.029768	-0.721766	3.357007
H	-5.622416	-1.416830	3.962938
H	-4.782748	0.139562	3.988052
H	-5.639348	-0.378433	2.517660
C	1.783243	-4.429932	-3.395587
H	1.517108	-5.307205	-3.996611
H	2.366229	-3.756088	-4.033715
H	2.410121	-4.750521	-2.560352
C	-0.364492	-3.263201	-4.071069
H	0.190477	-2.562227	-4.705557
H	-0.666911	-4.124267	-4.679013
H	-1.264893	-2.759853	-3.708820
C	3.100204	4.263666	-2.719865
H	4.026730	4.466084	-3.269354
H	2.263148	4.545470	-3.368785
H	3.077447	4.891164	-1.825474
C	3.051149	1.894405	-3.619068
H	3.001818	0.834387	-3.356144
H	2.198671	2.130550	-4.266860
H	3.979218	2.069419	-4.176025
C	2.594696	-3.767544	3.730622
H	3.447772	-3.924003	4.401006
H	1.681862	-3.934466	4.314052
H	2.637302	-4.506126	2.926741
C	-2.891410	-1.895446	4.048149
H	-2.613495	-1.049333	4.687505
H	-3.453042	-2.621520	4.647772
H	-1.973887	-2.372208	3.692872
C	2.554647	-1.297807	4.302216
H	1.635341	-1.427833	4.885407
H	3.415828	-1.412230	4.971500
H	2.561704	-0.282549	3.896658
H	5.090183	0.324665	0.827396
O	4.871136	-0.882964	-0.828559
O	6.101677	-0.491070	-1.079911

H	0.688058	-1.915141	4.652868
H	2.111386	-1.655601	3.628879
H	2.095463	-3.000345	4.791677
H	-0.826589	-3.955806	4.238425
H	0.576086	-5.023109	4.375589
H	-0.444644	-5.084554	2.918134
H	3.186815	-0.152764	-4.742206
H	3.012465	-1.590434	-3.722458
H	4.558489	-1.275193	-4.544327
H	4.668198	1.796166	-3.962809
H	6.030880	0.685019	-3.775458
H	5.518282	1.693796	-2.402400
H	-5.031375	-1.954700	0.577343
H	0.627585	5.340893	0.220447
H	-1.747425	0.722488	4.645272
H	-2.313140	-0.695284	3.743286
H	-3.394420	0.094183	4.914622
H	-2.713375	3.042246	4.118328
H	-4.347774	2.423058	4.390156
H	-3.947859	3.219805	2.850131
H	-2.069285	-2.912243	-4.528020
H	-3.133323	-1.933788	-3.501787
H	-3.748572	-3.433272	-4.230905
H	-1.224453	-5.187565	-3.688178
H	-2.886686	-5.706776	-3.381730
H	-1.686741	-5.763903	-2.068731
H	-4.212614	4.670612	-1.149107
H	-3.307850	3.465369	-0.203196
H	-4.492064	2.930520	-1.408074
H	-3.734694	4.940161	-3.657492
H	-3.996273	3.209666	-3.908270
H	-2.468694	3.956479	-4.431449
H	5.072191	3.116526	1.803783
H	4.124316	2.427853	0.464482
H	4.901040	1.350071	1.635792
H	4.188098	2.945342	4.207004
H	3.998421	1.197165	4.030350
H	2.606285	2.193017	4.521182
C	-0.015472	-0.050006	-0.569098
H	4.334018	-3.233820	0.275596
O	-0.194950	-0.028081	-2.112337
O	0.486684	-0.881114	-2.838452

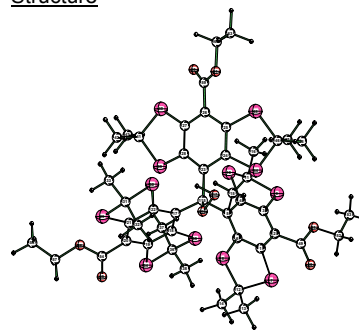
**1-CO<sub>2</sub>Et-a-ooH**  
Structure



Coordinates

C	0.695141	3.467495	-1.236705
C	1.814111	3.881571	-0.478043
C	2.320783	3.013857	0.521537
C	1.758244	1.738090	0.702434
C	0.638223	1.310304	-0.049178
C	0.128442	2.195104	-1.028341
C	0.043971	-0.054063	0.083976
S	-0.031442	4.451576	-2.523707
S	-1.143549	1.714237	-2.168806
S	3.678659	3.410758	1.606307

**1-CO<sub>2</sub>Et-b-ooH**  
Structure



Coordinates

C	-2.239615	-3.088364	-1.188262
C	-3.259011	-2.850372	-0.243783
C	-3.086987	-1.802244	0.687825
C	-1.982945	-0.934605	0.587331
C	-1.029379	-1.073482	-0.454614
C	-1.151762	-2.191721	-1.315405
S	-2.267475	-4.485709	-2.282499
S	-0.021465	-2.590181	-2.642306
S	-4.213448	-1.491244	2.037364
S	-1.897691	0.315401	1.859894

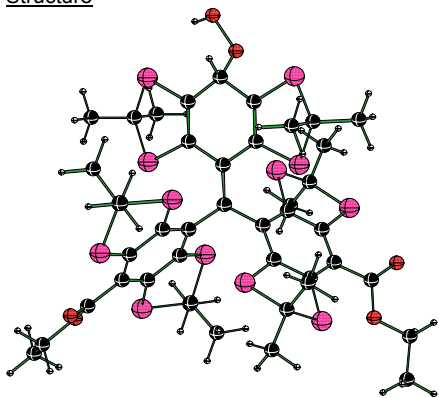
S	2.539143	0.700547	1.914624	C	-3.007943	-0.539624	3.061507
C	3.317526	2.086540	2.853076	C	-0.479444	-4.373253	-2.748925
C	-1.576472	3.428945	-2.697058	C	-0.316112	-4.832368	-4.203566
C	-1.995545	3.409154	-4.171633	C	0.372125	-5.228205	-1.800994
C	-2.692415	3.994694	-1.809390	C	-2.220686	-1.476659	3.985482
C	2.362339	2.615142	3.930899	C	-3.763516	0.521280	3.871795
C	4.637149	1.603617	3.464696	C	1.541915	-0.494382	-0.242361
C	-1.321930	-0.229643	0.260058	C	1.810049	-1.613642	0.573900
C	-2.176446	0.761002	0.930215	C	3.141356	-2.061611	0.770717
C	-3.515043	0.593906	1.108459	C	4.226550	-1.412237	0.159409
C	-4.298264	-0.526321	0.465283	C	3.973441	-0.280962	-0.640953
C	-3.376575	-1.565739	-0.126061	C	2.658090	0.170836	-0.822705
C	-2.027861	-1.434936	-0.201787	C	-0.303764	1.416995	-0.299343
C	0.973459	-1.223000	0.047579	C	-1.448216	2.029215	-0.904852
C	1.918834	-1.414820	-0.986483	C	-1.788132	3.369790	-0.623910
C	2.845327	-2.472725	-0.952539	C	-1.024906	4.133981	0.274378
C	2.849005	-3.376304	0.132050	C	0.016688	3.510103	0.979073
C	1.917208	-3.195799	1.177262	C	0.379749	2.171208	0.699045
C	0.988826	-2.139288	1.130121	S	5.256537	0.636901	-1.473153
S	-4.134570	-2.994437	-0.850961	S	2.556494	1.715040	-1.728971
S	-1.214299	-2.747553	-1.106738	C	4.114447	1.453189	-2.681114
C	-2.733389	-3.291571	-2.029373	C	3.875523	0.560012	-3.903718
C	-2.915485	-2.461206	-3.302829	C	4.694838	2.813514	-3.079592
C	-2.623935	-4.786917	-2.336205	S	3.366900	-3.500055	1.787660
S	-4.385540	1.755351	2.113650	S	0.589204	-2.599946	1.425831
S	-1.484394	2.200899	1.744831	C	1.757208	-3.307626	2.671406
C	-2.865552	2.407112	2.958096	C	1.905554	-2.375033	3.879824
C	-2.597880	1.594410	4.229685	C	1.248765	-4.690816	3.092478
C	-3.048689	3.896051	3.267426	S	1.573727	1.515596	1.857692
S	-0.043414	-1.955128	2.566162	S	0.849962	4.338678	2.311264
S	1.882356	-4.214748	2.630775	C	2.244249	3.133827	2.439509
C	0.184877	-3.689383	3.172175	C	3.437493	3.586794	1.589789
C	-0.883351	-4.614450	2.576213	C	2.642419	2.988223	3.914294
C	0.132509	-3.695301	4.704315	S	-2.600184	1.235049	-2.022782
S	1.917198	-0.432442	-2.462142	S	-3.260361	4.001185	-1.405473
S	3.944211	-2.573856	-2.349677	C	-4.030107	2.333732	-1.630062
C	3.665138	-0.828372	-2.917623	C	-4.788742	1.900503	-0.372515
C	4.639323	0.127576	-2.218988	C	-4.953283	2.370568	-2.853513
C	3.815052	-0.768551	-4.441075	C	-4.485427	-3.685971	-0.326238
C	2.441838	5.175959	-0.841368	O	-4.624595	-4.625905	-1.090065
O	2.049501	5.891381	-1.748648	O	-5.475896	-3.276532	0.490814
O	3.522536	5.489273	-0.100341	C	-6.705012	-4.038544	0.433595
C	4.188903	6.728225	-0.439400	C	-7.685484	-3.402759	1.400530
C	5.369246	6.887494	0.499549	C	5.589755	-1.970646	0.371287
C	-5.162157	0.037820	-0.713915	O	5.811878	-3.135149	0.646919
O	-4.749144	0.843149	-1.512437	O	6.562894	-1.046688	0.257123
O	-6.388008	-0.524747	-0.778705	C	7.920977	-1.531427	0.403928
C	-7.188406	-0.160220	-1.937184	C	8.850596	-0.341362	0.266944
C	-8.500287	-0.913584	-1.842046	C	-1.323186	5.565399	0.561632
C	3.808756	-4.504124	0.248696	O	-1.099051	6.111548	1.625749
O	4.098199	-5.044721	1.301567	O	-1.833420	6.210798	-0.503431
O	4.313199	-4.898133	-0.936711	C	-2.195157	7.598544	-0.296107
C	5.286383	-5.969372	-0.890728	C	-2.699127	8.141781	-1.619292
C	5.690651	-6.283610	-2.318261	H	0.734963	-4.760139	-4.507342
H	-2.902312	2.805958	-4.296420	H	-0.920338	-4.227445	-4.884271
H	-1.206880	2.999079	-4.807369	H	-0.616558	-5.881986	-4.304805
H	-2.225531	4.426313	-4.510041	H	1.430682	-5.161787	-2.079616
H	-3.587249	3.367021	-1.884129	H	0.061725	-6.278819	-1.856979
H	-2.940877	5.015431	-2.125925	H	0.271719	-4.890642	-0.766058
H	-2.383547	4.022263	-0.761142	H	-1.490260	-0.903192	4.568757
H	2.146694	1.827117	4.661983	H	-1.683011	-2.233755	3.410288
H	1.416088	2.941869	3.491162	H	-2.904091	-1.982832	4.678034
H	2.816826	3.465628	4.453317	H	-4.449355	0.036783	4.576642
H	5.127683	2.425238	3.999637	H	-4.338750	1.187202	3.224193
H	5.318840	1.226795	2.698355	H	-3.058762	1.123218	4.456708

H	4.446296	0.803944	4.189412
H	-2.051952	-2.597070	-3.964234
H	-3.005082	-1.396242	-3.071086
H	-3.819786	-2.780687	-3.835203
H	-1.768555	-4.972823	-2.995653
H	-3.524374	-5.131294	-2.858025
H	-2.498645	-5.376588	-1.424624
H	-1.683575	1.953399	4.716948
H	-2.470635	0.533973	3.996848
H	-3.435413	1.697546	4.929999
H	-2.147725	4.293569	3.748891
H	-3.884006	4.037435	3.963158
H	-3.244855	4.472925	2.360392
H	-0.714760	-5.645209	2.911226
H	-0.859969	-4.594216	1.483518
H	-1.881448	-4.298250	2.901356
H	0.292805	-4.712446	5.080571
H	-0.854595	-3.367448	5.050413
H	0.893058	-3.039187	5.134520
H	5.672440	-0.140523	-2.470943
H	4.526183	0.085059	-1.132335
H	4.454665	1.158261	-2.543065
H	4.839057	-1.033294	-4.729092
H	3.624566	0.250257	-4.797295
H	3.122221	-1.451035	-4.939511
H	3.469839	7.547616	-0.342796
H	4.497651	6.680855	-1.488421
H	6.070809	6.054285	0.392180
H	5.038164	6.927537	1.541845
H	5.899343	7.818081	0.268434
H	-6.622172	-0.426612	-2.833982
H	-7.327534	0.924738	-1.933842
H	-9.122593	-0.676580	-2.711724
H	-9.056061	-0.632172	-0.941203
H	-8.330389	-1.994481	-1.823545
H	4.830181	-6.829039	-0.390679
H	6.135414	-5.642540	-0.281948
H	4.824229	-6.594801	-2.910262
H	6.422573	-7.098818	-2.321796
H	6.142112	-5.410814	-2.799708
O	-5.085451	-1.291678	1.397121
O	-6.211299	-0.512946	1.875102
H	-6.852691	-0.704512	1.161631

H	3.183597	1.048470	-4.600025
H	3.446658	-0.403160	-3.615179
H	4.822932	0.377382	-4.424099
H	4.015213	3.327951	-3.768601
H	5.648415	2.673980	-3.601415
H	4.862854	3.450886	-2.207763
H	0.943164	-2.261209	4.391860
H	2.248004	-1.382117	3.575540
H	2.632198	-2.791186	4.587833
H	0.275994	-4.603189	3.589914
H	1.945108	-5.144555	3.807220
H	1.145072	-5.357969	2.233121
H	3.801405	4.557333	1.948739
H	3.160379	3.686133	0.537833
H	4.253606	2.857885	1.658649
H	3.011875	3.946352	4.297865
H	3.453183	2.257553	4.017283
H	1.797330	2.667825	4.528363
H	-5.611237	2.597844	-0.171489
H	-4.130689	1.874527	0.499205
H	-5.205462	0.896346	-0.510860
H	-5.785888	3.061140	-2.675532
H	-5.380648	1.377019	-3.030507
H	-4.417838	2.686974	-3.752174
H	-6.482622	-5.078174	0.693556
H	-7.072534	-4.026100	-0.597133
H	-7.881573	-2.360395	1.130295
H	-7.299202	-3.426966	2.424115
H	-8.633701	-3.950964	1.375101
H	8.103593	-2.290832	-0.362807
H	8.008893	-2.016444	1.380663
H	9.888590	-0.671197	0.384864
H	8.638838	0.411202	1.032996
H	8.746400	0.127339	-0.716361
H	-1.311867	8.134948	0.063219
H	-2.956586	7.645563	0.488806
H	-1.925677	8.071597	-2.390579
H	-2.975764	9.195396	-1.502613
H	-3.578837	7.588486	-1.961583
C	0.111418	-0.033558	-0.706063
O	0.421773	-0.134673	-2.155965
O	-0.161237	0.828583	-3.035933
H	0.573344	1.482280	-3.054614

### 2-CO<sub>2</sub>Et-a-ooH

#### Structure

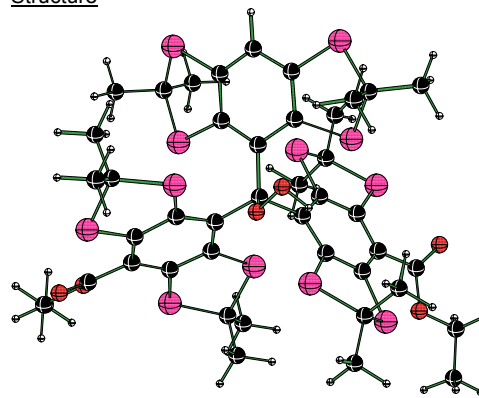


#### Coordinates

C	3.471520	-0.466944	-1.112756
C	3.819286	-1.514523	-0.236984
C	2.891268	-1.919733	0.748324
C	1.637439	-1.292082	0.841205
C	1.281731	-0.221268	-0.014104
C	2.217336	0.163873	-1.006225

### 2-CO<sub>2</sub>Et-b-ooH

#### Structure



#### Coordinates

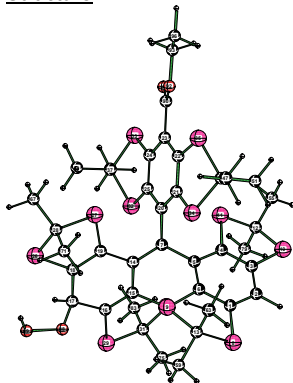
C	-3.087426	-0.301536	1.453221
C	-3.853513	-1.039499	0.536721
C	-3.387977	-1.181850	-0.783901
C	-2.177840	-0.583394	-1.184736
C	-1.351894	0.095791	-0.250381
C	-1.834641	0.230299	1.077613

C	-0.045286	0.453193	0.046970	S	-3.639970	0.004422	3.111512
S	4.556340	0.137126	-2.382502	S	-0.964686	1.052157	2.401105
S	1.901031	1.452612	-2.188683	S	-4.265415	-2.132390	-2.009067
S	3.201541	-3.203664	1.945107	S	-1.770968	-0.835161	-2.913170
S	0.552637	-1.916046	2.103623	C	-3.472627	-1.318153	-3.458443
C	1.903958	-2.635839	3.141430	C	-1.961353	0.358617	3.798890
C	3.214550	0.935589	-3.386713	C	-1.315433	-0.911955	4.363908
C	2.652630	-0.054425	-4.414370	C	-2.091407	1.439002	4.880963
C	3.785070	2.183799	-4.069715	C	-4.269024	-0.078202	-3.885921
C	2.472525	-1.581044	4.097744	C	-3.355328	-2.327415	-4.606846
C	1.360780	-3.849425	3.902642	C	0.324799	2.023777	0.016920
C	-0.143601	1.837298	0.074569	C	-0.619448	3.081874	-0.130128
C	0.905469	2.697660	0.651108	C	-0.296027	4.391641	0.274254
C	0.808933	4.051845	0.673822	C	0.915881	4.671972	0.891645
C	-1.374802	3.916931	-0.491472	C	1.783840	3.625633	1.173101
C	-1.307650	2.561340	-0.467884	C	1.500959	2.305908	0.764591
C	-1.261488	-0.413238	0.082400	C	1.228844	-0.390194	-0.629552
C	-1.491923	-1.441158	-0.860973	C	1.185895	-1.662002	0.000225
C	-2.588033	-2.315633	-0.748537	C	2.323035	-2.502559	0.003044
C	-3.496806	-2.176634	0.322609	C	3.496441	-2.136995	-0.678736
C	-3.283900	-1.154425	1.272981	C	3.511615	-0.939458	-1.411063
C	-2.187262	-0.281238	1.147879	C	2.398789	-0.072780	-1.386979
S	-2.755412	4.672103	-1.304590	S	3.298567	3.913374	2.055502
S	-2.652579	1.729163	-1.314622	S	2.681147	1.111650	1.390448
C	-3.138906	3.186908	-2.353842	C	3.377627	2.195073	2.734236
C	-2.321583	3.228121	-3.648418	C	2.553779	2.078521	4.021248
C	-4.642994	3.127209	-2.632750	C	4.837763	1.796856	2.970097
S	2.058184	4.987221	1.493967	S	-1.522553	5.657552	0.080742
S	2.309985	2.043283	1.551318	S	-2.337483	2.926022	-0.630743
C	2.612832	3.573934	2.563571	C	-2.553535	4.697084	-1.125403
C	1.798250	3.535958	3.860263	C	-2.071878	4.942271	-2.559806
C	4.113525	3.696543	2.842283	C	-4.026989	5.077507	-0.950966
S	-1.968080	0.878473	2.477385	S	2.585006	1.371905	-2.416687
S	-4.309434	-0.935787	2.705292	S	4.894519	-0.468583	-2.418456
C	-3.713491	0.781303	3.087104	C	4.427949	1.316839	-2.552037
C	-4.589019	1.824740	2.382074	C	5.110349	2.147776	-1.459684
C	-3.725123	0.979887	4.607057	C	4.819150	1.823141	-3.947669
S	-0.510083	-1.619943	-2.327052	S	-0.212462	-2.360262	0.870400
S	-2.727074	-3.541188	-2.032409	S	2.177772	-4.049791	0.878801
C	-0.968537	-3.389017	-2.607163	C	0.341364	-4.116817	0.752307
C	-0.056000	-4.323195	-1.803531	C	-0.102190	-4.737502	-0.577986
C	-0.906898	-3.696574	-4.106697	C	-0.222741	-4.892763	1.947194
C	5.163393	-2.128520	-0.391171	C	-5.149393	-1.606497	1.005157
O	6.107022	-1.573404	-0.925168	O	-5.836911	-1.100691	1.871870
O	5.232908	-3.383586	0.094246	O	-5.468567	-2.763359	0.394413
C	6.529370	-4.024411	0.019582	C	-6.742095	-3.348297	0.765010
C	6.384036	-5.420121	0.594713	C	-6.884745	-4.654251	0.007656
C	-4.663741	-3.073682	0.523166	C	4.715034	-2.994720	-0.702553
O	-5.226596	-3.226769	1.592991	O	5.498700	-3.040419	-1.631519
O	-5.064282	-3.688430	-0.606166	O	4.883960	-3.693842	0.436635
C	-6.173551	-4.609893	-0.470258	C	6.020500	-4.591526	0.468734
C	-6.466749	-5.181605	-1.843891	C	6.039383	-5.257194	1.831180
H	1.852432	0.416858	-4.997466	H	-0.315455	-0.685166	4.752955
H	2.242466	-0.940206	-3.922085	H	-1.211412	-1.680522	3.595234
H	3.445688	-0.374451	-5.100956	H	-1.927092	-1.311329	5.182065
H	3.007505	2.683490	-4.659169	H	-1.105240	1.686805	5.290659
H	4.589733	1.899819	-4.758136	H	-2.707746	1.067957	5.708317
H	4.181139	2.892857	-3.339018	H	-2.546264	2.349451	4.483780
H	1.691621	-1.238665	4.786554	H	-3.779842	0.412499	-4.736299
H	2.848610	-0.713831	3.548146	H	-4.346316	0.642113	-3.066138
H	3.296117	-2.008164	4.682401	H	-5.283392	-0.365026	-4.187542
H	2.157911	-4.306812	4.500341	H	-4.352621	-2.639697	-4.937973
H	0.957012	-4.602009	3.220872	H	-2.791863	-3.213462	-4.304601
H	0.567875	-3.537962	4.592174	H	-2.851675	-1.867475	-5.464814
H	-2.516638	2.325233	-4.238558	H	1.154823	5.683686	1.204422
H	-1.249884	3.273906	-3.436740	H	2.566787	1.042992	4.381286
H	-2.598590	4.105579	-4.245433	H	1.514599	2.371745	3.852190
H	-4.879307	2.230185	-3.216159	H	2.975424	2.727111	4.798371
H	-4.953272	3.996792	-3.223538	H	4.893164	0.760012	3.320944
H	-5.222820	3.105360	-1.706727	H	5.279282	2.432810	3.746158



