I. DFT-Optimized Cartesian Coordinates for DELTA50 Compounds

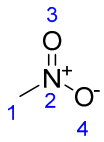
Optimized geometries *in vacuo* at the B3LYP/6-31G(d) level from Gaussian 16, Revision C.01 [1] for each compound in the DELTA50 training set are provided below. Optimized coordinates of the dominant conformer (≥ 98%) are provided. Experimental proton and carbon chemical shifts were referenced to TMS at 0.00 ppm (see acquired spectra in Section II).

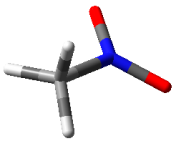
For conformer determinations and Boltzmann weightings, a mixed torsional, low-mode sampling search in MacroModel was performed with the OPLS4 force field [2], as implemented in Schrodinger software suite, version 2021-1 [3]. DFT Gibbs free energies were then calculated at the level of M06-2X/6-31+G(d,p) including the SMD solvent model for chloroform. The Boltzmann probabilities were calculated using the following equation.

$$p_i = \frac{e^{-\varepsilon_i/kT}}{\sum_{j=1}^{M} e^{-\varepsilon_j/kT}}$$

where p_i is the probability of the i^{th} state
ε_i is the energy of the i^{th} state
k is the Boltzmann constant
T is temperature
M is the number of states

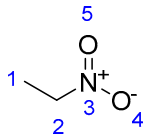
Compound 1: **Nitromethane**

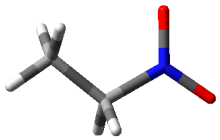




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-1.325474	-0.000005	-0.002538	62.49
2	-	N	0.174089	0.000000	-0.011776	-
3	-	O	0.731302	1.092955	0.003254	-
4	-	O	0.731302	-1.092950	0.003254	-
5	C1	H	-1.665785	-0.906616	-0.499708	4.33
6	C1	H	-1.665789	0.906569	-0.499774	4.33
7	C1	H	-1.635114	0.000035	1.045083	4.33

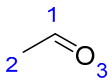
Compound 2: **Nitroethane**

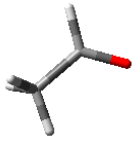




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-1.878328	0.098482	-0.000511	12.31
2	-	C	-0.627705	-0.758597	0.000661	70.47
3	-	N	0.654059	0.052770	0.000123	-
4	-	O	1.697683	-0.592331	-0.000557	-
5	-	O	0.570845	1.276342	0.000288	-
6	C1	H	-2.754961	-0.558268	-0.000005	1.59
7	C1	H	-1.922726	0.738517	0.884010	1.59
8	C1	H	-1.922383	0.736632	-0.886423	1.59
9	C2	H	-0.544965	-1.399815	-0.880815	4.42
10	C2	H	-0.545407	-1.397857	0.883625	4.42

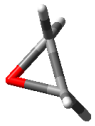
Compound 3: **Acetaldehyde**





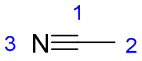
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.234239	0.399962	-0.000002	199.97
2	-	C	-1.171113	-0.148450	0.000001	30.99
3	-	O	1.237659	-0.277271	0.000001	-
4	C1	H	0.302577	1.512156	0.000003	9.80
5	C2	H	-1.713937	0.218871	-0.880943	2.21
6	C2	H	-1.154729	-1.240768	-0.000028	2.21
7	C2	H	-1.713936	0.218830	0.880963	2.21

Compound 4: **Oxirane**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	0.000001	0.855353	0.000000	-
2	-	C	-0.734442	-0.371867	-0.000001	40.94
3	-	C	0.734441	-0.371867	0.000001	40.94
4	C3	H	1.274772	-0.595107	0.920457	2.69
5	C3	H	1.274774	-0.595106	-0.920455	2.69
6	C2	H	-1.274772	-0.595105	-0.920458	2.69
7	C2	H	-1.274775	-0.595106	0.920454	2.69