H	2.102911	2.675960	4.468502
H	0.728757	3.445209	3.651584
H	1.963501	4.452625	4.439174
H	4.455801	2.845689	3.442641
H	4.316799	4.608185	3.416139
H	4.691384	3.726070	1.915619
H	-5.627102	1.736290	2.724779
H	-4.566771	1.691002	1.297393
H	-4.229959	2.835777	2.608777
H	-4.749823	0.897943	4.987818
H	-3.358068	1.981127	4.861192
H	-3.103207	0.237356	5.112810
H	-0.364717	-5.365292	-1.949425
H	-0.097419	-4.096932	-0.734620
H	0.982855	-4.214988	-2.136141
H	-1.213860	-4.732577	-4.290930
H	0.121100	-3.588042	-4.471182
H	-1.556595	-3.030755	-4.680171
H	7.250017	-3.418861	0.578248
H	6.847958	-4.038385	-1.027165
H	5.649881	-6.001956	0.028591
H	6.061887	-5.381579	1.639752
H	7.347470	-5.939494	0.547348
H	-7.027263	-4.063271	-0.058229
H	-5.895634	-5.385081	0.250736
H	-6.725475	-4.387503	-2.551301
H	-7.311740	-5.875964	-1.779672
H	-5.601478	-5.724963	-2.235660
C	-0.326380	4.825245	0.080955
H	-0.762050	5.494608	0.834302
O	0.263107	5.687209	-0.928645
O	-0.566301	6.869976	-1.049730
H	-1.127570	6.615706	-1.808970

**3-CO<sub>2</sub>Et-a-ooH**  
Structure

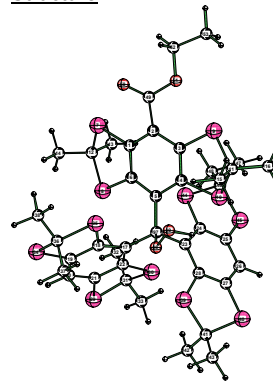


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C	0.722282	-3.909134	0.685694
C	0.299235	-2.574941	0.801240
C	0.847186	-1.564500	-0.029386
C	1.787275	-1.969793	-1.013685
C	0.424204	-0.139698	0.042583
S	3.417049	-3.693707	-2.343871
S	2.531125	-0.870783	-2.199051
S	-0.039718	-5.092659	1.767886
S	-0.939452	-2.288502	2.043481
C	-0.576827	-3.828748	3.019934
C	3.058493	-2.200750	-3.389332
C	1.359967	0.883993	0.081517
C	2.706893	0.707304	0.654838
C	3.628597	1.703878	0.675648

H	5.433014	1.890552	2.058637
H	-2.690099	4.372820	-3.264739
H	-1.031493	4.633888	-2.687725
H	-2.155731	6.007037	-2.807276
H	-4.651313	4.487187	-1.631623
H	-4.173853	6.134287	-1.201905
H	-4.365956	4.908072	0.073868
H	6.200700	2.080664	-1.561169
H	4.827563	1.799002	-0.464445
H	4.815698	3.200404	-1.547057
H	5.906645	1.769542	-4.077018
H	4.524742	2.872773	-4.064158
H	4.342461	1.235541	-4.735990
H	0.258056	-5.770706	-0.649548
H	0.293167	-4.174584	-1.427870
H	-1.196107	-4.739073	-0.647838
H	0.114389	-5.935193	1.910173
H	-1.318170	-4.898752	1.910486
H	0.096185	-4.454591	2.896407
H	-7.536112	-2.636564	0.518052
H	-6.750862	-3.494449	1.849196
H	-6.070008	-5.341545	0.256432
H	-6.876261	-4.485415	-1.073448
H	-7.833248	-5.132385	0.275769
H	6.926318	-4.007555	0.279830
H	5.915515	-5.315916	-0.345095
H	6.126950	-4.512837	2.628898
H	6.896563	-5.936302	1.896874
H	5.125661	-5.835789	1.997863
C	0.042196	0.651789	-0.668390
O	0.098343	0.798343	-2.127066
O	-0.490852	1.973258	-2.705846
H	-1.338673	1.589847	-3.019072

**3-CO<sub>2</sub>Et-b-ooH**  
Structure



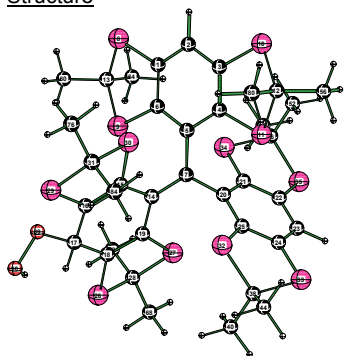
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C	-3.779939	0.444352	-0.045718
C	-3.242267	-0.695615	-0.673531
C	-1.847411	-0.862742	-0.760237
C	-0.946432	0.121290	-0.271208
C	-1.499923	1.173676	0.500000
S	-3.487848	2.751646	1.495997
S	-0.570469	2.325183	1.506726
S	-4.251455	-1.993008	-1.361244
S	-1.361190	-2.482031	-1.376352
C	-2.898898	-2.762254	-2.361784
C	-1.991477	2.848971	2.571691
C	-2.133968	1.931627	3.792205
C	-1.770394	4.306550	2.992296
C	-2.814251	-2.112946	-3.748548
C	-3.147974	-4.270859	-2.464836

C	3.419216	3.056909	0.073175	C	1.436869	1.264139	-0.254838
C	2.028298	3.210309	-0.468322	C	1.184800	2.481552	-0.961587
C	1.084293	2.235165	-0.440855	C	1.945612	3.635518	-0.694576
C	-1.041865	0.141797	0.083222	C	2.986711	3.610012	0.222864
C	-1.942598	-0.373400	-0.876849	C	3.273659	2.425149	0.887127
C	-3.331717	-0.188179	-0.759618	C	2.518319	1.253648	0.664742
C	-3.860307	0.522058	0.339822	C	1.170182	-1.352075	-0.176867
C	-2.975329	1.043059	1.308341	C	0.746543	-2.057917	0.983749
C	-1.585613	0.867342	1.171892	C	1.296478	-3.317799	1.293754
S	1.623166	4.744221	-1.258322	C	2.249776	-3.906552	0.473364
S	-0.456865	2.662222	-1.253578	C	2.700400	-3.216554	-0.645972
C	0.263660	4.016878	-2.295976	C	2.192043	-1.943884	-0.970403
S	5.164321	1.432499	1.498838	S	4.648863	2.333917	2.004948
S	3.189626	-0.764365	1.557542	S	3.101030	-0.136983	1.627933
C	4.505983	0.069482	2.573919	C	3.992311	0.862572	2.912368
S	-0.591964	1.481689	2.511847	C	3.032680	1.291323	4.027805
S	-3.525383	1.876013	2.776243	C	5.154320	0.027622	3.457630
S	-1.388744	-1.153622	-2.369993	S	1.472377	5.152030	-1.479604
S	-4.312387	-0.879556	-2.074560	S	-0.139511	2.755619	-2.124260
C	-2.988585	-2.023769	-2.695902	C	0.508088	4.341356	-2.836319
C	-1.879040	2.641847	3.167157	C	1.414019	4.051551	-4.039406
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C	-1.754655	4.017277	2.500619	S	2.934417	-1.223768	-2.431693
H	-2.546177	4.683166	2.865192	S	3.905036	-3.928193	-1.734514
H	-0.782731	4.466204	2.737013	C	4.454136	-2.298891	-2.421505
H	-1.838389	3.938159	1.413621	C	5.548321	-1.680447	-1.544436
C	-1.732155	2.744399	4.689549	C	4.929052	-2.484764	-3.865882
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H	-2.506038	3.405036	5.097563	S	0.824936	-4.082566	2.821527
H	-1.819618	1.765614	5.167458	C	-0.700917	-3.060182	3.064558
C	-3.163987	-2.211797	-4.206040	C	-1.916325	-3.737398	2.422017
H	-2.378564	-2.868241	-4.598014	C	-0.920573	-2.820442	4.562196
H	-4.127675	-2.689849	-4.416395	C	-5.236548	0.747445	0.003791
H	-3.122934	-1.257146	-4.736429	O	-5.688450	1.872044	0.114449
C	-3.041697	-3.363144	-1.951537	O	-6.013772	-0.350364	-0.061108
H	-2.246536	-4.027020	-2.310143	C	-7.443919	-0.116924	-0.072447
H	-2.911615	-3.224598	-0.874896	C	-8.129489	-1.468488	-0.123187
H	-4.009090	-3.850128	-2.123583	H	-1.225712	1.971519	4.405236
C	-1.863880	-4.300632	3.701597	H	-2.296987	0.894151	3.488038
H	-1.675199	-5.221913	4.264720	H	-2.984971	2.250219	4.406292
H	-2.212079	-3.543033	4.412834	H	-0.873835	4.389809	3.617517
H	-2.656906	-4.489126	2.973986	H	-2.621456	4.659095	3.586790
C	4.342758	-1.752214	-4.092542	H	-1.653022	4.958507	2.123304
H	4.690150	-2.534769	-4.777124	H	-2.019081	-2.584244	-4.339855
H	4.150818	-0.852888	-4.688996	H	-2.607148	-1.042168	-3.675786
H	5.136068	-1.533031	-3.374181	H	-3.762840	-2.246773	-4.281484
C	1.940637	-2.504311	-4.392507	H	-2.339641	-4.749731	-3.029216
H	1.708065	-1.607335	-4.978709	H	-4.083596	-4.460375	-3.003401
H	2.254145	-3.301209	-5.077428	H	-3.212077	-4.736267	-1.478091
H	1.029802	-2.824813	-3.880010	H	3.569123	4.504710	0.420387
C	-0.808916	5.076549	-2.559715	H	2.657786	-4.882823	0.716547
H	-0.391692	5.897024	-3.154899	H	2.617571	0.406905	4.524894
H	-1.633516	4.638502	-3.133343	H	2.201887	1.879128	3.628138
H	-1.208516	5.485116	-1.628309	H	3.564906	1.897765	4.770363
C	0.837259	3.452282	-3.599007	H	4.770802	-0.871276	3.953673
H	1.607099	2.702395	-3.397974	H	5.714433	0.603897	4.203124
H	0.038365	2.977619	-4.180378	H	5.838300	-0.274930	2.660814
H	1.279393	4.256576	-4.199617	H	0.843994	3.539092	-4.823071
C	5.619535	-0.939120	2.868884	H	2.253568	3.412346	-3.754002
H	6.418860	-0.460145	3.446373	H	1.812135	4.988375	-4.447489
H	5.227724	-1.766765	3.471419	H	-1.276766	4.734628	-4.001239
H	6.044527	-1.346347	1.948411	H	-0.319843	6.177465	-3.641455
C	0.539121	-3.567822	4.037308	H	-1.320952	5.436930	-2.367870
H	0.220106	-2.801585	4.753431	H	6.430050	-2.332058	-1.522175
H	0.772103	-4.488274	4.585679	H	5.197420	-1.530082	-0.520005
H	1.448635	-3.216573	3.542733	H	5.842925	-0.704745	-1.948727
C	3.909439	0.645652	3.861747	H	5.819168	-3.124075	-3.892548
H	3.488736	-0.161814	4.472836	H	5.206319	-1.515791	-4.296826
H	4.684726	1.159317	4.442973	H	4.152694	-2.935547	-4.489146
H	3.110484	1.358622	3.640569	H	-2.099122	-4.707789	2.899244

H	3.637754	3.839041	0.811762
O	4.427664	3.192872	-0.964933
O	4.740591	4.601170	-1.107898
C	-5.315839	0.732545	0.550330
O	-5.817090	0.972845	1.634480
O	-6.034079	0.661513	-0.586835
C	-7.466584	0.823167	-0.446380
H	-7.843512	0.031462	0.208874
H	-7.658549	1.781476	0.045493
C	-8.074294	0.758201	-1.834245
H	-9.159782	0.889761	-1.766179
H	-7.670261	1.548153	-2.475109
H	-7.871790	-0.207473	-2.307394
H	4.134908	4.844814	-1.836022

**4-CO<sub>2</sub>Et-a-ooH**  
Structure

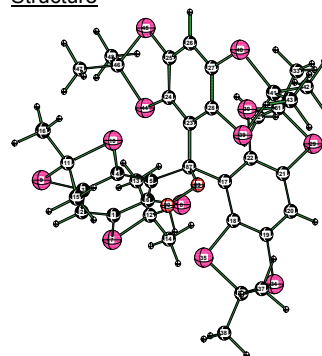


Coordinates

C	-1.500705	-3.416507	-0.842376
C	-2.620773	-3.511357	-0.022342
C	-2.942579	-2.443589	0.814757
C	-2.150437	-1.284527	0.843158
C	-0.983440	-1.181920	0.044754
C	-0.688128	-2.268372	-0.820054
C	-0.125274	0.033729	0.022422
S	-1.004321	-4.733213	-1.923539
S	0.686369	-2.301856	-1.949106
S	-4.384699	-2.457957	1.851189
S	-2.725517	-0.010327	1.941055
C	-3.755741	-1.139911	3.000796
C	-0.001211	-3.642076	-3.043622
C	1.253784	-0.061321	0.134615
C	1.916472	-1.155979	0.867288
C	3.266650	-1.258952	0.963814
C	4.231021	-0.335709	0.290918
C	3.522749	0.788373	-0.406590
C	2.173063	0.925839	-0.461713
C	-0.809428	1.351411	-0.124602
C	-1.736826	1.621297	-1.159987
C	-2.438632	2.838040	-1.204290
C	-2.245261	3.808230	-0.223618
C	-1.335374	3.565193	0.803067
C	-0.614759	2.359207	0.856542
S	4.517394	1.956476	-1.296075
S	1.600533	2.293246	-1.472990
C	3.158868	2.434515	-2.469665
S	3.957600	-2.527017	1.977958
S	1.012953	-2.331773	1.875224
C	2.430438	-2.717424	3.016456
S	0.416255	2.160438	2.293856
S	-1.115910	4.697625	2.149609
S	-1.999477	0.553527	-2.552346
S	-3.510137	3.097603	-2.594190
C	-3.636422	1.294085	-3.032198
H	-2.800607	4.740669	-0.255730

H	-1.762109	-3.896672	1.352112
H	-2.807044	-3.110977	2.549053
H	-1.106950	-3.773304	5.070841
H	-1.801668	-2.186969	4.716685
H	-0.054714	-2.338806	5.022468
H	-7.687471	0.504739	-0.939740
H	-7.707479	0.448275	0.826546
H	-7.859917	-2.077010	0.745765
H	-7.851001	-2.016489	-1.028520
H	-9.216118	-1.329093	-0.123171
C	0.567846	0.011918	-0.615962
O	0.782455	0.120169	-2.082921
O	-0.260102	-0.279680	-2.985213
H	-0.136359	-1.250774	-3.014267

**4-CO<sub>2</sub>Et-b-ooH**  
Structure



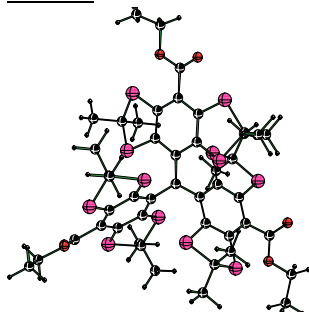
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C	-0.472094	-3.671207	0.553942
C	0.572951	-4.288456	-0.121360
C	1.481433	-3.502769	-0.821433
C	1.317734	-2.108577	-0.899849
C	0.185400	-1.475049	-0.316914
C	-0.667799	-2.274266	0.488560
S	-1.625791	-4.622544	1.511565
S	-1.974909	-1.694495	1.573111
S	2.928699	-4.208763	-1.565081
S	2.707994	-1.271859	-1.646754
C	3.293095	-2.729994	-2.631030
C	-2.058601	-3.220566	2.635793
C	-1.069612	-3.129246	3.802702
C	-3.498901	-3.384628	3.130614
C	2.551077	-2.834217	-3.967003
C	4.805752	-2.609918	-2.836373
C	-1.441126	0.591073	-0.152306
C	-2.611569	0.124215	-0.820278
C	-3.873880	0.683987	-0.563003
C	-4.022642	1.705502	0.366702
C	-2.902917	2.160515	1.047712
C	-1.616352	1.627189	0.800160
C	1.164567	0.905705	-0.205257
C	2.013808	0.607067	0.897142
C	3.123697	1.427289	1.184704
C	3.418385	2.537929	0.405712
C	2.583968	2.860842	-0.657367
C	1.462515	2.068595	-0.970291
S	-3.041162	3.490428	2.212685
S	-0.341609	2.408117	1.780369
C	-1.474179	3.061733	3.097370
C	-1.725718	1.998949	4.172324
C	-0.852633	4.328626	3.691847
S	-5.280758	0.005505	-1.405655
S	-2.702277	-1.274171	-1.940218
C	-4.283174	-0.766283	-2.764491
C	-4.021535	0.242108	-3.887999

C	0.498188	3.970647	2.717777
H	-3.241612	-4.401841	-0.039858
C	1.672621	4.641352	1.996965
H	1.680697	5.716600	2.212174
H	2.619296	4.207397	2.339624
H	1.605612	4.500418	0.915197
C	0.610911	4.119042	4.238092
H	1.541441	3.660714	4.592169
H	0.641204	5.180202	4.511120
H	-0.231027	3.647226	4.750132
C	-3.824784	1.152743	-4.544941
H	-3.883024	0.093170	-4.819211
H	-4.764859	1.624915	-4.852417
H	-3.002088	1.614956	-5.095892
C	-4.777983	0.631401	-2.253531
H	-4.837563	-0.433372	-2.507321
H	-4.624848	0.717484	-1.174425
H	-5.732110	1.107442	-2.508754
C	-4.937984	-0.350234	3.568316
H	-5.569861	-1.005880	4.178572
H	-4.574334	0.455795	4.215755
H	-5.547762	0.086036	2.773493
C	1.161971	-4.447136	-3.629680
H	0.777917	-5.271018	-4.242462
H	1.771928	-3.808462	-4.278828
H	1.799469	-4.858338	-2.843646
C	-0.886354	-3.044107	-4.141818
H	-0.289542	-2.396410	-4.794828
H	-1.327962	-3.844144	-4.747814
H	-1.694525	-2.447082	-3.711304
C	3.345435	3.887341	-2.913293
H	4.278001	3.993711	-3.479483
H	2.522701	4.185412	-3.572924
H	3.373206	4.567786	-2.058542
C	3.126863	1.473866	-3.661741
H	2.994316	0.440715	-3.329625
H	2.291955	1.731755	-4.323468
H	4.061951	1.542310	-4.230896
C	2.306900	-4.167137	3.492529
H	3.147025	-4.421046	4.149386
H	1.384937	-4.296204	4.071304
H	2.293307	-4.864406	2.651503
C	-2.901567	-1.756893	4.113229
H	-2.531059	-0.969636	4.780058
H	-3.499501	-2.464426	4.699810
H	-2.040151	-2.287394	3.698857
C	2.461278	-1.736493	4.192391
H	1.547090	-1.838384	4.789287
H	3.326157	-1.941249	4.834791
H	2.526957	-0.703428	3.840107
H	4.959220	0.048501	1.016630
O	4.990512	-1.161011	-0.635871
O	6.301668	-0.563165	-0.800435
H	6.152629	-0.025399	-1.603356

### 1-CO<sub>2</sub>Et<sup>+</sup> (cation)

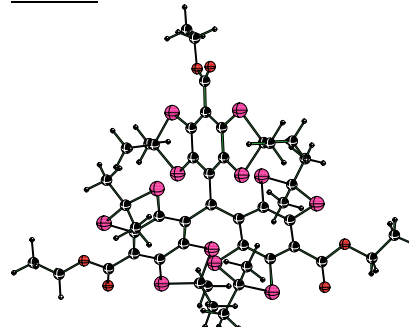
Structure



C	-4.997679	-2.019787	-3.276675
S	0.532783	2.672547	-2.373518
S	2.915690	4.268439	-1.683228
C	1.169634	4.417538	-2.283732
C	0.333427	5.263597	-1.317627
C	1.164116	5.008867	-3.696942
S	1.738758	-0.656795	2.128707
S	4.072861	1.073987	2.640383
C	3.460942	-0.664178	2.823338
C	4.358152	-1.638316	2.052705
C	3.386637	-1.024471	4.310839
H	-1.317204	-2.271041	4.438350
H	-0.045684	-3.003550	3.441817
H	-1.116067	-4.041662	4.409152
H	-3.779498	-2.534789	3.763397
H	-3.585794	-4.292239	3.739300
H	-4.202580	-3.448740	2.297337
H	2.737616	-1.938438	-4.569920
H	1.473645	-2.919019	-3.811327
H	2.897254	-3.714954	-4.520916
H	5.032841	-1.721374	-3.436320
H	5.182156	-3.482769	-3.382143
H	5.335687	-2.536339	-1.883500
H	-4.999292	2.137216	0.562198
H	4.277272	3.160368	0.637443
H	-0.781032	1.731955	4.659861
H	-2.152621	1.091584	3.736865
H	-2.418925	2.384035	4.929655
H	0.103540	4.088901	4.170557
H	-1.513088	4.745565	4.460862
H	-0.680362	5.088787	2.925889
H	-3.421237	-0.222122	-4.679521
H	-3.481978	1.116835	-3.515577
H	-4.971418	0.576433	-4.320957
H	-4.398239	-2.505164	-4.055346
H	-5.959147	-1.744194	-3.724675
H	-5.176908	-2.736510	-2.471745
H	0.741751	6.279289	-1.250655
H	0.320724	4.825298	-0.316139
H	-0.701362	5.324628	-1.675535
H	1.556061	6.032557	-3.680897
H	0.137995	5.054872	-4.080054
H	1.767794	4.410660	-4.383959
H	5.378764	-1.602971	2.452620
H	4.388446	-1.389399	0.989210
H	3.976349	-2.661170	2.151910
H	4.389820	-1.002429	4.752078
H	2.996159	-2.041329	4.433520
H	2.745423	-0.330746	4.859801
C	-0.053335	0.023211	-0.608472
H	0.702779	-5.364823	-0.064820
O	-0.230096	0.255368	-2.073401
O	0.133410	-0.789781	-2.991427
H	-0.771882	-1.129886	-3.169624

### 1-CO<sub>2</sub>Et<sup>-</sup> (anion)

Structure



## Coordinates

C	-2.613483	-2.549845	-1.245242
C	-3.672007	-2.268837	-0.347452
C	-3.535979	-1.220638	0.595493
C	-2.381777	-0.411008	0.598423
C	-1.270607	-0.732244	-0.252259
C	-1.434042	-1.787605	-1.199412
C	-0.000973	-0.032349	-0.122424
S	-2.711662	-3.783520	-2.511104
S	-0.310482	-2.030671	-2.535374
S	-4.775544	-0.799063	1.799394
S	-2.405988	0.948848	1.724444
C	-3.657086	0.217377	2.873220
C	-0.914447	-3.716747	-2.999983
C	-0.807311	-3.882422	-4.520738
C	-0.123573	-4.800912	-2.258459
C	-2.975397	-0.659407	3.929301
C	-4.467123	1.349097	3.514615
C	1.245900	-0.773400	-0.068876
C	1.340587	-2.028367	0.619935
C	2.575074	-2.699463	0.711016
C	3.718379	-2.184458	0.069116
C	3.633863	-0.976225	-0.655862
C	2.429624	-0.254852	-0.690491
C	0.006304	1.418759	0.029644
C	-0.737686	2.246495	-0.868169
C	-0.780442	3.641472	-0.702322
C	-0.103143	4.242647	0.380625
C	0.630996	3.443517	1.284463
C	0.716833	2.050778	1.099475
S	4.996830	-0.275136	-1.554948
S	2.488535	1.260400	-1.606694
C	3.941671	0.780111	-2.654700
C	3.485889	0.002794	-3.893319
C	4.718950	2.044614	-3.033830
S	2.594020	-4.219332	1.627729
S	0.002861	-2.824254	1.457577
C	1.066944	-3.825558	2.601792
C	1.406557	-3.026593	3.864564
C	0.336878	-5.129820	2.939267
S	1.544407	1.164885	2.381833
S	1.414392	4.101578	2.731419
C	2.494585	2.621880	3.028230
C	3.828398	2.759152	2.285514
C	2.702420	2.452724	4.537166
S	-1.454051	1.631988	-2.359309
S	-1.672141	4.541309	-1.945652
C	-2.594565	3.072808	-2.609157
C	-3.909902	2.865527	-1.851529
C	-2.829338	3.267474	-4.110832
C	-4.933495	-3.053103	-0.527116
O	-5.056511	-3.916151	-1.377846
O	-5.918927	-2.695680	0.301312
C	-7.183238	-3.407043	0.147705
C	-8.154245	-2.846496	1.166354
C	4.979426	-2.987383	0.156232
O	4.980716	-4.190922	0.328854
O	6.083226	-2.241079	0.051224
C	7.354542	-2.956894	0.092833
C	8.463305	-1.927963	0.013436
C	-0.154474	5.715206	0.649022
O	0.011580	6.186750	1.757583
O	-0.377406	6.442171	-0.449524
C	-0.470035	7.886848	-0.262590
C	-0.700955	8.511728	-1.622993
H	0.241899	-3.844559	-4.834980
H	-1.365534	-3.108316	-5.052453
H	-1.202134	-4.861175	-4.814710
H	0.933330	-4.768734	-2.547299
H	-0.522652	-5.788639	-2.516399

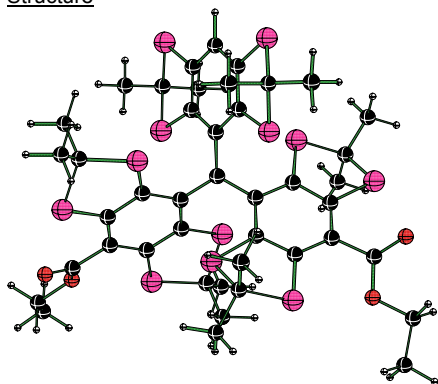
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C	-2.468029	-2.740838	-1.187220
C	-3.605858	-2.491734	-0.374675
C	-3.505018	-1.456260	0.594681
C	-2.345821	-0.681175	0.695162
C	-1.196908	-0.897691	-0.124969
C	-1.313967	-1.957177	-1.069844
C	0.004998	-0.068322	-0.027500
S	-2.460336	-3.977935	-2.469191
S	-0.073202	-2.205439	-2.324107
S	-4.783203	-1.080555	1.790399
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C	-3.664655	-0.194689	2.972459
C	-0.631271	-3.900021	-2.790684
C	-0.381952	-4.122025	-4.286986
C	0.095930	-4.955283	-1.945997
C	-3.047293	-1.187611	3.965868
C	-4.464550	0.892228	3.698130
C	1.326420	-0.680334	-0.017277
C	1.607569	-1.896858	0.674717
C	2.877167	-2.481598	0.682230
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C	3.712838	-0.679726	-0.701636
C	2.439913	-0.102417	-0.702299
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C	5.271578	-2.551551	0.042903
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H	1.176914	-4.906714	-2.124406
H	-0.261194	-5.960122	-2.206723

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### 2-CO<sub>2</sub>Et<sup>+</sup> (cation)

#### Structure



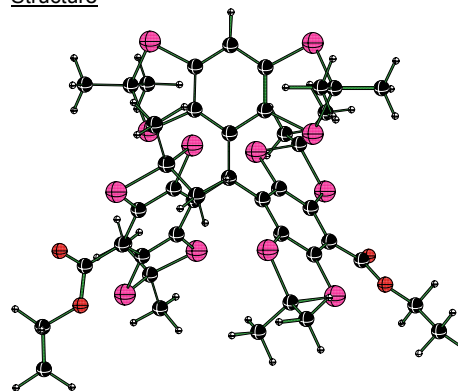
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H	2.391116	-1.809095	3.587239
H	2.713603	-3.278072	4.536813
H	0.080961	-4.788559	3.780588
H	1.694677	-5.516420	3.786480
H	0.696753	-5.585684	2.314558
H	4.295775	3.883387	2.239538
H	3.506779	2.993643	0.915776
H	4.419481	2.105674	2.147040
H	3.381694	3.662697	4.635672
H	3.491745	1.899807	4.524298
H	1.940403	2.665331	4.943561
H	-4.974398	3.359860	-1.535468
H	-3.970593	2.450348	-0.381369
H	-4.770521	1.596192	-1.711365
H	-4.159494	3.674969	-3.952218
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H	-2.578280	3.021272	-4.445462
H	-6.954590	-4.664928	0.029448
H	-7.399007	-3.463171	-1.183230
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H	-7.871446	-3.171900	1.852955
H	-9.125962	-3.545778	0.648358
H	7.634913	-3.060925	-1.052086
H	7.790801	-2.853954	0.693889
H	9.642020	-1.636262	-0.502800
H	8.589880	-0.479496	0.343414
H	8.439320	-0.690546	-1.410222
H	-0.114299	8.240992	-0.123697
H	-1.781243	8.001310	0.404190
H	-0.862985	8.135188	-2.539258
H	-1.702147	9.437874	-1.667199
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### 2-CO<sub>2</sub>Et<sup>-</sup> (anion)

#### Structure



#### Coordinates

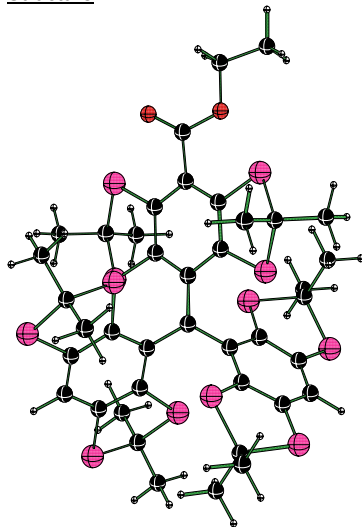
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C	1.537170	-1.282358	0.734346	C	-1.676263	-1.149863	-0.771807
C	1.261527	-0.144763	-0.096454	C	-1.288207	-0.053912	0.063772
C	2.280241	0.289453	-1.008331	C	-2.300077	0.405624	0.964905
C	-0.006981	0.555286	-0.010874	C	0.032917	0.545672	-0.003052
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S	2.072959	1.591872	-2.189002	S	-1.983433	1.704379	2.149158
S	3.065396	-3.202136	1.887712	S	-3.265775	-2.995727	-1.947681
S	0.375715	-2.008537	1.849738	S	-0.558547	-1.825935	-1.988639
C	1.643954	-2.743404	2.984474	C	-1.890247	-2.489081	-3.080887
C	3.414267	1.016429	-3.335687	C	-3.337568	1.212190	3.304171
C	2.860794	0.010839	-4.350966	C	-2.835016	0.172827	4.314903
C	4.031708	2.236233	-4.027834	C	-3.875501	2.459141	4.013933
C	2.070753	-1.725331	4.046886	C	-2.369781	-1.414163	-4.064441
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C	-1.087471	2.697616	-0.745537	C	1.181830	2.634064	0.865965
C	-1.252737	-0.200687	0.120702	C	1.227649	-0.287910	-0.149421
C	-1.562683	-1.265408	-0.777399	C	1.447083	-1.449646	0.652721
C	-2.757032	-1.996042	-0.644646	C	2.591942	-2.246148	0.539893
C	-3.650582	-1.702894	0.408411	C	3.612569	-1.920870	-0.392452
C	-3.347686	-0.670087	1.322384	C	3.417061	-0.773620	-1.203985
C	-2.176884	0.094682	1.167516	C	2.264300	0.008899	-1.083057
S	-2.330519	4.890590	-1.771601	S	2.616178	4.664125	1.966574
S	-2.460469	1.949514	-1.563506	S	2.365485	1.721220	1.837778
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C	-1.943154	3.234356	-3.993098	C	1.737467	3.157956	4.147815
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S	-0.609580	-1.612232	-2.225161	S	0.344290	-1.849243	1.996098
S	-3.052822	-3.228652	-1.887234	S	2.692607	-3.615842	1.683360
C	-1.294527	-3.318128	-2.475355	C	0.896343	-3.603338	2.139731
C	-0.499038	-4.346733	-1.664834	C	0.095213	-4.502715	1.189366
C	-1.286544	-3.646310	-3.972053	C	0.750255	-4.063440	3.594430
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O	5.218646	-3.294132	0.181970	O	-5.404627	-3.054695	-0.220734
C	6.532242	-3.930368	0.183170	C	-6.728568	-3.610668	-0.220806
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C	-4.912606	-2.475048	0.637607	C	4.836617	-2.704350	-0.584711
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O	-5.402036	-3.025065	-0.478078	O	5.123663	-3.536660	0.453839
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H	0.759870	-4.739563	2.859927	H	-1.031029	-4.493606	-3.121225
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### 3-CO<sub>2</sub>Et<sup>+</sup> (cation)

Structure



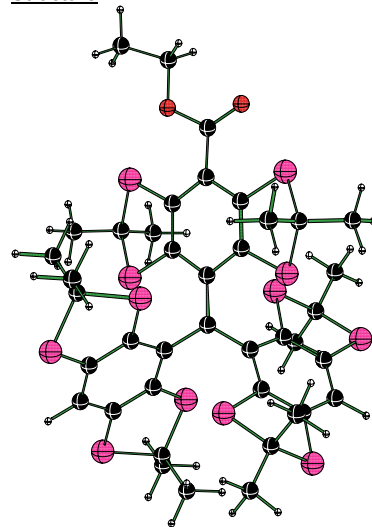
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H	-0.304470	-4.034655	3.893356
H	1.324643	-3.427062	4.272562
H	-7.388819	-2.970730	-0.817301
H	-7.115585	-3.611603	0.803860
H	-5.966136	-5.635950	-0.187372
H	-6.245767	-4.992923	-1.815180
H	-7.626557	-5.481309	-0.804656
H	7.154474	-3.744622	0.105887
H	6.139655	-5.001027	-0.604778
H	6.554778	-4.568355	2.422554
H	7.301969	-5.863225	1.459640
H	5.540040	-5.832601	1.705319

### 3-CO<sub>2</sub>Et<sup>-</sup> (anion)

Structure



Coordinates

C	2.866404	-1.487688	0.868718
C	3.772544	-0.691792	0.120187
C	3.216697	0.349978	-0.670209
C	1.841488	0.580554	-0.694665
C	0.901743	-0.213578	0.043737
C	1.490761	-1.257699	0.830825
C	-0.523171	0.029230	0.009386
S	3.426702	-2.776435	1.970678
S	0.501720	-2.296530	1.896336
S	4.191930	1.374004	-1.770693



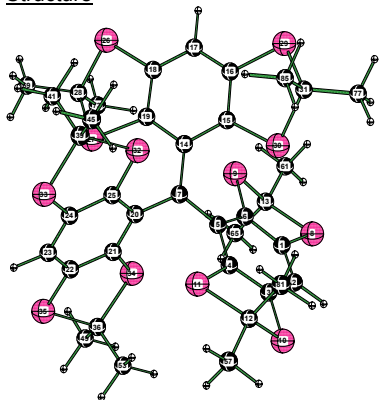
S	-1.204695	-1.963770	-1.793982	S	1.288303	1.887484	-1.780736
C	-2.681057	-1.939106	-2.916078	C	2.774360	1.828154	-2.872894
C	-2.004947	2.641347	3.077182	C	1.893184	-2.767227	3.014751
C	-2.125922	1.615901	4.209681	C	2.035268	-1.752936	4.157634
C	-1.815017	4.062039	3.619638	C	1.650650	-4.180079	3.556175
C	-2.485627	-0.924484	-4.047547	C	2.595540	0.777625	-3.976802
C	-2.914182	-3.352753	-3.459357	C	3.024500	3.217695	-3.467415
C	1.419881	1.137246	-0.037960	C	-1.465089	-1.092125	-0.015338
C	1.079584	2.307136	-0.808191	C	-1.261618	-2.231471	-0.850363
C	1.935267	3.417768	-0.812230	C	-2.154788	-3.312737	-0.867878
C	3.087300	3.433649	-0.023826	C	-3.310256	-3.311322	-0.089758
C	3.436599	2.320249	0.738780	C	-3.553607	-2.198350	0.715595
C	2.652918	1.155479	0.709302	C	-2.661941	-1.119550	0.760206
C	1.111579	-1.355523	0.008538	C	-1.044708	1.408606	0.003335
C	0.673418	-2.334826	0.958419	C	-0.591606	2.392381	0.929837
C	1.239698	-3.619966	0.958831	C	-1.097293	3.700194	0.936508
C	2.197702	-3.973901	0.008690	C	-2.086634	4.097835	0.038201
C	2.621467	-3.044913	-0.943935	C	-2.555230	3.157998	-0.878984
C	2.112928	-1.737258	-0.943732	C	-2.047787	1.851425	-0.906433
S	4.909887	2.292175	1.718944	S	-5.005527	-2.082251	1.744106
S	3.284466	-0.171320	1.687697	S	-3.122219	0.193257	1.877289
C	4.346114	0.889458	2.797380	C	-4.245915	-0.856576	2.917331
C	3.529409	1.404781	3.985408	C	-3.447685	-1.581463	4.007101
C	5.556945	0.068940	3.249271	C	-5.344602	0.023707	3.517795
S	1.469472	4.810837	-1.796418	S	-1.746530	-4.673806	-1.942941
S	-0.336650	2.471846	-1.853796	S	0.117525	-2.373581	-1.973069
C	0.353126	3.840498	-2.918829	C	-0.674053	-3.651536	-3.064095
C	1.138004	3.259937	-4.098321	C	-1.524256	-2.983179	-4.150559
C	-0.804453	4.729220	-3.382662	C	0.417791	-4.537779	-3.669125
S	2.637259	-0.737747	-2.305174	S	-2.625993	0.845238	-2.258287
S	3.726764	-3.490927	-2.248869	S	-3.727567	3.592867	-2.146508
C	4.157219	-1.742033	-2.710512	C	-4.165918	1.833449	-2.561858
C	5.357742	-1.248635	-1.898348	C	-5.307999	1.342843	-1.663612
C	4.413671	-1.660744	-4.218026	C	-4.538346	1.740882	-4.044254
S	-0.415186	-2.005141	2.310421	S	0.531129	2.007435	2.258916
S	0.761294	-4.720339	2.257120	S	-0.514533	4.781938	2.224449
C	-0.788133	-3.792658	2.696974	C	0.998445	3.768989	2.605935
C	-1.971711	-4.284509	1.858972	C	2.167929	4.201721	1.713404
C	-1.053938	-3.928199	4.198905	C	1.342683	3.914146	4.091036
C	-5.182021	0.843137	0.127625	C	5.200384	-0.995088	0.197962
O	-5.632324	1.927184	0.444073	O	5.682978	-2.049319	0.592838
O	-5.930256	-0.218060	-0.190582	O	6.000089	0.039541	-0.195838
C	-7.375114	-0.011100	-0.200970	C	7.407267	-0.238421	-0.232043
C	-8.028036	-1.344539	-0.501143	C	8.108319	1.013073	-0.731449
H	-1.224247	1.628632	4.832951	H	1.122218	-1.735094	4.765904
H	-2.261753	0.603361	3.819150	H	2.200982	-0.746603	3.763371
H	-2.988002	1.859961	4.840647	H	2.883983	-2.019450	4.800951
H	-0.919337	4.113394	4.248830	H	0.737089	-4.203518	4.163092
H	-2.671475	4.336994	4.245175	H	2.484183	-4.488811	4.199565
H	-1.723219	4.792629	2.812538	H	1.548230	-4.902273	2.742320
H	-1.628939	-1.210958	-4.668175	H	1.747643	1.045897	-4.618874
H	-2.308131	0.081214	-3.656451	H	2.397855	-0.207428	-3.545685
H	-3.380034	-0.896427	-4.680166	H	3.501731	0.715053	-4.593272
H	-2.067653	-3.662820	-4.081921	H	2.178677	3.514944	-4.098974
H	-3.808695	-3.365527	-4.091796	H	3.922332	3.206731	-4.098094
H	-3.045437	-4.079131	-2.653718	H	3.154824	3.967689	-2.682993
H	3.720024	4.316376	-0.011207	H	-4.001092	-4.147843	-0.111356
H	2.613912	-4.977106	0.007698	H	-2.480836	5.109061	0.052695
H	3.177352	0.562260	4.591625	H	-2.976775	-0.849470	4.674288
H	2.660021	1.979692	3.654866	H	-2.658007	-2.195451	3.566280
H	4.153582	2.050123	4.613436	H	-4.108698	-2.228044	4.598298
H	5.229530	-0.786919	3.849630	H	-4.901352	0.777449	4.179295
H	6.206835	0.684182	3.881012	H	-6.033149	-0.583254	4.118576
H	6.139052	-0.296361	2.399924	H	-5.914204	0.535700	2.737976
H	0.474496	2.661486	-4.733167	H	-0.890677	-2.357527	-4.790984
H	1.958468	2.622151	-3.757978	H	-2.291076	-2.345529	-3.702916
H	1.558261	4.072013	-4.702044	H	-2.017156	-3.741950	-4.771884
H	-1.486277	4.157237	-4.021634	H	1.082152	-3.936860	-4.301646
H	-0.416881	5.562290	-3.979269	H	-0.028944	-5.315366	-4.301192