Compound 5: **Acetonitrile**

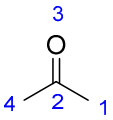


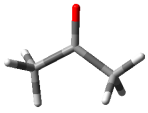
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.280559	0.000022	0.000032	116.33
2	-	C	-1.181127	-0.000005	-0.000006	1.91
3	-	N	1.440866	-0.000010	-0.000013	-
4	C2	H	-1.560884	-0.950715	0.387217	2.01
5	C2	H	-1.560927	0.810703	0.629685	2.01
6	C2	H	-1.560842	0.139978	-1.016971	2.01

Compound 6: **Cyclopropane**

Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-0.492427	-0.718224	0.000003	-3.15
2	-	C	-0.375776	0.785563	-0.000007	-3.15
3	-	C	0.868266	-0.067308	0.000002	-3.15
4	C1	H	-0.827012	-1.206263	0.911497	0.25
5	C1	H	-0.827011	-1.206266	-0.911490	0.25
6	C3	H	1.458202	-0.113027	-0.911499	0.25
7	C3	H	1.458179	-0.113014	0.911519	0.25
8	C2	H	-0.631365	1.319196	0.911510	0.25
9	C2	H	-0.631371	1.319189	-0.911526	0.25

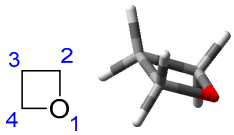
Compound 7: **Acetone**





Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	1.293088	-0.614813	0.000004	30.94
2	-	C	-0.000003	0.185303	0.000026	206.93
3	-	O	0.000030	1.400974	-0.000010	-
4	-	C	-1.293122	-0.614774	-0.000013	30.94
5	C1	H	-1.341564	-1.267122	0.881099	2.17
6	C1	H	-2.148522	0.063608	-0.000211	2.17
7	C1	H	-1.341318	-1.267479	-0.880857	2.17
8	C4	H	1.341193	-1.267740	0.880691	2.17
9	C4	H	1.341663	-1.266896	-0.881290	2.17
10	C4	H	2.148524	0.063541	0.000546	2.17

Compound 8: **Oxetane**

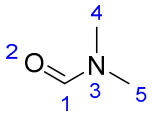


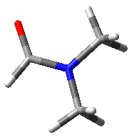
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	0.000000	-1.072579	0.000125	-
2	-	C	1.036814	-0.064801	-0.000084	72.55
3	-	C	-0.000000	1.077698	0.000082	22.35
4	-	C	-1.036814	-0.064801	-0.000084	72.55
5	C2	H	1.672620	-0.132539	0.892519	4.76
6	C2	H	1.672232	-0.132514	-0.892972	4.76
7	C3	H	-0.000000	1.710902	0.890879	2.70
8	C3	H	-0.000000	1.711261	-0.890459	2.70
9	C4	H	-1.672620	-0.132539	0.892519	4.76
10	C4	H	-1.672232	-0.132514	-0.892972	4.76

Compound 9: **Methyl acetate**

Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	-	C	0.000000	0.493825	0.000000	171.55
2	-	C	-1.133612	1.492846	0.000000	20.71
3	-	O	1.180758	0.763097	0.000000	-
4	-	O	-0.476542	-0.773738	0.000000	-
5	-	C	0.523356	-1.804412	0.000000	51.62
6	C2	H	-1.765505	1.345823	0.882046	2.06
7	C2	H	-0.725713	2.504101	0.000000	2.06
8	C2	H	-1.765505	1.345823	-0.882046	2.06
9	C5	H	-0.026169	-2.746405	0.000000	3.67
10	C5	H	1.155351	-1.728879	-0.889147	3.67
11	C5	H	1.155351	-1.728879	0.889147	3.67

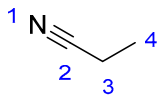
Compound 10: **N,N-Dimethylformamide (DMF)**





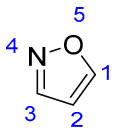
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.697924	-0.825549	0.000000	162.52
2	-	O	0.209607	-1.943285	0.000000	-
3	-	N	0.000000	0.348854	0.000000	-
4	-	C	0.665195	1.635661	0.000000	31.44
5	-	C	-1.452628	0.332528	0.000000	36.48
6	C1	H	1.792762	-0.653290	0.000000	8.02
7	C4	H	0.394574	2.221023	0.889346	2.89
8	C4	H	1.749320	1.489175	0.000000	2.89
9	C4	H	0.394574	2.221023	-0.889346	2.89
10	C5	H	-1.846975	0.839609	-0.890461	2.96
11	C5	H	-1.777086	-0.708689	0.000000	2.96
12	C5	H	-1.846975	0.839609	0.890461	2.96