H	-1.366921	5.133279	-2.537871
H	6.236140	-1.863322	-2.125035
H	5.163970	-1.302816	-0.823838
H	5.584127	-0.207763	-2.156347
H	5.285772	-2.269695	-4.479968
H	4.637024	-0.627573	-4.506364
H	3.554352	-2.012123	-4.793755
H	-2.165083	-5.341072	2.075971
H	-1.777124	-4.180434	0.788176
H	-2.871024	-3.707946	2.103801
H	-1.242752	-4.977884	4.448916
H	-1.948393	-3.359483	4.476275
H	-0.208911	-3.572294	4.792807
H	-7.602028	0.746502	-0.956608
H	-7.664392	0.387090	0.775272
H	-7.775038	-2.087290	0.261629
H	-7.716622	-1.726655	-1.477971
H	-9.115942	-1.220298	-0.511687

H	1.016741	-5.015145	-2.889747
H	-6.204451	1.956323	-1.821193
H	-5.026916	1.395766	-0.608492
H	-5.547077	0.298541	-1.897005
H	-5.435754	2.337382	-4.249387
H	-4.764082	0.700990	-4.308955
H	-3.724523	2.096661	-4.681124
H	2.419206	5.253572	1.901306
H	1.917706	4.083118	0.656046
H	3.048564	3.583066	1.922780
H	1.603516	4.954474	4.321199
H	2.212151	3.292628	4.335982
H	0.505208	3.611160	4.724570
H	7.590257	-1.097074	-0.888100
H	7.742979	-0.520657	0.772022
H	7.906362	1.861841	-0.069884
H	7.763942	1.275999	-1.736537
H	9.191903	0.848292	-0.764441

#### 4-CO<sub>2</sub>Et<sup>+</sup> (cation)

Structure

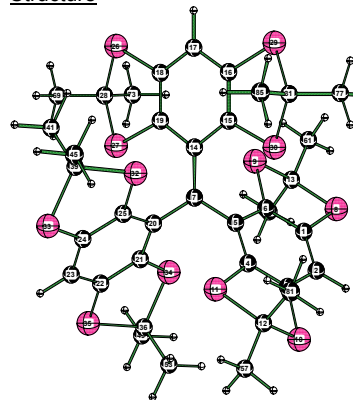


Coordinates

C	3.184530	1.938054	-0.709366
C	4.079607	1.308624	0.157822
C	3.665207	0.230050	0.937353
C	2.349208	-0.254097	0.850833
C	1.386621	0.425712	0.024050
C	1.842522	1.536988	-0.769162
C	0.003433	0.005025	-0.003695
S	3.679739	3.297492	-1.726478
S	0.857293	2.444177	-1.926526
S	4.782862	-0.626326	2.009478
S	2.023364	-1.666865	1.859203
C	3.443266	-1.395851	3.040317
C	2.285140	3.096599	-2.936727
C	-1.051098	0.993148	-0.038727
C	-0.961710	2.205268	0.733433
C	-1.994764	3.151712	0.675654
C	-3.088167	2.964119	-0.171662
C	-3.198273	1.802395	-0.934073
C	-2.225776	0.792696	-0.847385
C	-0.327320	-1.415866	0.005302
C	0.294939	-2.321569	-0.912641
C	-0.056507	-3.680858	-0.908070
C	-0.974292	-4.174747	0.020136
C	-1.575502	-3.314635	0.940427
C	-1.286192	-1.941000	0.930091
S	-4.593045	1.508739	-1.983186
S	-2.565307	-0.634182	-1.830821
C	-3.745857	0.209454	-3.004771
S	-1.833033	4.603966	1.672386
S	0.338663	2.610520	1.863878

#### 4-CO<sub>2</sub>Et<sup>-</sup> (anion)

Structure

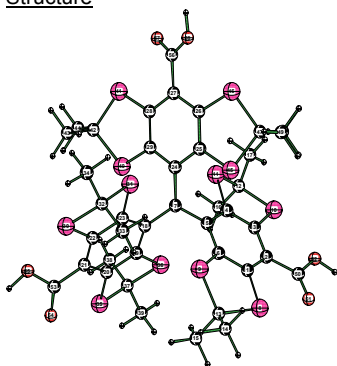


Coordinates

C	-2.945328	2.333208	0.741598
C	-3.943000	1.858022	-0.108265
C	-3.637443	0.763447	-0.916921
C	-2.371761	0.164813	-0.892015
C	-1.325521	0.623826	-0.033925
C	-1.679838	1.733548	0.794521
C	-0.004928	0.004171	0.005165
S	-3.223939	3.716902	1.831097
S	-0.567244	2.426879	2.007474
S	-4.830487	0.069890	-2.047199
S	-2.152184	-1.184548	-2.039333
C	-3.544586	-0.680873	-3.159303
C	-1.899329	3.215961	3.033067
C	1.191364	0.837358	0.067992
C	1.340622	2.028840	-0.708066
C	2.488457	2.829544	-0.637228
C	3.566931	2.488000	0.177649
C	3.465122	1.317923	0.930297
C	2.317275	0.517060	0.887752
C	0.121213	-1.460057	-0.023509
C	-0.647575	-2.315846	0.820931
C	-0.518603	-3.710931	0.790189
C	0.382267	-4.338982	-0.069422
C	1.153838	-3.532455	-0.905637
C	1.029925	-2.136597	-0.891647
S	4.780818	0.776469	2.006579
S	2.354060	-0.913124	1.954893
C	3.663230	-0.241930	3.087320
S	2.511878	4.290990	-1.658826
S	0.104342	2.583490	-1.871242

C	-0.648542	3.830123	2.875112	C	1.265681	3.633609	-2.869566
S	-2.021168	-1.017308	2.247059	S	1.960721	-1.280859	-2.149323
S	-2.641783	-3.912417	2.217060	S	2.243159	-4.232283	-2.128624
S	1.359791	-1.835244	-2.238348	S	-1.712949	-1.682249	2.103072
S	0.629500	-4.702277	-2.177094	S	-1.457896	-4.633156	1.989852
C	2.026403	-3.544500	-2.582500	C	-2.662185	-3.258985	2.333530
H	-3.863530	3.722606	-0.227763	H	4.455334	3.109336	0.222845
H	-1.222106	-5.232181	0.026036	H	0.480281	-5.419805	-0.086371
C	-3.373740	-2.250483	2.614867	C	3.177467	-2.652910	-2.428591
H	5.107960	1.653340	0.215171	H	-4.922267	2.324169	-0.140329
C	-4.600651	-1.976084	1.740962	C	4.353716	-2.536627	-1.451703
H	-5.374194	-2.725468	1.943040	H	5.049722	-3.373570	-1.594047
H	-5.009147	-0.984378	1.966329	H	4.890545	-1.595531	-1.620330
H	-4.351556	-2.012192	0.677160	H	4.002675	-2.542628	-0.416670
C	-3.709045	-2.186362	4.107674	C	3.652751	-2.615644	-3.883951
H	-4.126000	-1.204675	4.358332	H	4.168248	-1.668973	-4.085572
H	-4.469772	-2.936594	4.349596	H	4.365454	-3.428077	-4.072459
H	-2.828637	-2.367000	4.728702	H	2.814400	-2.713508	-4.578353
C	2.362701	-3.653910	-4.072341	C	-3.135717	-3.354351	3.786825
H	3.167069	-2.955666	-4.329011	H	-3.821410	-2.528815	4.012394
H	2.721277	-4.663944	-4.298704	H	-3.681448	-4.292216	3.948554
H	1.494428	-3.441173	-4.700310	H	-2.293979	-3.311589	4.482667
C	3.242893	-3.833601	-1.698803	C	-3.840397	-3.327258	1.354221
H	4.049006	-3.126697	-1.925771	H	-4.534610	-2.499526	1.542220
H	2.997453	-3.747483	-0.636992	H	-3.493669	-3.246701	0.320754
H	3.606661	-4.849409	-1.890175	H	-4.378653	-4.276520	1.473751
C	3.913790	-2.755543	3.562983	C	-4.121949	-1.925027	-3.838294
H	4.763776	-2.619281	4.240435	H	-4.963006	-1.649612	-4.486746
H	3.112603	-3.238086	4.133503	H	-3.358001	-2.398464	-4.466495
H	4.217884	-3.418505	2.749483	H	-4.468240	-2.654345	-3.101514
C	1.898165	4.464769	-3.504674	C	-1.334102	4.464003	3.715670
H	2.736237	4.880656	-4.074583	H	-2.115239	4.965907	4.300316
H	1.052150	4.361949	-4.193263	H	-0.530891	4.182434	4.407362
H	1.627000	5.168350	-2.714255	H	-0.932761	5.168302	2.982694
C	2.662230	2.104134	-4.039724	C	-2.455003	2.218567	4.056155
H	1.821286	1.971188	-4.730000	H	-1.656245	1.892611	4.733508
H	3.520837	2.483516	-4.604866	H	-3.255200	2.682199	4.647600
H	2.926362	1.127703	-3.624497	H	-2.856992	1.334205	3.554737
C	-4.774360	-0.817043	-3.487053	C	4.456078	-1.405077	3.687869
H	-5.487409	-0.337070	-4.166193	H	5.249505	-1.026624	4.344318
H	-4.275636	-1.616704	-4.045677	H	3.795189	-2.036641	4.293504
H	-5.327220	-1.258574	-2.654602	H	4.908332	-2.021767	2.906951
C	-2.980982	0.842271	-4.170406	C	3.032595	0.630914	4.178280
H	-2.242912	1.568145	-3.818349	H	2.462530	1.451447	3.734825
H	-2.458547	0.066561	-4.741801	H	2.346994	0.029673	4.787632
H	-3.680568	1.356814	-4.838460	H	3.810088	1.052445	4.828408
C	0.302699	4.900416	3.417132	C	0.486021	4.799952	-3.481981
H	-0.264270	5.651445	3.977986	H	1.157930	5.445972	-4.060919
H	1.023158	4.449391	4.108512	H	-0.281494	4.419979	-4.167080
H	0.848562	5.400276	2.613644	H	-0.002005	5.398750	-2.708924
C	3.020760	-0.460166	4.176109	C	-3.061809	0.347377	-4.188755
H	2.196623	-0.907180	4.743554	H	-2.279209	-0.093239	-4.818244
H	3.864071	-0.295670	4.856043	H	-3.894361	0.668343	-4.828103
H	2.690567	0.509512	3.793324	H	-2.643098	1.226000	-3.691077
C	-1.402724	3.112917	3.997949	C	1.960024	2.793694	-3.947755
H	-0.693209	2.615747	4.669260	H	1.215085	2.381270	-4.639202
H	-1.983167	3.837885	4.579438	H	2.669436	3.409637	-4.515508
H	-2.088807	2.359489	3.601387	H	2.503605	1.959351	-3.496799

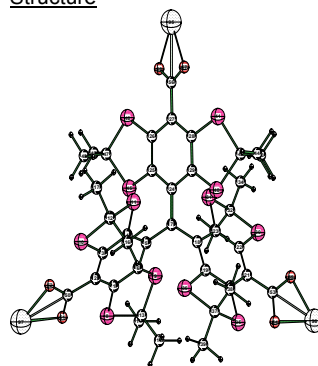
**1-CO<sub>2</sub>H**  
Structure



Coordinates

C	-1.576003	-3.351450	-0.961775
C	-2.694126	-3.403191	-0.097727
C	-2.916771	-2.326662	0.799164
C	-2.069420	-1.207299	0.784376
C	-0.942656	-1.136940	-0.081244
C	-0.729899	-2.226789	-0.962495
C	-0.037568	0.028040	-0.067636
S	-1.197436	-4.627077	-2.135126
S	0.476908	-2.174208	-2.260788
S	-4.235899	-2.274164	1.997492
S	-2.484006	0.099843	1.916075
C	-3.464814	-0.966906	3.060807
C	0.499743	-3.995333	-2.563296
C	0.763719	-4.254770	-4.050908
C	1.552246	-4.677193	-1.679725
C	-2.558438	-1.603789	4.121259
C	-4.574368	-0.127989	3.704090
C	1.422368	-0.168037	-0.041674
C	2.026906	-1.151340	0.784476
C	3.420985	-1.323102	0.813828
C	4.260295	-0.525996	0.006476
C	3.675619	0.443876	-0.837664
C	2.282969	0.625260	-0.847243
C	-0.595865	1.394775	-0.047248
C	-1.610898	1.789925	-0.961152
C	-2.154756	3.086270	-0.946030
C	-1.693784	4.037803	-0.007938
C	-0.691900	3.661868	0.914187
C	-0.149699	2.364915	0.890109
S	4.599967	1.477463	-1.956816
S	1.679683	1.881238	-1.954733
C	3.161270	1.852865	-3.063511
C	3.012121	0.775941	-4.144112
C	3.352748	3.242278	-3.679921
S	4.042779	-2.578401	1.907746
S	1.104990	-2.232740	1.855143
C	2.526831	-2.619623	2.976556
C	2.628372	-1.581158	4.099978
C	2.351066	-4.034647	3.537367
S	0.973149	1.982040	2.208467
S	-0.097376	4.743126	2.190228
C	1.420643	3.740935	2.566562
C	2.594661	4.190622	1.688379
C	1.748544	3.881301	4.056955
S	-2.143330	0.745992	-2.293209
S	-3.385498	3.420189	-2.187609
C	-3.736107	1.640872	-2.577851
C	-4.838899	1.093821	-1.663780
C	-4.121115	1.522580	-4.056272
C	-3.614099	-4.551091	-0.244898
O	-3.451986	-5.472516	-1.027104

**1-CO<sub>2</sub>Na**  
Structure

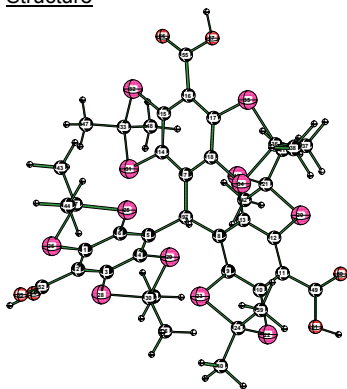


Coordinates

C	-1.796540	-3.261211	-0.911063
C	-2.905881	-3.231739	-0.042691
C	-3.044411	-2.141708	0.843581
C	-2.133194	-1.074661	0.814946
C	-1.012760	-1.081673	-0.060646
C	-0.880712	-2.194055	-0.932743
C	-0.033998	0.021956	-0.063138
S	-1.509378	-4.577149	-2.073551
S	0.316608	-2.235146	-2.244745
S	-4.355048	-2.032313	2.045319
S	-2.467184	0.262222	1.939129
C	-3.521217	-0.733639	3.082865
C	0.226076	-4.059869	-2.505298
C	0.484086	-4.370358	-3.983820
C	1.232592	-4.781557	-1.599404
C	-2.660470	-1.391809	4.168972
C	-4.589758	0.176579	3.698198
C	1.409711	-0.269465	-0.047630
C	1.958412	-1.282423	0.783718
C	3.337762	-1.544141	0.803469
C	4.218716	-0.825042	-0.025429
C	3.691244	0.172670	-0.865061
C	2.316414	0.456904	-0.864706
C	-0.503022	1.421793	-0.047064
C	-1.500317	1.876729	-0.952137
C	-1.954430	3.206077	-0.936957
C	-1.424317	4.134162	-0.021020
C	-0.433748	3.704605	0.882959
C	0.015940	2.373441	0.873753
S	4.699635	1.124730	-1.982492
S	1.802661	1.754912	-1.969735
C	3.282971	1.629233	-3.072865
C	3.048703	0.584624	-4.171371
C	3.577546	3.008120	-3.672556
S	3.893541	-2.807825	1.929687
S	0.976128	-2.287528	1.879429
C	2.378731	-2.733777	3.000805
C	2.546650	-1.678561	4.101110
C	2.118869	-4.121246	3.596857
S	1.126551	1.933812	2.188616
S	0.273058	4.772270	2.118652
C	1.716541	3.659945	2.487623
C	2.900719	3.991263	1.570809
C	2.094814	3.810848	3.964883
S	-2.120719	0.867515	-2.274008
S	-3.168584	3.641844	-2.161923
C	-3.636884	1.886424	-2.559664
C	-4.779988	1.415615	-1.651397
C	-4.027297	1.799122	-4.038889
C	-3.966657	-4.281193	-0.125544
O	-3.805264	-5.248079	-0.938360

O	-4.711130	-4.500072	0.545934
C	5.718372	-0.772561	0.068363
O	6.229147	-1.812408	0.441838
O	6.467915	0.290372	-0.308856
C	-2.229381	5.415253	0.081652
O	-2.141185	6.128389	1.064498
O	-2.823537	5.848935	-1.054323
H	1.757946	-3.886529	-4.329803
H	0.016355	-3.766702	-4.681223
H	0.743333	-5.332009	-4.252486
H	2.554985	-4.312000	-1.930624
H	1.525390	-5.762253	-1.836685
H	1.370574	-4.475666	-0.620614
H	-2.096836	-0.823930	4.738163
H	-1.760857	-2.189772	3.656876
H	-3.144950	-2.265415	4.769857
H	-5.188267	-0.755364	4.360692
H	-5.220360	0.327867	2.949766
H	-4.136931	0.666221	4.319743
H	2.144452	0.995115	-4.776991
H	2.870177	-0.212584	-3.699137
H	3.909424	0.748135	-4.773779
H	2.496181	3.492566	-4.316102
H	4.248366	3.253349	-4.311807
H	3.456114	4.011871	-2.911013
H	1.722290	-1.600664	4.716978
H	2.745003	-0.572128	3.695266
H	3.492697	-1.800993	4.737878
H	1.446110	-4.089138	4.153544
H	3.202396	-4.292343	4.177950
H	2.277418	-4.776439	2.738265
H	2.823568	5.245395	1.882269
H	2.362450	4.075985	0.626073
H	3.485902	3.591991	1.909982
H	1.978605	4.926654	4.293015
H	2.633042	3.284485	4.308153
H	0.913718	3.556652	4.683021
H	-5.766777	1.657695	-1.817583
H	-4.556554	1.170503	-0.610266
H	-5.027893	0.038444	-1.891537
H	-5.047983	2.075165	-4.248460
H	-4.302883	0.473096	-4.314379
H	-3.336359	1.914965	-4.707650
H	7.396807	-0.006361	-0.275314
H	-3.168517	6.740156	-0.857590
H	-5.228308	-5.300420	0.336844

**1-CO<sub>2</sub>H-H**  
Structure

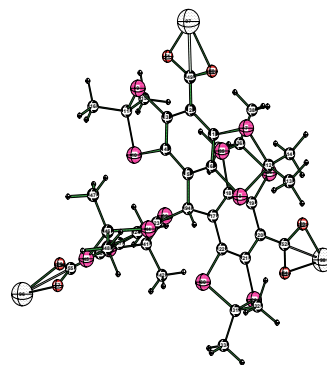


Coordinates

C	2.861090	-2.583529	-0.961944
C	2.625574	-3.533339	0.053302
C	1.532835	-3.342946	0.925455

O	-5.008525	-4.149359	0.595253
C	5.685204	-1.115719	-0.014702
O	6.070280	-2.258616	0.392759
O	6.482229	-0.206788	-0.413934
C	-1.904634	5.550453	-0.008650
O	-1.714440	6.243257	1.041863
O	-2.482239	6.000428	-1.049889
H	1.501909	-4.073547	-4.264053
H	-0.225998	-3.848606	-4.630337
H	0.394323	-5.448682	-4.162079
H	2.257483	-4.490011	-1.858570
H	1.134127	-5.867690	-1.720387
H	1.064995	-4.532725	-0.548020
H	-2.156452	-0.626325	4.771312
H	-1.895793	-2.034448	3.724419
H	-3.288377	-2.003483	4.828838
H	-5.249505	-0.406106	4.352534
H	-5.197331	0.655459	2.926200
H	-4.120479	0.955952	4.310339
H	2.216578	0.890614	-4.816650
H	2.805716	-0.390201	-3.739712
H	3.950573	0.476802	-4.786810
H	2.748730	3.328127	-4.314932
H	4.480100	2.963139	-4.293995
H	3.726946	3.758784	-2.892417
H	1.640599	-1.621831	4.716421
H	2.729495	-0.690112	3.671023
H	3.394777	-1.938922	4.746507
H	1.203338	-4.111943	4.200247
H	2.946531	-4.408043	4.256711
H	2.016093	-4.878093	2.815119
H	3.230246	5.023613	1.742953
H	2.625366	3.885693	0.518016
H	3.740529	3.315433	1.771654
H	2.429682	4.835893	4.163988
H	2.923805	3.138479	4.216124
H	1.248095	3.586312	4.618497
H	-5.660262	2.054569	-1.795770
H	-4.490205	1.457648	-0.597848
H	-5.053927	0.380580	-1.888328
H	-4.898370	2.435603	-4.235880
H	-4.303580	0.770453	-4.298922
H	-3.207108	2.118075	-4.686939
Na	-2.695171	7.902821	0.009761
Na	8.117939	-1.598392	0.004905
Na	-5.755864	-5.997608	-0.301165

**1-CO<sub>2</sub>Na-H**  
Structure



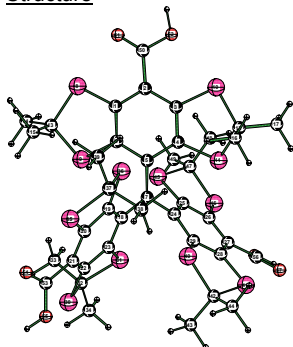
Coordinates

C	1.718973	-3.412725	0.915417
C	2.753224	-3.386888	-0.038984
C	2.866223	-2.263426	-0.881767

C	0.696013	-2.211670	0.791834	C	2.006865	-1.154361	-0.729546
C	0.923638	-1.253813	-0.220378	C	0.986070	-1.158388	0.243082
C	2.015391	-1.469333	-1.090594	C	0.871591	-2.301436	1.062911
C	0.679700	1.353822	-0.243113	S	1.438761	-4.781386	2.017380
C	-1.456884	-0.161149	-0.185605	S	-0.288729	-2.390481	2.413841
C	-2.192670	-1.086199	-0.957832	S	4.099386	-2.147121	-2.161947
C	-3.579803	-1.251402	-0.810154	S	2.347543	0.226411	-1.802173
C	-4.276938	-0.478748	0.141316	C	3.282509	-0.744460	-3.062370
C	-3.558246	0.455084	0.916538	C	-0.257196	-4.231580	2.551017
C	-2.164392	0.610384	0.756261	C	-0.473502	-4.632958	4.014223
C	1.676542	1.612010	0.717844	C	-1.325566	-4.849246	1.639056
C	2.239267	2.899964	0.848077	C	2.335274	-1.285022	-4.141601
C	1.834500	3.956733	-0.000075	C	4.363330	0.152745	-3.676835
C	0.821720	3.712625	-0.956293	C	-1.458366	-0.215626	0.228983
C	0.281837	2.420102	-1.079017	C	-1.970935	-1.125040	-0.717569
S	-1.426709	1.858404	1.794346	C	-3.362549	-1.306752	-0.865574
S	-4.347202	1.507892	2.109828	C	-4.275676	-0.597519	-0.066022
C	-2.793924	1.896393	3.040766	C	-3.774306	0.306911	0.883698
S	-4.339844	-2.438372	-1.898700	C	-2.389454	0.492929	1.017678
S	-1.418086	-2.155909	-2.154894	C	0.575413	1.429833	0.251362
C	-2.958309	-2.441770	-3.137877	C	1.589908	1.908966	1.111837
S	2.366457	-0.394942	-2.464768	C	2.129220	3.198632	0.981838
S	4.164750	-2.731391	-2.156529	C	1.645724	4.068823	-0.009935
C	4.121132	-0.947718	-2.671879	C	0.630679	3.614620	-0.868781
S	1.125115	-4.462043	2.248615	C	0.105006	2.308954	-0.748343
S	-0.548906	-2.053363	2.053340	S	-4.813558	1.252127	1.977447
C	-0.608932	-3.851306	2.467274	S	-1.898053	1.718739	2.215922
S	2.348968	0.375458	1.804814	C	-3.459491	1.610383	3.201694
S	3.479867	3.100252	2.103452	C	-3.362438	0.488523	4.242633
C	3.036024	1.562397	3.040829	C	-3.728675	2.965117	3.864177
S	-0.868169	2.183586	-2.420044	S	-3.892330	-2.485318	-2.090613
S	0.195320	4.923901	-2.100033	S	-0.964296	-2.147267	-1.780817
C	-1.314982	3.967163	-2.591140	C	-2.292228	-2.474660	-3.026390
C	-2.489101	4.318192	-1.668991	C	-2.305648	-1.386597	-4.107242
C	-1.640455	4.269425	-4.058001	C	-2.063372	-3.860883	-3.639491
C	-3.158301	-1.330663	-4.175010	S	-1.068235	1.861841	-2.009892
C	-2.883858	-3.821566	-3.799173	S	-0.036756	4.628688	-2.170449
C	-2.900123	3.312937	3.617048	C	-1.558158	3.594969	-2.415800
C	-2.554368	0.862547	4.147652	C	-2.690385	4.068043	-1.495094
C	5.049545	-0.107061	-1.787107	C	-1.973752	3.662179	-3.889258
C	4.510618	-0.847904	-4.150426	S	2.219443	0.948495	2.475318
C	-1.013145	-4.012361	3.936594	S	3.390979	3.656156	2.149296
C	-1.569081	-4.599025	1.534785	C	3.791280	1.909560	2.643777
C	4.310840	0.965726	3.649112	C	4.871992	1.323624	1.726400
C	1.998876	1.877313	4.126180	C	4.234753	1.895691	4.110238
C	-5.739412	-0.577393	0.345588	C	3.765513	-4.485885	-0.086052
O	-6.432714	0.292886	0.838649	O	3.645030	-5.456277	0.730680
O	-6.265040	-1.762093	-0.048975	O	4.729645	-4.393968	-0.912726
C	3.536959	-4.698439	0.123947	C	-5.750297	-0.800644	-0.212757
O	4.233758	-5.084817	-0.796497	O	-6.163033	-1.884490	-0.737057
O	3.562245	-5.307068	1.332541	O	-6.527182	0.121857	0.196182
C	2.561571	5.239952	0.112925	C	2.204308	5.450536	-0.142361
O	3.534782	5.423086	0.823706	O	2.061807	6.057432	-1.251860
O	2.080500	6.232824	-0.671222	O	2.799594	5.956789	0.862789
H	-2.718613	5.387670	-1.746224	H	-1.462147	-4.306355	4.358338
H	-2.255285	4.087456	-0.626271	H	0.288264	-4.196122	4.664781
H	-3.379472	3.746751	-1.955883	H	-0.434542	-5.724505	4.112457
H	-1.875333	5.333256	-4.178319	H	-2.326742	-4.529034	1.951805
H	-2.522173	3.699922	-4.373555	H	-1.273691	-5.943967	1.690767
H	-0.803922	4.017992	-4.714444	H	-1.179974	-4.544270	0.599248
H	-2.327597	-1.328390	-4.890141	H	1.840879	-0.456328	-4.662851
H	-3.203037	-0.348282	-3.696877	H	1.563161	-1.919099	-3.698578
H	-4.093898	-1.492460	-4.723277	H	2.897157	-1.878441	-4.873771
H	-2.054908	-3.851785	-4.515349	H	4.952977	-0.414129	-4.407619
H	-3.807737	-4.022182	-4.353751	H	5.038070	0.544020	-2.911298
H	-2.739116	-4.613475	-3.060227	H	3.903618	0.996559	-4.204985
H	-3.726790	3.364715	4.335063	H	-2.553883	0.697473	4.953265
H	-3.071668	4.053410	2.831983	H	-3.158049	-0.473183	3.763835
H	-1.980705	3.574757	4.153385	H	-4.305968	0.406297	4.796116
H	-3.383976	0.881498	4.864555	H	-2.930381	3.206595	4.575752

H	-1.623477	1.086711	4.681565
H	-2.476527	-0.146693	3.735239
H	6.081839	-0.463877	-1.884428
H	4.758801	-0.170062	-0.734927
H	5.011694	0.945631	-2.090497
H	5.539196	-1.200162	-4.289893
H	4.470972	0.195630	-4.483151
H	3.847372	-1.444892	-4.781146
H	-2.027554	-3.627429	4.092307
H	-0.327687	-3.480859	4.601425
H	-1.018200	-5.073538	4.210906
H	-2.589669	-4.219456	1.660164
H	-1.560952	-5.670344	1.768749
H	-1.284554	-4.470561	0.487019
H	4.750470	1.670466	4.364548
H	5.053523	0.739569	2.880156
H	4.075942	0.044125	4.194093
H	2.408570	2.603065	4.839103
H	1.731005	0.962770	4.668577
H	1.088421	2.295178	3.689051
H	-7.228403	-1.690096	0.087227
H	4.160768	-6.071775	1.238231
H	2.668351	6.997013	-0.522329
C	0.041444	-0.023199	-0.527429
H	0.007949	-0.048768	-1.626877

**1-CO<sub>2</sub>H+**  
Structure

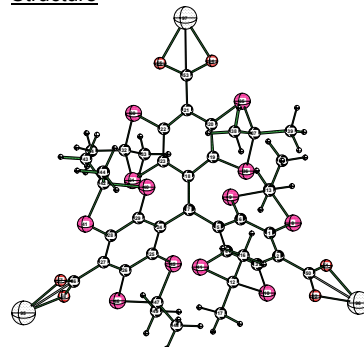


Coordinates

C	-2.968794	-2.219705	0.942023
C	-2.808614	-3.252667	-0.015402
C	-1.669875	-3.265811	-0.856898
C	-0.666596	-2.283184	-0.708319
C	-0.874317	-1.167022	0.173059
C	-2.021452	-1.186629	1.022308
C	0.029587	-0.027262	0.163603
S	-4.284452	-2.179526	2.123904
S	-2.191434	-0.091859	2.392997
S	-1.356949	-4.508532	-2.088473
S	0.781646	-2.519359	-1.684801
C	-0.018742	-3.578757	-2.971676
C	-3.987405	-0.430876	2.691917
C	-4.266957	-0.344408	4.197080
C	-4.865846	0.542981	1.898635
C	-0.610630	-2.713543	-4.089957
C	1.013534	-4.574868	-3.511021
C	-0.490792	1.328560	0.104780
C	-1.631907	1.657793	-0.700052
C	-2.043374	3.000379	-0.833875
C	-1.386755	4.022716	-0.121566
C	-0.305838	3.706813	0.733595
C	0.162700	2.386898	0.815990
C	1.471191	-0.251763	0.121345
C	2.089752	-1.155169	1.041106
C	3.464072	-1.439666	0.968037

H	-4.671232	2.928635	4.423459
H	-3.792673	3.765752	3.122962
H	-1.348450	-1.366966	-4.641916
H	-2.469409	-0.399319	-3.667910
H	-3.108183	-1.583822	-4.829019
H	-1.111534	-3.885529	-4.183369
H	-2.860051	-4.090957	-4.357242
H	-2.048705	-4.638457	-2.871704
H	-2.954119	5.107331	-1.728101
H	-2.393175	4.013042	-0.444200
H	-3.579212	3.440218	-1.629243
H	-2.236680	4.692146	-4.158600
H	-2.859204	3.039296	-4.063701
H	-1.168761	3.323147	-4.546323
H	5.788954	1.921470	1.800772
H	4.543859	1.319188	0.683392
H	5.100381	0.291209	2.016876
H	5.150472	2.487104	4.229772
H	4.458180	0.871425	4.431050
H	3.463167	2.309297	4.764453
C	0.032357	0.015596	0.553321
H	0.008514	0.019978	1.653295
Na	3.132370	7.741678	-0.356027
Na	5.481111	-6.283467	-0.113059
Na	-8.196533	-1.135468	-0.447136

**1-CO<sub>2</sub>Na+**  
Structure



Coordinates

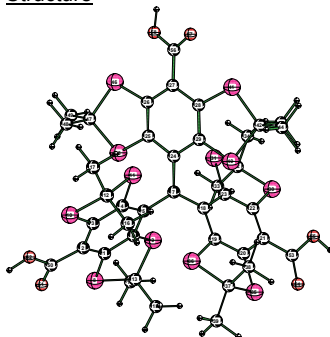
C	2.614622	-2.618280	-0.920424
C	2.271474	-3.648802	-0.017885
C	1.148964	-3.499940	0.822283
C	0.318484	-2.366765	0.714693
C	0.692058	-1.280718	-0.146263
C	1.834278	-1.454437	-0.987964
C	-0.043535	-0.025220	-0.123964
S	3.963224	-2.744265	-2.064861
S	2.188318	-0.370972	-2.338330
S	0.671776	-4.726485	2.016249
S	-1.133287	-2.392586	1.719514
C	-0.480617	-3.606769	2.952591
C	3.920885	-0.961283	-2.606140
C	4.247181	-0.886982	-4.102259
C	4.907375	-0.131502	-1.775772
C	0.266391	-2.879254	4.076867
C	-1.648944	-4.433760	3.499700
C	0.666260	1.238012	-0.067298
C	1.861578	1.389020	0.712486
C	2.512197	2.631328	0.782975
C	2.052474	3.725855	0.028318
C	0.900431	3.590085	-0.766954
C	0.183874	2.382626	-0.785032
C	-1.500636	-0.042813	-0.093168
C	-2.240247	-0.835410	-1.025898
C	-3.643594	-0.873291	-0.983682

C	4.249232	-0.847210	-0.046462	C	-4.344473	-0.147122	-0.002676
C	3.660620	0.050280	-0.964625	C	-3.635244	0.636020	0.930143
C	2.294522	0.380013	-0.864978	C	-2.233459	0.707923	0.882083
S	0.534910	4.902230	1.743814	S	0.264523	4.918127	-1.760655
S	1.544408	2.144915	1.900380	S	-1.270456	2.392392	-1.794974
C	1.224605	3.654559	2.929112	C	-0.734605	3.809097	-2.865082
C	0.223599	3.351462	4.048055	C	0.105510	3.304500	-4.043269
C	2.556144	4.170097	3.484375	C	-1.978577	4.563922	-3.344251
S	-3.431717	3.311020	-1.891663	S	3.938081	2.736371	1.839294
S	-2.584626	0.496327	-1.628505	S	2.587940	0.111537	1.702415
C	-3.269578	1.725692	-2.838528	C	3.470168	1.259637	2.861230
C	-2.325105	1.891220	-4.034080	C	2.556034	1.663298	4.023147
C	-4.662182	1.261782	-3.278571	C	4.743809	0.570349	3.361357
S	1.669046	1.412119	-2.151603	S	-1.471221	1.576116	2.219985
S	4.548729	0.752900	-2.326945	S	-4.436010	1.508063	2.251583
C	3.316474	2.100161	-2.656623	C	-2.969767	2.574054	2.661875
C	3.645026	3.352524	-1.835938	C	-2.999761	3.877350	1.854857
C	3.293159	2.398181	-4.159781	C	-2.958460	2.846749	4.169992
S	1.252593	-1.787070	2.459800	S	-1.498996	-1.624458	-2.419977
S	4.100625	-2.511357	2.230587	S	-4.451414	-1.810311	-2.254404
C	2.449910	-3.169839	2.767803	C	-2.928623	-2.757514	-2.751903
C	2.068553	-4.413300	1.958270	C	-2.796811	-4.045057	-1.930743
C	2.495648	-3.463182	4.271333	C	-2.991615	-3.051429	-4.254460
C	-3.823434	-4.345398	0.003354	C	3.032535	-4.948657	-0.032662
O	-4.695614	-4.434656	0.845318	O	4.020414	-5.054211	-0.820162
O	-3.686355	-5.251625	-0.981271	O	2.627172	-5.886045	0.719299
C	-1.907831	5.411860	-0.276093	C	2.789226	5.039140	0.075351
O	-3.046106	5.669774	-0.608774	O	4.023009	5.013119	0.362465
O	-0.982271	6.359347	-0.035499	O	2.132761	6.092674	-0.177643
C	5.699281	-1.153660	-0.223539	C	-5.849340	-0.205215	0.047146
O	6.286022	-1.034557	-1.279154	O	-6.415120	0.059725	1.149369
O	6.304063	-1.558013	0.908286	O	-6.463457	-0.516978	-1.016170
H	-4.097578	0.676764	4.556610	H	4.231152	0.153828	-4.445805
H	-3.636154	-1.030891	4.766590	H	3.539296	-1.467612	-4.698538
H	-5.316268	-0.590795	4.393082	H	5.256006	-1.275890	-4.281373
H	-4.686311	1.573337	2.226487	H	4.886164	0.917983	-2.092216
H	-5.922462	0.305610	2.067282	H	5.924239	-0.516961	-1.916241
H	-4.666093	0.480681	0.825724	H	4.666457	-0.174065	-0.710366
H	0.185622	-2.158738	-4.599073	H	-0.414271	-2.211553	4.617980
H	-1.335168	-1.995562	-3.695452	H	1.093254	-2.282361	3.681779
H	-1.117107	-3.350088	-4.824141	H	0.675526	-3.609853	4.784442
H	0.542559	-5.235388	-4.247124	H	-1.274447	-5.183292	4.206169
H	1.438247	-5.188542	-2.713065	H	-2.186655	-4.948808	2.699693
H	1.824330	-4.041305	-4.019073	H	-2.351599	-3.791313	4.042691
H	0.633055	2.593826	4.725744	H	-0.489232	2.636725	-4.677215
H	-0.723842	2.980829	3.646832	H	0.986518	2.756628	-3.697155
H	0.022114	4.261944	4.623394	H	0.443236	4.152890	-4.649886
H	2.995090	3.428166	4.160478	H	-2.603681	3.913126	-3.966109
H	2.388190	5.084100	4.064567	H	-1.679478	5.419644	-3.960118
H	3.271058	4.388583	2.687438	H	-2.575150	4.930571	-2.505225
H	-2.227643	0.943436	-4.576261	H	2.265121	0.781041	4.605418
H	-1.328547	2.212039	-3.717768	H	1.646968	2.152379	3.662100
H	-2.726971	2.643806	-4.721632	H	3.082250	2.360220	4.685701
H	-4.593830	0.313792	-3.823577	H	4.492276	-0.328248	3.936254
H	-5.100098	2.000549	-3.958768	H	5.293392	1.244223	4.028336
H	-5.333811	1.133526	-2.426312	H	5.399828	0.287719	2.534296
H	4.633958	3.729859	-2.119579	H	-3.904737	4.445168	2.101359
H	3.651028	3.139082	-0.763519	H	-2.996765	3.681005	0.779237
H	2.904785	4.137601	-2.027313	H	-2.125305	4.494330	2.092604
H	4.271622	2.775025	-4.477148	H	-3.858219	3.404645	4.453039
H	2.554989	3.177159	-4.381084	H	-2.092614	3.462202	4.439800
H	3.055630	1.507123	-4.745803	H	-2.927762	1.919192	4.746762
H	2.806403	-5.205569	2.127928	H	-3.665310	-4.689043	-2.112164
H	2.032067	-4.199145	0.886764	H	-2.742352	-3.832668	-0.859447
H	1.085285	-4.781176	2.272915	H	-1.891602	-4.591699	-2.219945
H	3.232023	-4.248498	4.474101	H	-3.856435	-3.688515	-4.471675
H	1.521729	-3.830543	4.613045	H	-2.094698	-3.593763	-4.574517
H	2.762800	-2.575502	4.849488	H	-3.078389	-2.133775	-4.841231
H	7.232031	-1.765092	0.683719	Na	-8.352751	-0.295747	0.128562
H	-1.425793	7.225578	-0.121203	Na	4.265398	-7.136260	-0.098212