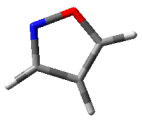
Compound 11: **Propionitrile**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	-1.370404	-1.429413	0.000000	-
2	-	C	-0.773054	-0.434092	0.000000	120.68
3	-	C	0.000000	0.812731	0.000000	10.92
4	-	C	-1.519806	0.567322	0.000000	10.48
5	C3	H	-0.293533	1.398433	0.879652	2.36
6	C3	H	-0.293533	1.398433	-0.879652	2.36
7	C2	H	2.048163	1.525644	0.000000	1.30
8	C2	H	1.825611	0.003809	0.886224	1.30
9	C2	H	1.825611	0.003809	-0.886224	1.30

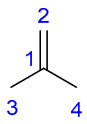
Compound 12: **Isoxazole**

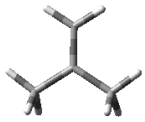




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	1.127837	0.000000	157.64
2	-	C	1.128139	0.368535	0.000000	103.47
3	-	C	0.617674	-0.960436	0.000000	149.02
4	-	N	-0.694334	-0.995568	0.000000	-
5	-	O	-1.093882	0.345149	0.000000	-
6	C1	H	-0.184497	0.345149	0.000000	8.48
7	C2	H	2.156947	2.192680	0.000000	6.38
8	C3	H	1.164069	-1.895339	0.000000	8.31

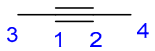
Compound 13: **Isobutylene (2-Methylpropene)**





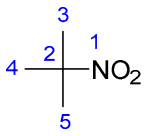
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	-0.000000	0.122960	142.45
2	-	C	0.000000	-0.000000	1.459489	110.47
3	-	C	0.000000	1.278083	-0.678954	24.13
4	-	C	-0.000000	-1.278083	-0.678954	24.13
5	C2	H	0.000000	-0.924634	2.031659	4.66
6	C2	H	0.000000	0.924634	2.031659	4.66
7	C3	H	0.000000	2.163190	-0.035443	1.73
8	C3	H	0.880040	1.332255	-1.334921	1.73
9	C3	H	-0.880040	1.332255	-1.334921	1.73
10	C4	H	-0.000000	-2.163190	-0.035443	1.73
11	C4	H	-0.880040	-1.332255	-1.334921	1.73
12	C4	H	0.880040	-1.332255	-1.334921	1.73

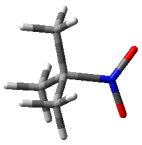
Compound 14: **2-Butyne**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	0.000000	0.604587	74.54
2	-	C	0.000000	0.000000	-0.604587	74.54
3	-	C	0.000000	0.000000	2.066081	3.37
4	-	C	0.000000	0.000000	-2.066081	3.37
5	C3	H	0.000000	1.021502	2.466253	1.75
6	C3	H	-0.884647	-0.510751	2.466253	1.75
7	C3	H	0.884647	-0.510751	2.466253	1.75
8	C4	H	0.000000	1.021502	-2.466253	1.75
9	C4	H	0.884647	-0.510751	-2.466253	1.75
10	C4	H	-0.884647	-0.510751	-2.466253	1.75

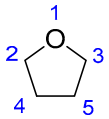
Compound 15: **t-Butyl nitrate (2-Methyl-2-nitropropane)**

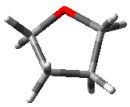




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	-0.146964	-0.975496	0.000000	-
2	-	C	0.063658	0.559662	0.000000	85.06
3	-	C	-1.299721	1.246854	0.000000	27.87
4	-	C	0.866281	0.878877	1.268433	27.87
5	-	C	0.866281	0.878877	-1.268433	27.87
6	C3	H	-1.143931	2.331156	0.000000	1.62
7	C3	H	-1.883032	0.980536	-0.884879	1.62
8	C3	H	-1.883032	0.980536	0.884879	1.62
9	C4	H	1.069422	1.954161	1.303318	1.62
10	C4	H	0.303440	0.609249	2.168502	1.62
11	C4	H	1.816375	0.340115	1.273084	1.62
12	C5	H	1.069422	1.954161	-1.303318	1.62
13	C5	H	0.303440	0.609249	-2.168502	1.62
14	C5	H	1.816375	0.340115	-1.273084	1.62
15	-	O	-1.293622	-1.411438	0.000000	-
16	-	O	0.866281	-1.670614	0.000000	-