H -4.378817 -5.926977 -0.844160

**1-CO<sub>2</sub>H-**  
Structure

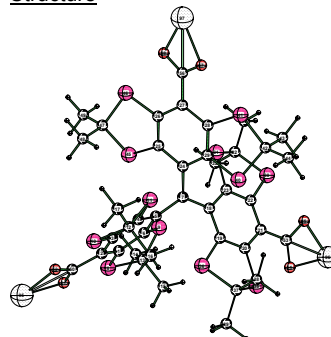


Coordinates

C	-2.318085	-2.911048	-0.913472
C	-3.453186	-2.667946	-0.094852
C	-3.405583	-1.546831	0.779332
C	-2.300346	-0.691454	0.782718
C	-1.158080	-0.899644	-0.049671
C	-1.219212	-2.044364	-0.895922
C	-0.020448	0.019249	-0.062040
S	-2.255757	-4.250800	-2.084502
S	0.006569	-2.319062	-2.159952
S	-4.683345	-1.154897	1.969726
S	-2.370193	0.678340	1.921200
C	-3.597782	-0.110359	3.048997
C	-0.444067	-4.081532	-2.462523
C	-0.213756	-4.416602	-3.940916
C	0.372716	-5.008612	-1.551769
C	-2.892112	-0.983349	4.094434
C	-4.449099	0.976427	3.713057
C	1.342823	-0.491961	-0.053170
C	1.739087	-1.616978	0.731275
C	3.053584	-2.090956	0.752738
C	4.069175	-1.476222	-0.021413
C	3.698917	-0.367984	-0.825628
C	2.384068	0.105539	-0.829204
C	-0.256856	1.469706	-0.044525
C	-1.198592	2.095667	-0.914565
C	-1.437097	3.475227	-0.907264
C	-0.732249	4.324517	-0.014758
C	0.205295	3.726259	0.864677
C	0.431422	2.344776	0.845865
S	4.820515	0.449970	-1.954617
S	2.057248	1.476948	-1.924677
C	3.485745	1.133243	-3.042968
C	3.098305	0.115104	-4.122445
C	3.970101	2.446693	-3.664722
S	3.388803	-3.454400	1.853772
S	0.594822	-2.481894	1.794784
C	1.895830	-3.161135	2.916144
C	2.223353	-2.161502	4.032541
C	1.419871	-4.498981	3.490972
S	1.491660	1.718455	2.132784
S	1.093466	4.657392	2.095558
C	2.343834	3.327631	2.437416
C	3.553513	3.483512	1.506338
C	2.763383	3.408162	3.909312
S	-2.008425	1.168175	-2.201277
S	-2.612570	4.060288	-2.117430
C	-3.360016	2.398486	-2.457155
C	-4.526624	2.131545	-1.497072
C	-3.819800	2.349352	-3.918352
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Na 4.013183 7.223892 0.152815

**1-CO<sub>2</sub>Na-**  
Structure

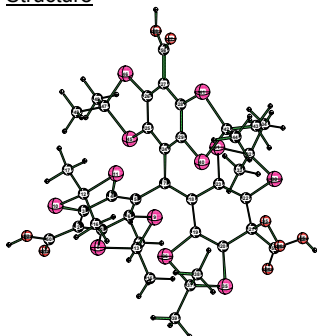


Coordinates

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C	-2.202943	-0.935596	0.813185
C	-1.053556	-1.021834	-0.029515
C	-1.004823	-2.175171	-0.867951
C	-0.017265	0.012337	-0.060251
S	-1.802209	-4.500857	-2.023446
S	0.227909	-2.321826	-2.149734
S	-4.507853	-1.692537	2.029344
S	-2.433715	0.432184	1.934655
C	-3.559494	-0.481720	3.073287
C	-0.027274	-4.125976	-2.431317
C	0.220779	-4.447022	-3.909858
C	0.902464	-4.946249	-1.525588
C	-2.749565	-1.226730	4.143726
C	-4.542585	0.503768	3.713994
C	1.393332	-0.356057	-0.053575
C	1.910326	-1.422537	0.744634
C	3.265374	-1.767595	0.754207
C	4.204814	-1.074950	-0.040167
C	3.720806	-0.018276	-0.841406
C	2.366912	0.329987	-0.842053
C	-0.406095	1.430942	-0.050748
C	-1.410129	1.948685	-0.921158
C	-1.798518	3.293596	-0.910611
C	-1.191501	4.219070	-0.033115
C	-0.187944	3.735985	0.835792
C	0.183539	2.385526	0.830413
S	4.774861	0.889659	-1.965244
S	1.912673	1.663258	-1.939529
C	3.378691	1.466327	-3.045705
C	3.091037	0.431894	-4.141899
C	3.740658	2.825921	-3.651696
S	3.748596	-3.067035	1.883878
S	0.866453	-2.373011	1.841539
C	2.241252	-2.902889	2.955088
C	2.477090	-1.857821	4.053852
C	1.904097	-4.270330	3.557991
S	1.311634	1.888964	2.119049
S	0.622656	4.777290	2.038635
C	2.000041	3.579867	2.389892
C	3.183889	3.835986	1.447333
C	2.420975	3.723737	3.856508
S	-2.113778	0.944689	-2.213566
S	-3.033451	3.769668	-2.108508
C	-3.581804	2.031966	-2.476315
C	-4.724755	1.621390	-1.537239
C	-4.016371	1.948550	-3.943648
C	-4.269616	-3.984115	-0.127838

O	-4.711189	-4.469336	-1.043723
O	-5.708678	-3.179418	0.485147
C	5.423553	-2.024441	0.039475
O	5.726680	-3.142264	0.434327
O	6.398224	-1.160414	-0.369933
C	-0.932774	5.772042	0.068128
O	-0.591285	6.487219	1.000830
O	-1.538234	6.323775	-1.022375
H	0.849863	-4.318185	-4.190256
H	-0.790408	-3.755385	-4.592663
H	-0.506551	-5.454107	-4.144172
H	1.443153	-4.906052	-1.766866
H	0.077861	-6.053588	-1.713785
H	0.215455	-4.760284	-0.499009
H	-2.240708	-0.364664	4.723429
H	-2.274651	-1.744170	3.609733
H	-3.630350	-1.485590	4.732736
H	-5.209597	0.522268	4.360230
H	-4.948712	1.599957	2.967272
H	-3.818533	1.617972	4.340015
H	2.298603	0.521059	-4.753473
H	2.736808	-0.812269	-3.670349
H	3.964804	-0.118250	-4.754436
H	3.180080	2.881787	-4.288243
H	4.839600	2.265033	-4.308536
H	4.247553	3.172217	-2.895699
H	1.333603	-1.972315	4.645459
H	2.556944	-1.208268	3.613838
H	3.018952	-2.557636	4.676520
H	0.527278	-4.349578	4.110578
H	2.197639	-4.935592	4.129671
H	1.178690	-5.210249	2.696768
H	4.022952	4.463988	1.658995
H	3.254340	3.399396	0.458258
H	4.294499	2.701416	1.710504
H	3.243040	4.373213	4.114195
H	3.492387	2.621394	4.138111
H	1.903990	3.295586	4.575294
H	-5.308465	2.890122	-1.632201
H	-4.192365	2.156525	-0.456558
H	-4.956503	1.141727	-1.690829
H	-4.604386	3.095296	-4.095431
H	-4.242238	1.363521	-4.145989
H	-2.989897	2.541787	-4.603086
H	-1.646189	7.265947	-0.798225
H	7.222325	-1.679218	-0.335744
H	-6.392635	-3.828288	0.239184

**1-CO<sub>2</sub>H-a-oo-radical**  
Structure

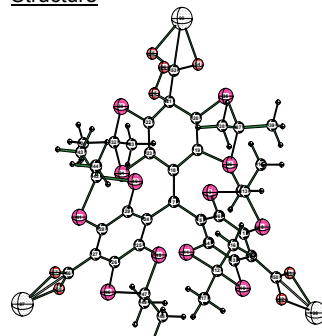


Coordinates

C	-2.674272	-2.678215	-0.918401
C	-3.657425	-2.486811	0.081320
C	-3.447315	-1.494066	1.071118
C	-2.306112	-0.675209	1.013666

O	-4.182937	-4.979480	-0.930939
O	-5.324644	-3.764882	0.566675
C	5.637976	-1.440176	-0.032331
O	5.976994	-2.604101	0.382748
O	6.496088	-0.581057	-0.441450
C	-1.592525	5.643592	-0.024749
O	-1.287288	6.366198	0.987858
O	-2.232050	6.111302	-1.031171
H	1.260702	-4.223693	-4.179258
H	-0.441710	-3.866104	-4.556790
H	0.051570	-5.514704	-4.100720
H	1.952573	-4.737024	-1.764143
H	0.714417	-6.019824	-1.662812
H	0.740140	-4.694873	-0.474303
H	-2.185628	-0.513568	4.758103
H	-2.035976	-1.912789	3.679495
H	-3.418935	-1.804906	4.794874
H	-5.239115	-0.028399	4.374894
H	-5.119338	1.036289	2.953188
H	-4.003028	1.239603	4.322957
H	2.256517	0.765055	-4.771366
H	2.820391	-0.531201	-3.700848
H	3.977930	0.290097	-4.773974
H	2.919179	3.193451	-4.278890
H	4.630210	2.734224	-4.288386
H	3.942100	3.565411	-2.872179
H	1.579145	-1.748946	4.674970
H	2.706647	-0.882890	3.615371
H	3.316536	-2.159900	4.694425
H	0.997214	-4.203392	4.171771
H	2.720256	-4.611317	4.208023
H	1.742424	-5.017665	2.776726
H	3.562201	4.858175	1.584155
H	2.884256	3.710909	0.403521
H	3.995627	3.127036	1.651289
H	2.812854	4.732001	4.042639
H	3.219051	3.009431	4.094124
H	1.578274	3.545587	4.529729
H	-5.581704	2.296774	-1.664564
H	-4.403301	1.658011	-0.492829
H	-5.046107	0.595343	-1.754709
H	-4.877072	2.605706	-4.123317
H	-4.323074	0.924700	-4.190745
H	-3.204578	2.242696	-4.614090
Na	-6.189956	-5.515243	-0.349163
Na	8.022819	-2.044385	-0.015146
Na	-2.257367	8.013789	-0.014162

**1-CO<sub>2</sub>H-a-oo-radical**  
Structure



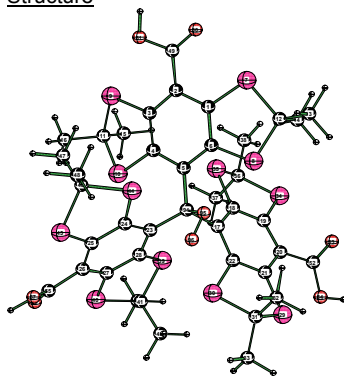
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C	-1.924758	-3.230872	-0.899367
C	-2.962052	-3.247516	0.054518
C	-3.017869	-2.218691	1.017849
C	-2.101830	-1.153848	0.977611

C	-1.313776	-0.858602	0.023818	C	-1.054760	-1.122594	0.028364
C	-1.521754	-1.870345	-0.942776	C	-0.990282	-2.179253	-0.913456
C	-0.122079	0.032391	-0.088073	C	-0.093983	0.014944	-0.066520
S	-2.837376	-3.865541	-2.225672	S	-1.759448	-4.461876	-2.173084
S	-0.448281	-2.083532	-2.343404	S	0.152833	-2.170577	-2.278348
S	-4.558956	-1.159079	2.422340	S	-4.232578	-2.164127	2.319063
S	-2.190698	0.601922	2.241004	S	-2.352444	0.136379	2.172383
C	-3.336859	-0.207396	3.441851	C	-3.319958	-0.909908	3.346842
C	-1.078101	-3.754534	-2.820569	C	-0.049798	-3.956075	-2.706443
C	-1.066337	-3.877371	-4.349271	C	0.064778	-4.122731	-4.226652
C	-0.229833	-4.853810	-2.168196	C	1.001628	-4.802848	-1.976705
C	-2.566253	-1.153385	4.371448	C	-2.379796	-1.615412	4.333094
C	-4.081324	0.872461	4.234637	C	-4.337449	-0.030391	4.081381
C	1.167747	-0.479148	-0.153445	C	1.280187	-0.193296	-0.084365
C	1.567428	-1.752849	0.457395	C	1.929099	-1.339933	0.563731
C	2.869193	-2.157913	0.511185	C	3.285324	-1.475104	0.620265
C	4.003040	-1.295122	0.050680	C	4.220580	-0.417446	0.135535
C	3.541832	-0.193392	-0.849630	C	3.551475	0.551030	-0.779308
C	2.248920	0.233406	-0.850960	C	2.199164	0.721238	-0.777505
C	-0.348756	1.509095	-0.102324	C	-0.652377	1.398012	-0.118465
C	-1.278215	2.136306	-0.966488	C	-1.668315	1.783022	-1.025404
C	-1.518510	3.522131	-0.908728	C	-2.221800	3.075154	-0.997260
C	-0.823469	4.323032	0.024779	C	-1.774271	4.024783	-0.060826
C	0.098630	3.712755	0.903179	C	-0.766825	3.659637	0.851515
C	0.330533	2.325918	0.838955	C	-0.216992	2.365238	0.826375
S	4.701293	0.653710	-1.888927	S	4.526060	1.588110	-1.837973
S	1.918738	1.615185	-1.935860	S	1.599332	2.015668	-1.857604
C	3.398034	1.337352	-3.019965	C	3.102277	2.042874	-2.937086
C	3.079569	0.333278	-4.131404	C	2.964471	1.023985	-4.074303
C	3.865366	2.680664	-3.586876	C	3.306643	3.460918	-3.478939
S	3.243964	-3.649946	1.379516	S	3.942905	-2.839815	1.537179
S	0.432767	-2.805323	1.351493	S	1.024051	-2.558875	1.512010
C	1.729321	-3.572434	2.440206	C	2.450588	-2.987208	2.621693
C	1.978040	-2.707697	3.679264	C	2.533500	-2.014415	3.801840
C	1.292654	-4.990848	2.814898	C	2.299201	-4.435497	3.092712
S	1.402448	1.671260	2.095303	S	0.932100	1.992530	2.131528
S	0.973347	4.601709	2.165681	S	-0.160142	4.755499	2.114904
C	2.243846	3.277304	-2.458050	C	1.361309	3.754287	2.492078
C	3.452671	3.470913	1.535029	C	2.539894	4.206288	1.620875
C	2.657845	3.303541	3.933420	C	1.687829	3.891330	3.983305
S	-2.099332	1.265011	-2.273778	S	-2.211710	0.741800	-2.354109
S	-2.701651	4.145466	-2.083224	S	-3.461344	3.429176	-2.224248
C	-3.467063	2.496065	-2.452920	C	-3.803497	1.644533	-2.622689
C	-4.603669	2.197321	-1.468128	C	-4.899441	1.089308	-1.703993
C	-3.962683	2.490853	-3.902635	C	-4.201385	1.530371	-4.097776
C	-4.894524	-3.290026	-0.020841	C	-4.040348	-4.281540	-0.009324
O	-5.129788	-4.086335	-0.913745	O	-3.975308	-5.173256	-0.916671
O	-5.801187	-3.058417	0.957021	O	-4.999093	-4.212478	0.825978
C	5.164883	-2.111552	-0.547671	C	5.591341	-0.929186	-0.379609
O	5.028395	-3.209634	-1.031556	O	5.716589	-2.170637	-0.584392
O	6.328125	-1.441180	-0.519078	O	6.493393	-0.064989	-0.550960
C	-1.032331	5.783603	0.153828	C	-2.362261	5.401249	-0.037115
O	-0.748224	6.437928	1.140029	O	-2.247876	6.087132	1.028856
O	-1.556271	6.362604	-0.951965	O	-2.948505	5.824185	-1.084653
H	-0.039043	-3.811761	-4.726330	H	1.063939	-3.826933	-4.568569
H	-1.665352	-3.093564	-4.818965	H	-0.679686	-3.519279	-4.751710
H	-1.465914	-4.852919	-4.649948	H	-0.079111	-5.174767	-4.501437
H	0.806049	-4.793621	-2.522467	H	2.011436	-4.510122	-2.289104
H	-0.632133	-5.840731	-2.427336	H	0.854948	-5.865224	-2.209272
H	-0.223761	-4.754515	-1.079919	H	0.929949	-4.670133	-0.894339
H	-1.832944	-0.587916	4.958407	H	-1.840242	-0.877238	4.938833
H	-2.032684	-1.917700	3.799922	H	-1.644091	-2.225322	3.801560
H	-3.258588	-1.652846	5.059704	H	-2.954730	-2.268039	5.001884
H	-4.788035	0.407896	4.931874	H	-4.941322	-0.641621	4.763001
H	-4.631107	1.546511	3.573359	H	-5.005772	0.475218	3.379862
H	-3.371411	1.461580	4.826220	H	-3.822313	0.726866	4.684092
H	2.281683	0.726422	-4.772102	H	2.105056	1.279497	-4.705539
H	2.747386	-0.622126	-3.716518	H	2.810809	0.015393	-3.680573
H	3.969751	0.155110	-4.746335	H	3.869986	1.022133	-4.693972
H	3.083830	3.109769	-4.224065	H	2.457816	3.749546	-4.109732

H	4.756846	2.537710	-4.208392
H	4.100860	3.393476	-2.792833
H	1.059787	-2.632203	4.273799
H	2.292997	-1.698291	3.401810
H	2.763691	-3.155826	4.298796
H	0.368638	-4.957433	3.403281
H	2.060827	-5.468855	3.433491
H	1.121954	-5.606685	1.928284
H	3.939252	4.429914	1.750748
H	3.152949	3.463616	0.483684
H	4.177115	2.662942	1.688536
H	3.126319	4.264891	4.173912
H	3.396154	2.518122	4.131518
H	1.799849	3.157305	4.594290
H	-5.388155	2.957844	-1.560118
H	-4.244754	2.194872	-0.435274
H	-5.040209	1.215021	-1.682339
H	-4.750279	3.241809	-4.033278
H	-4.393676	1.513858	-4.149145
H	-3.152549	2.705682	-4.603819
O	4.537333	-0.565996	1.297297
O	5.295655	-1.339517	2.043993
H	-1.682201	7.304592	-0.731331
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**1-CO<sub>2</sub>H-b-oo-radical**  
Structure

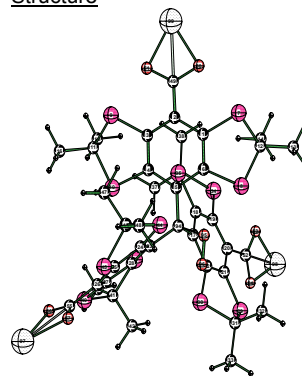


Coordinates

C	0.196224	3.778092	-0.907699
C	1.288945	4.094263	-0.073969
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C	1.419294	1.738225	0.586338
C	0.406915	1.388045	-0.344321
C	-0.217414	2.435571	-1.071538
S	-0.701819	5.016419	-1.805617
S	-1.527598	2.220241	-2.269636
S	3.144536	3.361344	1.920620
S	2.225764	0.580963	1.683005
C	2.810366	1.835953	2.902793
C	-2.169948	3.943286	-2.167643
C	-2.739604	4.331884	-3.538070
C	-3.226404	4.093899	-1.065978
C	1.754352	2.102132	3.982245
C	4.121825	1.340293	3.524442
C	-1.456362	-0.447187	-0.187445
C	-2.193351	0.328937	0.740216
C	-3.575343	0.110985	0.934030
C	-4.264679	-0.876254	0.203708
C	-3.533584	-1.704702	-0.667422
C	-2.143405	-1.515058	-0.828032
C	1.103658	-1.124476	-0.340181
C	2.313338	-1.062246	-1.089378
C	3.324250	-2.029071	-0.927634

H	4.209713	3.501754	-4.099650
H	3.404718	4.188001	-2.669032
H	1.619442	-2.073119	4.405129
H	2.653107	-0.984773	3.454896
H	3.392645	-2.265137	4.435854
H	1.390899	-4.544776	3.696832
H	3.150981	-4.716612	3.723426
H	2.243430	-5.127595	2.248276
H	2.782857	5.255201	1.832916
H	2.301136	4.113150	0.558135
H	3.421922	3.588511	1.825865
H	1.917443	4.936595	4.222722
H	2.571663	3.293222	4.234256
H	0.851419	3.564557	4.606384
H	-5.829019	1.654395	-1.846589
H	-4.609001	1.163123	-0.652413
H	-5.090587	0.033949	-1.932291
H	-5.127082	2.088839	-4.281531
H	-4.389020	0.482696	-4.360837
H	-3.419902	1.923434	-4.752985
O	4.549317	0.443786	1.398570
O	5.509580	-0.063286	2.133177
Na	-3.328010	7.686331	0.001432
Na	-5.860433	-5.968671	-0.148045
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**1-CO<sub>2</sub>Na-b-oo-radical**  
Structure



Coordinates

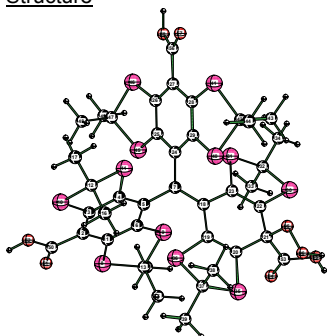
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C	1.413715	1.697818	0.603863
C	0.409282	1.379242	-0.345439
C	-0.191195	2.453410	-1.057650
S	-0.632731	5.058842	-1.745482
S	-1.490866	2.281762	-2.278420
S	3.124434	3.310803	1.992151
S	2.212595	0.513882	1.677637
C	2.802927	1.742164	2.920756
C	-2.111661	4.009640	-2.135489
C	-2.677117	4.436131	-3.496032
C	-3.170038	4.142396	-1.032817
C	1.752705	1.967746	4.016255
C	4.118957	1.233600	3.522010
C	-1.476126	-0.433929	-0.241887
C	-2.210085	0.327929	0.702378
C	-3.591065	0.108415	0.897230
C	-4.286522	-0.854447	0.151142
C	-3.562600	-1.663919	-0.733844
C	-2.173844	-1.481528	-0.904707
C	1.075791	-1.137887	-0.387766
C	2.295868	-1.071767	-1.118882
C	3.302101	-2.039431	-0.944042

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 C 2.012749 -3.100712 0.811539  
 C 0.984768 -2.146461 0.635778  
 S -4.265666 -3.039007 -1.589229  
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 C 4.187839 -4.128497 0.209223  
 O 4.340269 -4.754862 1.240722  
 O 4.943560 -4.369905 -0.886255  
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 H 4.636947 -0.279779 -4.416734  
 C 0.000287 -0.091274 -0.633491  
 O -0.183099 -0.008145 -2.154513

C 3.135792 -3.089574 -0.028796  
 C 1.965813 -3.135932 0.743341  
 C 0.939931 -2.180708 0.565918  
 S -4.332779 -2.982064 -1.648842  
 S -1.406296 -2.765561 -1.871813  
 C -2.918928 -3.190783 -2.831498  
 C -3.072809 -2.255677 -4.037635  
 C -2.836687 -4.657513 -3.265826  
 S -4.410524 1.105643 2.124633  
 S -1.533453 1.605047 1.760699  
 C -2.855764 1.491936 3.046013  
 C -2.536813 0.397264 4.071419  
 C -2.999177 2.860062 3.722007  
 S -0.371806 -2.299203 1.770878  
 S 1.747959 -4.345802 2.031243  
 C -0.068694 -4.059360 2.239078  
 C -0.876478 -5.014474 1.351955  
 C -0.434486 -4.238538 3.717877  
 S 2.691867 0.186574 -2.322688  
 S 4.778372 -1.858019 -1.922563  
 C 4.520480 -0.052745 -2.253390  
 C 5.153308 0.802947 -1.149363  
 C 5.108057 0.290237 -3.627443  
 C 1.924195 5.437206 0.032632  
 O 1.391775 6.361075 -0.661868  
 O 2.981418 5.611267 0.721100  
 C -5.765734 -1.028090 0.317573  
 O -6.440918 -0.040361 0.749428  
 O -6.279421 -2.151801 0.014162  
 C 4.205288 -4.128502 0.132790  
 O 4.287190 -4.743770 1.243253  
 O 4.981228 -4.346343 -0.850712  
 H -3.544207 3.818066 -3.758478  
 H -1.927996 4.343742 -4.286525  
 H -3.016155 5.478316 -3.453230  
 H -4.040559 3.516186 -1.262781  
 H -3.500575 5.185743 -0.951639  
 H -2.773714 3.826954 -0.064317  
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 H 0.817176 2.336625 3.589042  
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 H -3.992112 -2.499131 -4.584360  
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 H -3.801801 2.827376 4.468629  
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 H -0.652747 -6.053958 1.623070  
 H -0.636473 -4.869902 0.295966  
 H -1.951341 -4.840257 1.481246  
 H -0.234734 -5.270329 4.031169  
 H -1.503386 -4.048550 3.871819  
 H 0.140147 -3.561977 4.355260  
 H 6.235973 0.627491 -1.113793  
 H 4.728139 0.563114 -0.171610  
 H 4.975869 1.867490 -1.343677  
 H 6.191373 0.119705 -3.624863  
 H 4.940582 1.348740 -3.858861  
 H 4.658761 -0.317533 -4.416780  
 C -0.013574 -0.087163 -0.670051  
 O -0.181639 0.031044 -2.191957

O	0.259769	-1.019139	-2.887435
H	5.602378	-5.039178	-0.621351
H	-7.209018	-2.120838	0.206730
H	3.184635	6.614495	0.448917

**1-CO<sub>2</sub>H-a-ooH**  
Structure

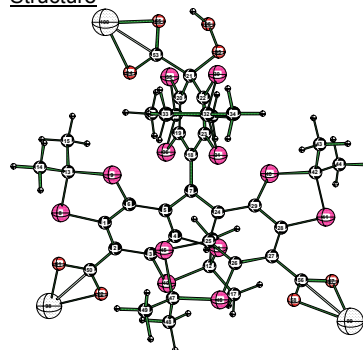


Coordinates

C	-2.014238	-3.163598	-0.919221
C	-3.052949	-3.172330	0.041365
C	-3.092412	-2.146586	1.019094
C	-2.151526	-1.102661	0.981588
C	-1.105199	-1.084085	0.031217
C	-1.056744	-2.131562	-0.918345
C	-0.124818	0.038083	-0.063633
S	-1.872260	-4.373443	-2.208670
S	0.097961	-2.137087	-2.268773
S	-4.289431	-2.046517	2.335432
S	-2.358683	0.184232	2.187638
C	-3.320876	-0.853650	3.373802
C	-0.145131	-3.912202	-2.722268
C	-0.025304	-4.063790	-4.243599
C	0.875820	-4.795618	-1.993708
C	-2.378660	-1.610605	4.318049
C	-4.295967	0.037288	4.150543
C	1.244329	-0.189731	-0.074583
C	1.881168	-1.345700	0.570241
C	3.231370	-1.508448	0.626462
C	4.214236	-0.491030	0.095612
C	3.521248	0.544276	-0.755207
C	2.175445	0.722695	-0.757123
C	-0.665536	1.430150	-0.118024
C	-1.674103	1.827354	-1.027426
C	-2.232157	3.118931	-0.992398
C	-1.782469	4.057806	-0.037053
C	-0.776879	3.678310	0.879881
C	-0.225665	2.384219	0.835747
S	4.515595	1.623258	-1.747747
S	1.606641	2.033121	-1.835710
C	3.126404	2.048214	-2.902244
C	3.017800	1.005520	-4.018312
C	3.332811	3.458499	-3.460216
S	3.861600	-2.921810	1.481393
S	0.949358	-2.573777	1.485429
C	2.366859	-3.110401	2.556619
C	2.487479	-2.217840	3.794922
C	2.182070	-4.582747	2.932336
S	0.931308	1.995384	2.126760
S	-0.186433	4.745112	2.169147
C	1.341998	3.752782	2.532144
C	2.518602	4.239236	1.677338
C	1.656255	3.860155	4.028547
S	-2.203835	0.792683	-2.365682
S	-3.473284	3.451869	-2.223862
C	-3.810782	1.670538	-2.621881

O	0.246234	-0.974039	-2.941815
Na	5.982690	-5.839914	0.394839
Na	-8.218539	-1.307295	0.581880
Na	2.983959	7.686989	0.028830

**1-CO<sub>2</sub>Na-a-ooH**  
Structure

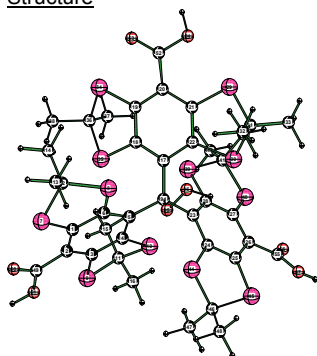


Coordinates

C	-0.573467	3.605812	-0.861831
C	0.346224	4.293324	-0.045141
C	1.140349	3.553216	0.855525
C	1.065622	2.150054	0.887242
C	0.155497	1.444304	0.067163
C	-0.651751	2.202284	-0.815837
C	0.083368	-0.047784	0.033226
S	-1.631384	4.422992	-2.036807
S	-1.699015	1.436231	-2.030968
S	2.288289	4.306692	1.990193
S	2.182838	1.334559	2.001237
C	2.447507	2.808767	3.082080
C	-2.703309	2.941514	-2.389658
C	-3.084568	2.948092	-3.874985
C	-3.952853	2.966078	-1.498286
C	1.393732	2.848968	4.196260
C	3.866073	2.760760	3.659469
C	-1.125181	-0.716075	0.176894
C	-2.259972	-0.180723	0.944260
C	-3.423945	-0.862612	1.125533
C	-3.750610	-2.155517	0.419567
C	-2.551544	-2.683228	-0.319846
C	-1.362997	-2.040990	-0.417879
C	1.366535	-0.795683	-0.134152
C	2.285441	-0.511562	-1.171730
C	3.532038	-1.156813	-1.245633
C	3.899178	-2.112260	-0.281558
C	2.996399	-2.413775	0.755347
C	1.748566	-1.767939	0.827855
S	-2.768065	-4.209487	-1.195261
S	-0.187714	-2.828984	-1.518519
C	-1.463526	-3.807605	-2.450409
C	-2.057595	-2.969039	-3.587098
C	-0.822790	-5.096809	-2.968192
S	-4.636100	-0.187543	2.219876
S	-2.142398	1.362274	1.855695
C	-3.451611	0.943724	3.091662
C	-2.845818	0.214898	4.297212
C	-4.176503	2.224488	3.515547
S	0.766180	-2.149126	2.262789
S	3.374029	-3.562953	2.059631
C	1.616881	-3.749339	2.636048
C	0.928650	-4.907998	1.903548
C	1.614439	-3.972843	4.152540
S	1.890197	0.556300	-2.531364
S	4.568256	-0.716915	-2.624027
C	3.650016	0.852802	-3.016260

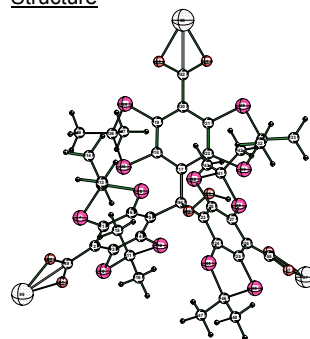
C	-4.895179	1.108272	-1.695101
C	-4.216844	1.558089	-4.094950
C	-4.090040	-4.217622	-0.088605
O	-4.124560	-5.051327	-0.977826
O	-5.057688	-4.174560	0.857202
C	5.312252	-1.187350	-0.746251
O	5.111877	-2.125150	-1.476219
O	6.529634	-0.599447	-0.615056
C	-2.331345	5.428213	0.073510
O	-2.238525	6.133246	1.061675
O	-2.943800	5.867581	-1.051227
H	0.984429	-3.791762	-4.572619
H	-0.748738	-3.434781	-4.767871
H	-0.194820	-5.108142	-4.530901
H	1.894898	-4.523663	-2.292867
H	0.704676	-5.849667	-2.244438
H	0.796519	-4.677526	-0.910181
H	-1.806264	-0.900320	4.926138
H	-1.671924	-2.227369	3.756103
H	-2.956204	-2.260988	4.985869
H	-4.900658	-0.571092	4.833109
H	-4.964560	0.580408	3.478230
H	-3.741477	0.762397	4.757080
H	2.161966	1.238553	-4.662347
H	2.877016	0.001359	-3.609130
H	3.929198	1.007959	-4.628197
H	2.491732	3.730579	-4.107897
H	4.243554	3.493689	-4.069068
H	3.414048	4.199570	-2.661274
H	1.575110	-2.291094	4.398749
H	2.635195	-1.172124	3.513408
H	3.341623	-2.533563	4.405443
H	1.276836	-4.705297	3.538018
H	3.030701	-4.926368	3.534914
H	2.099348	-5.217064	2.046209
H	2.744793	5.286528	1.911979
H	2.289437	4.163938	0.611108
H	3.408123	3.630940	1.878054
H	1.872921	4.901883	4.292244
H	2.544989	3.266276	4.271156
H	0.820108	3.510353	4.639076
H	-5.829808	1.665288	-1.831499
H	-4.599103	1.182414	-0.645159
H	-5.078933	0.052798	-1.926471
H	-5.149330	2.106686	-4.270819
H	-4.396413	0.508953	-4.355882
H	-3.443900	1.958496	-4.755556
O	4.789111	0.329861	1.148626
O	5.717197	-0.435032	1.961123
H	-3.292029	6.754280	-0.840878
H	7.119985	-1.061996	-1.240663
H	-5.676919	-4.895247	0.636408
H	6.543370	-0.271480	1.465127

**1-CO<sub>2</sub>H-b-ooH**  
Structure



C	4.233539	2.029643	-2.224191
C	3.719191	1.106558	-4.525638
C	0.543784	5.767759	-0.195244
O	-0.192736	6.401956	-1.017386
O	1.466310	6.327148	0.482260
C	-4.888814	-1.926416	-0.650743
O	-4.683942	-1.056793	-1.534262
O	-5.926472	-2.666297	-0.596627
C	5.229553	-2.794134	-0.355803
O	5.699979	-3.318958	0.702568
O	5.831006	-2.816463	-1.477976
H	-3.708614	2.076707	-4.109941
H	-2.198941	2.927799	-4.514692
H	-3.667906	3.846561	-4.111106
H	-4.571635	2.081262	-1.692146
H	-4.542064	3.870434	-1.698585
H	-3.677441	2.956129	-0.440648
H	1.477849	1.958706	4.831216
H	0.384428	2.875194	3.776489
H	1.535369	3.741604	4.818327
H	4.051384	3.648142	4.276831
H	4.617000	2.723097	2.866272
H	3.987592	1.879679	4.300633
H	-1.266780	-2.662924	-4.282050
H	-2.543161	-2.070739	-3.195033
H	-2.800616	-3.560523	-4.139259
H	-0.019594	-4.860239	-3.675624
H	-1.566228	-5.702154	-3.500578
H	-0.405345	-5.691108	-2.151423
H	-2.118395	0.863504	4.800200
H	-2.333361	-0.698433	3.984070
H	-3.632192	-0.056548	5.012080
H	-3.477977	2.905879	4.015230
H	-4.975051	1.988802	4.229052
H	-4.612693	2.739376	2.655967
H	1.453557	-5.848582	2.113425
H	0.926508	-4.743953	0.822895
H	-0.112058	-5.003601	2.234783
H	2.139424	-4.904494	4.395785
H	0.586131	-4.068079	4.520817
H	2.102410	-3.148319	4.678228
H	5.285827	2.179977	-2.496257
H	4.178290	1.846610	-1.147790
H	3.678196	2.949553	-2.443038
H	4.761099	1.253293	-4.834784
H	3.165973	2.017126	-4.784548
H	3.301835	0.268478	-5.089636
O	-4.075829	-3.241890	1.309261
O	-5.377252	-3.043302	1.920095
H	-5.933414	-3.168073	1.112770
Na	0.915695	8.206995	-0.468341
Na	7.437922	-3.912265	-0.489996
Na	-6.514897	-1.774859	-2.520044

**1-CO<sub>2</sub>Na-b-ooH**  
Structure





## Coordinates

C	3.434229	-1.862036	-0.901073
C	3.296868	-2.945626	-0.008562
C	2.113651	-3.051046	0.757340
C	1.053115	-2.134071	0.575894
C	1.162490	-1.062569	-0.346913
C	2.368881	-0.954965	-1.094754
S	4.908325	-1.591399	-1.850334
S	2.656795	0.255196	-2.369675
S	1.854393	-4.323743	1.980365
S	-0.384922	-2.480802	1.576111
C	0.508265	-3.433722	2.872395
C	4.495744	0.142648	-2.358813
C	5.002856	0.370961	-3.789656
C	5.126333	1.148263	-1.387584
C	1.086360	-2.500215	3.942910
C	-0.453958	-4.457756	3.485300
C	0.251246	1.437208	-0.293128
C	1.349289	1.861707	0.493725
C	1.652311	3.234037	0.628095
C	0.850455	4.216509	0.018450
C	-0.325848	3.813128	-0.643230
C	-0.634373	2.443348	-0.764574
C	-1.427170	-0.537495	-0.292881
C	-2.066158	-1.504561	-1.116082
C	-3.403071	-1.886632	-0.883961
C	-4.125216	-1.335454	0.194101
C	-3.470740	-0.460215	1.080425
C	-2.139397	-0.056251	0.837955
S	-1.497889	4.964923	-1.330328
S	-2.296144	2.148784	-1.391349
C	-2.400223	3.718864	-2.356901
C	-1.754861	3.587609	-3.741599
C	-3.872437	4.132464	-2.463557
S	3.078580	3.653453	1.603465
S	2.411791	0.789292	1.455932
C	3.012774	2.106432	2.610109
C	2.063392	2.269237	3.803122
C	4.428358	1.743612	3.072091
S	-1.425470	0.913304	2.149180
S	-4.244930	0.122655	2.566677
C	-3.014654	1.461953	2.916152
C	-3.485995	2.799078	2.332872
C	-2.812459	1.561354	4.433993
S	-1.292991	-2.319708	-2.510537
S	-4.084379	-3.097391	-1.996420
C	-2.445852	-3.766511	-2.522656
C	-1.963343	-4.859803	-1.561925
C	-2.557006	-4.293062	-3.958043
C	4.380864	-3.956392	0.008352
O	5.400406	-3.889476	-0.655596
O	4.146355	-5.026043	0.802999
C	1.294143	5.628284	0.117713
O	2.445191	5.974775	0.303009
O	0.292138	6.530821	0.005376
C	-5.541454	-1.679649	0.471094
O	-6.068268	-1.620306	1.565971
O	-6.235288	-2.044419	-0.631565
H	4.759934	1.388319	-4.118454
H	4.559355	-0.339848	-4.491095
H	6.093564	0.265317	-3.824440
H	4.871315	2.172555	-1.684210
H	6.218379	1.044467	-1.393694
H	4.765957	0.990726	-0.368694
H	0.276638	-1.959938	4.446984
H	1.762589	-1.764971	3.498671
H	1.642089	-3.081346	4.688434
H	0.065050	-5.051440	4.246674
H	-0.855894	-5.134416	2.727045
H	-1.287983	-3.944547	3.977249

## Coordinates

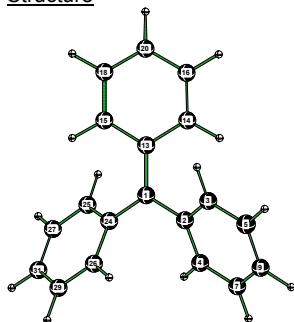
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C	1.048497	-2.128438	0.560504
C	1.169858	-1.057238	-0.360112
C	2.391809	-0.949126	-1.086396
S	4.953292	-1.575383	-1.790564
S	2.695285	0.253043	-2.369610
S	1.877892	-4.311732	1.982338
S	-0.407876	-2.504758	1.523617
C	0.469982	-3.459805	2.827976
C	4.534068	0.152536	-2.318185
C	5.069321	0.380772	-3.738572
C	5.133395	1.171422	-1.340321
C	0.985328	-2.526150	3.931396
C	-0.488308	-4.512132	3.397306
C	0.256960	1.438402	-0.314130
C	1.344062	1.865811	0.488531
C	1.633995	3.238886	0.637637
C	0.841222	4.218771	0.024641
C	-0.319071	3.813112	-0.650863
C	-0.624871	2.446075	-0.789373
C	-1.418391	-0.536911	-0.347215
C	-2.049933	-1.495346	-1.185841
C	-3.385129	-1.883915	-0.959629
C	-4.114823	-1.362622	0.120203
C	-3.475778	-0.485744	1.008313
C	-2.147448	-0.067219	0.779741
S	-1.472693	4.990223	-1.326896
S	-2.279713	2.161258	-1.442704
C	-2.372549	3.753058	-2.374555
C	-1.722252	3.638541	-3.758944
C	-3.843667	4.168538	-2.484733
S	3.035043	3.669009	1.651415
S	2.401745	0.793205	1.460252
C	2.969618	2.106078	2.635177
C	2.000133	2.242591	3.815817
C	4.380644	1.751517	3.117113
S	-1.455807	0.906502	2.103098
S	-4.275798	0.089524	2.490098
C	-3.059867	1.440524	2.847758
C	-3.532512	2.772656	2.253132
C	-2.874992	1.550983	4.366943
S	-1.277610	-2.289568	-2.593295
S	-4.086294	-3.064315	-2.092948
C	-2.447528	-3.722360	-2.640997
C	-1.966072	-4.843763	-1.711380
C	-2.560920	-4.212708	-4.088809
C	4.359646	-3.988504	0.117493
O	5.429091	-3.851043	-0.558205
O	4.125762	-5.011903	0.838315
C	1.206278	5.668214	0.126551
O	2.428743	5.966314	0.310242
O	0.278607	6.532789	0.019752
C	-5.546057	-1.759352	0.329116
O	-6.015060	-1.726734	1.511032
O	-6.225067	-2.105488	-0.688599
H	4.822212	1.393661	-4.079140
H	4.647717	-0.338652	-4.444937
H	6.162107	0.286486	-3.750408
H	4.849933	2.190503	-1.630278
H	6.228620	1.097831	-1.341743
H	4.772456	0.997683	-0.324250
H	0.148339	-2.002731	4.408824
H	1.666373	-1.775637	3.520752
H	1.522465	-3.104750	4.693393
H	0.024085	-5.113613	4.157898
H	-0.857255	-5.179578	2.614292
H	-1.345117	-4.026925	3.879660



H	-2.294343	2.844614	-4.342303
H	-0.708214	3.282291	-3.667938
H	-1.800575	4.549409	-4.265438
H	-4.432022	3.389996	-3.043878
H	-3.954358	5.091068	-2.988418
H	-4.335678	4.232217	-1.478785
H	2.010310	1.335747	4.375676
H	1.053310	2.525423	3.472323
H	2.423888	3.066107	4.464495
H	4.416457	0.798688	3.627307
H	4.811718	2.518009	3.746519
H	5.114435	1.644463	2.227330
H	-4.442831	3.085742	2.785850
H	-3.617401	2.734217	1.250461
H	-2.751045	3.585253	2.542457
H	-3.751247	1.855170	4.917656
H	-2.067243	2.330592	4.667975
H	-2.482997	0.609584	4.857611
H	-2.664566	-5.702980	-1.564756
H	-1.875784	-4.481186	-0.539948
H	-0.977382	-5.223157	-1.874588
H	-3.255808	-5.136718	-3.998303
H	-1.581406	-4.656424	-4.300622
H	-2.902771	-3.516983	-4.645609
C	0.000908	-0.051225	-0.682619
O	0.120652	-0.217586	-2.153004
O	-0.256664	0.856415	-3.025736
H	-7.127673	-2.290685	-0.323011
H	0.713580	7.410380	0.037915
H	4.921315	-5.609420	0.697979
H	-1.229294	0.752609	-3.064910

H	-2.262319	2.909594	-4.376768
H	-0.678792	3.322244	-3.682721
H	-1.754715	4.610111	-4.266597
H	-4.404039	3.436218	-3.077819
H	-3.921317	5.136048	-2.994782
H	-4.310156	4.255254	-1.500058
H	1.936745	1.297128	4.367815
H	0.996144	2.503927	3.470978
H	2.347152	3.026885	4.500096
H	4.366347	0.810251	3.679076
H	4.754950	2.532713	3.789692
H	5.075411	1.648124	2.279808
H	-4.494793	3.058294	2.696749
H	-3.654859	2.698720	1.170253
H	-2.802433	3.564503	2.459624
H	-3.821664	1.839223	4.839643
H	-2.138007	2.327098	4.605837
H	-2.542175	0.603666	4.798124
H	-2.685419	-5.672336	-1.712958
H	-1.849547	-4.484123	-0.685310
H	-0.993790	-5.222492	-2.049302
H	-3.257228	-5.058021	-4.148371
H	-1.585762	-4.562305	-4.447932
H	-2.914663	-3.420048	-4.753310
C	0.013973	-0.047587	-0.713799
O	0.157116	-0.209478	-2.183202
O	-0.222621	0.862606	-3.059590
Na	-7.909131	-2.435008	0.668685
Na	1.818153	8.068651	0.278166
Na	6.065278	-5.796418	0.204147
H	-1.200275	0.796759	-3.053344

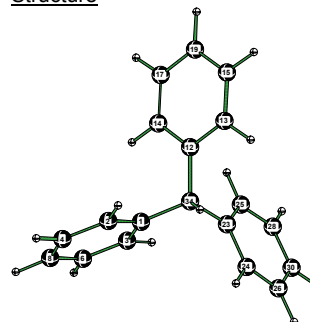
**CPh<sub>3</sub>**  
Structure



Coordinates

C	-0.001266	-0.004788	0.000316
C	1.207673	-0.831123	0.003163
C	2.384489	-0.413313	0.670744
C	1.251999	-2.078767	-0.665089
C	3.532107	-1.199551	0.673622
H	2.379325	0.529148	1.208949
C	2.404157	-2.858393	-0.665669
H	0.375071	-2.418525	-1.206795
C	3.552214	-2.426948	0.004980
H	4.414481	-0.856289	1.207775
H	2.409450	-3.805011	-1.200098
H	4.450297	-3.038562	0.006212
C	0.113505	1.456745	-0.000314
C	1.158339	2.113142	-0.693560
C	-0.815036	2.269700	0.692618
C	1.263999	3.500441	-0.696037
H	1.876404	1.519233	-1.250025
C	-0.701460	3.656406	0.693884
H	-1.617000	1.796588	1.250295
C	0.336884	4.282553	-0.001426
H	2.069783	3.975286	-1.250067

**CPh<sub>3</sub>-H**  
Structure

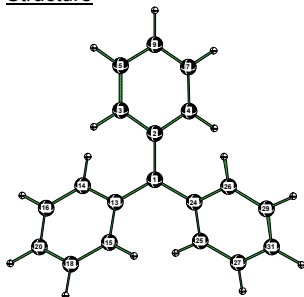


Coordinates

C	1.281540	-0.732472	-0.324454
C	2.442148	-0.557084	-1.092793
C	1.350790	-1.556367	0.805109
C	3.637217	-1.183830	-0.744286
H	2.405904	0.081224	-1.973225
C	2.548291	-2.183641	1.159554
H	0.461577	-1.718843	1.406729
C	3.694898	-2.001079	0.387289
H	4.522616	-1.037424	-1.357727
H	2.579498	-2.820884	2.039713
H	4.624461	-2.493450	0.660399
C	-0.007228	1.473690	-0.323263
C	-0.747450	2.390912	-1.083716
C	0.679357	1.944434	0.802314
C	-0.802875	3.738351	-0.731175
H	-1.288207	2.041122	-1.960706
C	0.622882	3.293820	1.160878
H	1.271625	1.255224	1.396658
C	-0.116740	4.195679	0.396413
H	-1.378895	4.431932	-1.338472
H	1.164867	3.638789	2.037802

H	-1.422571	4.252315	1.247588
H	0.422558	5.365766	-0.001913
C	-1.323277	-0.633766	-0.002635
C	-2.423601	-0.034739	-0.662991
C	-1.558325	-1.863895	0.658607
C	-3.679181	-0.633538	-0.665218
H	-2.274514	0.898756	-1.196073
C	-2.817130	-2.455951	0.658944
H	-0.742999	-2.338599	1.194951
C	-3.886876	-1.847425	-0.003933
H	-4.499519	-0.154419	-1.193641
H	-2.967197	-3.393882	1.187614
H	-4.868862	-2.312537	-0.004804

**CPh<sub>3</sub><sup>+</sup>**  
Structure

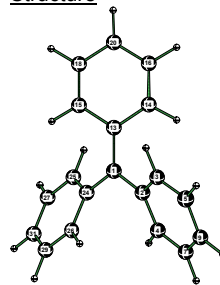


Coordinates

C	-0.000545	-0.000989	-0.001810
C	-0.253426	1.426358	-0.000373
C	-1.379768	1.964306	0.677453
C	0.620057	2.318139	-0.677922
C	-1.609073	3.332706	0.685926
H	-2.031507	1.302791	1.237557
C	0.364615	3.681904	-0.688422
H	1.460924	1.920646	-1.235598
C	-0.743920	4.192062	-0.002053
H	-2.456071	3.735842	1.231931
H	1.021979	4.351178	-1.234301
H	-0.933579	5.261463	-0.002657
C	-1.109411	-0.934146	-0.001746
C	-2.323925	-0.618965	-0.667697
C	-1.006914	-2.183807	0.665839
C	-3.378059	-1.521035	-0.674700
H	-2.403530	0.310386	-1.220774
C	-2.077217	-3.066629	0.676333
H	-0.104334	-2.421224	1.218057
C	-3.260184	-2.741166	0.001798
H	-4.290835	-1.282206	-1.211208
H	-1.998303	-4.006031	1.214229
H	-4.091716	-3.439839	0.003150
C	1.362641	-0.493890	-0.000989
C	1.701531	-1.694322	-0.680315
C	2.389265	0.213311	0.679605
C	3.010719	-2.153844	-0.687415
H	0.939303	-2.222896	-1.242194
C	3.689334	-0.271345	0.691643
H	2.139959	1.108530	1.238674
C	4.003971	-1.449409	0.003585
H	3.264265	-3.056301	-1.234531
H	4.460008	0.261062	1.239951
H	5.025297	-1.818835	0.005277

H	-0.155629	5.246051	0.672657
C	-1.273585	-0.742749	-0.322533
C	-1.728874	-1.810715	-1.109113
C	-1.995655	-0.411584	0.830625
C	-2.869227	-2.530319	-0.755039
H	-1.179265	-2.081987	-2.008120
C	-3.136889	-1.132683	1.190521
H	-1.671680	0.423133	1.445109
C	-3.578617	-2.193578	0.399922
H	-3.205885	-3.351335	-1.382932
H	-3.683740	-0.857958	2.088970
H	-4.469743	-2.750333	0.677419
C	0.000417	-0.001323	-0.740510
H	0.000089	-0.002040	-1.838732

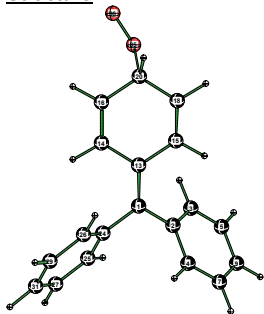
**CPh<sub>3</sub><sup>-</sup>**  
Structure



Coordinates

C	0.000501	-0.001896	-0.001720
C	1.325297	-0.611424	-0.000339
C	2.454464	0.003587	0.616856
C	1.595521	-1.868719	-0.617058
C	3.718130	-0.575620	0.611846
H	2.314248	0.954914	1.122085
C	2.858184	-2.450161	-0.609599
H	0.783362	-2.382009	-1.123803
C	3.946298	-1.815394	0.002013
H	4.538265	-0.057756	1.109931
H	3.000415	-3.409978	-1.107002
H	4.934847	-2.269671	0.003225
C	-0.133069	1.450795	-0.000876
C	0.820733	2.311860	-0.619238
C	-1.228011	2.121971	0.618849
C	0.694236	3.696265	-0.612123
H	1.670236	1.863853	-1.126796
C	-1.357449	3.506092	0.613109
H	-1.981040	1.525168	1.125516
C	-0.398297	4.322118	0.000768
H	1.453725	4.298727	-1.111175
H	-2.214587	3.958622	1.112473
H	-0.498528	5.405449	0.001081
C	-1.190927	-0.842689	-0.002083
C	-2.414514	-0.443550	-0.616881
C	-1.226800	-2.128281	0.614654
C	-3.551708	-1.243017	-0.609507
H	-2.450786	0.517461	-1.121889
C	-2.362646	-2.929679	0.609600
H	-0.334260	-2.485042	1.120527
C	-3.549359	-2.503547	0.000490
H	-4.453453	-0.882936	-1.105580
H	-2.327066	-3.899140	1.107375
H	-4.438877	-3.129937	0.001473

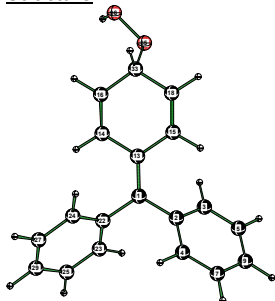
**CPh<sub>3</sub>-a-oo-radical**  
Structure



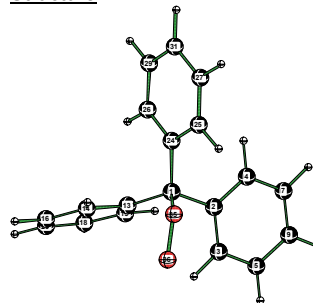
Coordinates

C	0.546899	0.003617	-0.086012
C	1.347299	-1.250016	-0.049642
C	0.989224	-2.324422	0.785491
C	2.516793	-1.371788	-0.823669
C	1.759384	-3.486613	0.827421
H	0.111831	-2.233424	1.418958
C	3.278783	-2.537140	-0.789972
H	2.817884	-0.546964	-1.462852
C	2.903214	-3.599838	0.035882
H	1.468346	-4.300389	1.486275
H	4.169648	-2.615545	-1.407454
H	3.502862	-4.505464	0.068024
C	-0.824781	-0.003919	-0.217949
C	-1.643708	1.184483	0.026577
C	-1.566432	-1.203630	-0.609107
C	-2.983735	1.179607	-0.086374
H	-1.144065	2.088430	0.357089
C	-2.903681	-1.221183	-0.756619
H	-0.998221	-2.095239	-0.850635
C	-3.756837	-0.030139	-0.487238
H	-3.566659	2.065283	0.151576
H	-3.406974	-2.122263	-1.096851
H	-4.462232	0.174889	-1.300791
C	1.325909	1.266256	0.032330
C	2.317832	1.402811	1.021471
C	1.129471	2.334295	-0.862415
C	3.061448	2.575473	1.131764
H	2.493761	0.583770	1.712657
C	1.882500	3.503593	-0.758775
H	0.393516	2.233583	-1.654778
C	2.847263	3.630950	0.241765
H	3.811900	2.665038	1.912685
H	1.719503	4.312314	-1.466233
H	3.433473	4.542241	0.323310
O	-4.683629	-0.400099	0.657529
O	-5.779576	0.330019	0.637402

**CPh<sub>3</sub>-a-ooH**  
Structure



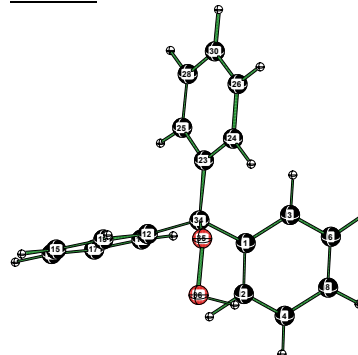
**CPh<sub>3</sub>-b-oo-radical**  
Structure



Coordinates

C	0.018501	0.006047	0.480921
C	1.318274	-0.676456	0.042337
C	1.545925	-2.023909	0.374591
C	2.302491	0.007088	-0.682786
C	2.732072	-2.655716	0.007741
H	0.793817	-2.570559	0.930267
C	3.486398	-0.631901	-1.059349
H	2.149281	1.043238	-0.961011
C	3.708198	-1.962845	-0.712207
H	2.890901	-3.695326	0.281824
H	4.234218	-0.081502	-1.624022
H	4.630630	-2.459062	-1.002146
C	-1.249844	-0.730896	0.051430
C	-2.452068	-0.503144	0.739376
C	-1.265454	-1.568732	-1.069203
C	-3.632305	-1.117284	0.328273
H	-2.461041	0.153614	1.602987
C	-2.452910	-2.175125	-1.488458
H	-0.349051	-1.751018	-1.620163
C	-3.637915	-1.956795	-0.788727
H	-4.550791	-0.937657	0.880589
H	-2.443833	-2.822591	-2.361225
H	-4.559913	-2.434025	-1.109823
C	-0.038051	1.495960	0.128280
C	0.660006	2.433298	0.906831
C	-0.745986	1.947150	-0.992408
C	0.636518	3.787822	0.576226
H	1.218213	2.102278	1.775311
C	-0.758094	3.301962	-1.328488
H	-1.293194	1.239004	-1.605544
C	-0.071104	4.227838	-0.543693
H	1.175534	4.499484	1.195926
H	-1.312587	3.631297	-2.203182
H	-0.086422	5.283303	-0.801924
O	0.033305	0.057610	2.009742
O	-0.116265	-1.110941	2.590011

**CPh<sub>3</sub>-b-ooH**  
Structure



Coordinates

C	0.585160	0.000534	-0.077922
C	1.427916	-1.226566	-0.044191
C	1.122846	-2.303353	0.808387
C	2.586793	-1.317864	-0.837837
C	1.932846	-3.438377	0.848677
H	0.252870	-2.236090	1.455022
C	3.389948	-2.455434	-0.804735
H	2.848142	-0.490361	-1.491055
C	3.066236	-3.521327	0.038673
H	1.680842	-4.254684	1.520536
H	4.272271	-2.509741	-1.437071
H	3.697298	-4.405471	0.069570
C	-0.785123	-0.050339	-0.200270
C	-1.639645	1.116568	0.035676
C	-1.495655	-1.278457	-0.566351
C	-2.977557	1.072604	-0.082090
H	-1.164630	2.033963	0.366667
C	-2.830406	-1.336634	-0.713333
H	-0.903729	-2.161033	-0.783083
H	-3.577207	1.951132	0.141922
H	-3.312321	-2.260314	-1.022198
C	1.326327	1.287696	0.031429
C	2.316875	1.459999	1.016320
C	1.096527	2.344982	-0.867945
C	3.026820	2.654322	1.117504
H	2.519932	0.650017	1.710903
C	1.814465	3.537037	-0.772775
H	0.360469	2.218560	-1.656547
C	2.778859	3.698614	0.223167
H	3.777583	2.769541	1.894927
H	1.624770	4.336774	-1.483960
H	3.338509	4.627133	0.297585
C	-3.729512	-0.158243	-0.491874
H	-4.332716	0.035054	-1.393088
O	-4.669952	-0.579517	0.533929
O	-5.768328	0.381279	0.520887
H	-5.658166	0.766843	1.408274

Coordinates

C	1.220846	-0.809802	-0.010677
C	1.199634	-2.215342	0.059646
C	2.386982	-0.192294	-0.484571
C	2.309399	-2.970435	-0.321266
H	0.303481	-2.718114	0.405151
C	3.495265	-0.948492	-0.871475
H	2.433051	0.887994	-0.559355
C	3.463461	-2.339961	-0.788812
H	2.266361	-4.054737	-0.258361
H	4.384230	-0.443555	-1.240345
H	4.326005	-2.928065	-1.090955
C	-1.339782	-0.568215	0.062635
C	-2.457499	-0.403744	0.890752
C	-1.510818	-1.190734	-1.180714
C	-3.711970	-0.860221	0.489550
H	-2.333673	0.075985	1.855286
C	-2.769641	-1.640576	-1.586718
H	-0.657267	-1.330475	-1.837044
C	-3.874470	-1.479787	-0.751492
H	-4.565653	-0.731273	1.149894
H	-2.880825	-2.121033	-2.555367
H	-4.853358	-1.834679	-1.062953
C	0.113468	1.502748	0.132433
C	0.816247	2.394774	0.957820
C	-0.467467	1.997519	-1.042438
C	0.925186	3.744167	0.618229
H	1.273199	2.033116	1.871127
C	-0.347228	3.344376	-1.386322
H	-1.025043	1.331580	-1.691720
C	0.346195	4.225313	-0.556086
H	1.466842	4.418513	1.276480
H	-0.806066	3.704444	-2.303425
H	0.432521	5.275853	-0.820695
C	0.015390	0.006340	0.499937
O	0.074288	0.061573	1.961216
O	-0.020064	-1.264911	2.527173
H	0.923227	-1.512644	2.572582

### Molecular oxygen

#### Structure



#### Coordinates

O	0.000000	0.000000	0.607296
O	0.000000	0.000000	-0.607296

### Hydroxyl radical

#### Structure



#### Coordinates

O	0.000000	0.000000	0.109213
H	0.000000	0.000000	-0.873701

### Water

#### Structure

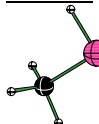


#### Coordinates

O	0.000000	0.000000	0.119720
H	0.000000	0.761560	-0.478879
H	0.000000	-0.761560	-0.478879

### Methylthiol

#### Structure

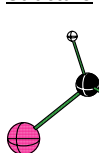


#### Coordinates

C	-1.164836	0.019536	0.000000
H	-1.531096	-1.009787	-0.000021
H	-1.535819	0.522757	0.895782
H	-1.535817	0.522792	-0.895763
S	0.667735	-0.087181	0.000000
H	0.907990	1.241915	0.000000

### CH3S radical

#### Structure

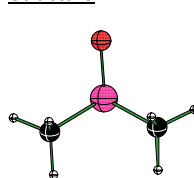


#### Coordinates

S	-0.697635	0.000002	-0.001831
C	1.115063	0.000011	-0.008304
H	1.436288	-0.000589	1.042807
H	1.517776	0.899835	-0.481373
H	1.517724	-0.899345	-0.482319

### DMSO

#### Structure

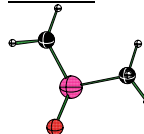


#### Coordinates

S	0.000012	0.242953	-0.439537
O	-0.000105	1.508325	0.387008
C	-1.363358	-0.822250	0.180119
H	-1.332320	-1.796498	-0.317507
H	-1.275418	-0.933848	1.264946
H	-2.300201	-0.313698	-0.059958
C	1.363419	-0.822104	0.180141
H	1.275249	-0.934271	1.264893
H	1.332738	-1.796125	-0.317956
H	2.300233	-0.313277	-0.059448

### CH2SOCH3 radical

#### Structure



#### Coordinates

S	-0.134927	-0.142875	-0.392320
O	-0.638960	-1.377494	0.309817
C	1.580437	0.210819	0.188535
H	1.911303	1.170434	-0.218137
H	1.588810	0.222705	1.280536
H	2.213105	-0.596367	-0.187792
C	-0.906676	1.298571	0.227718
H	-1.932933	1.194064	0.564051
H	-0.552335	2.258771	-0.137587

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