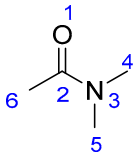
Compound 16: **Tetrahydrofuran (THF)**

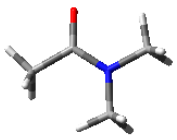




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	0.000000	-0.000000	1.251442	-
2	-	C	0.000000	1.172681	0.430760	67.99
3	-	C	-0.000000	-1.172681	0.430760	67.99
4	-	C	-0.307936	0.703722	-0.996748	25.62
5	-	C	0.307936	-0.703722	-0.996748	25.62
6	C2	H	-0.742265	1.877577	0.823672	3.75
7	C3	H	0.742265	-1.877577	0.823672	3.75
8	C3	H	0.987905	1.656495	0.483033	3.75
9	C2	H	-0.987905	-1.656495	0.483033	3.75
10	C4	H	-1.391540	0.644345	-1.155142	1.85
11	C5	H	1.391540	-0.644345	-1.155142	1.85
12	C4	H	0.110732	1.365421	-1.761405	1.85
13	C5	H	-0.110732	-1.365421	-1.761405	1.85

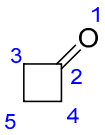
Compound 17: **N,N-Dimethylacetamide (DMAc)**

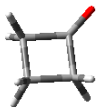




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	1.067377	-1.472559	0.000130	-
2	-	C	0.728849	-0.293308	-0.000029	170.66
3	-	N	-0.596288	0.083564	-0.000285	-
4	-	C	-1.623986	-0.946085	-0.000013	35.20
5	-	C	-1.083783	1.450223	0.000127	38.05
6	-	C	1.778984	0.813138	-0.000038	21.58
7	C4	H	-1.133732	-1.918451	-0.000364	2.94
8	C4	H	-2.261301	-0.855378	0.890146	2.94
9	C4	H	-2.262012	-0.855052	-0.889618	2.94
10	C5	H	-0.261812	2.164327	-0.000763	3.01
11	C5	H	-1.704698	1.640728	-0.886873	3.01
12	C5	H	-1.703029	1.640949	0.888265	3.01
13	C6	H	2.754921	0.326973	0.000021	2.08
14	C6	H	1.703172	1.453769	-0.886055	2.08
15	C6	H	1.703108	1.453846	0.885917	2.08

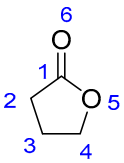
Compound 18: **Cyclobutanone**

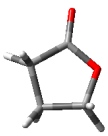




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	-0.000000	0.000000	1.883380	-
2	-	C	-0.000000	0.000000	0.680062	209.40
3	-	C	-0.000000	1.111393	-0.385557	47.74
4	-	C	-0.000000	-1.111393	-0.385557	47.74
5	-	C	0.000000	0.000000	-1.480192	9.71
6	C3	H	-0.887021	1.754218	-0.350761	3.09
7	C3	H	0.887021	1.754218	-0.350761	3.09
8	C4	H	-0.887021	-1.754218	-0.350761	3.09
9	C4	H	0.887021	-1.754218	-0.350761	3.09
10	C5	H	-0.887077	0.000000	-2.118265	2.01
11	C5	H	0.887077	-0.000000	-2.118265	2.01

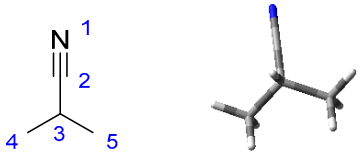
Compound 19: **Butyrolactone**





Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.889487	-0.001520	0.003368	177.65
2	-	C	-0.026980	1.209424	0.169334	27.80
3	-	C	-1.406468	0.669083	-0.219782	22.20
4	-	C	-1.269380	-0.822646	0.127783	68.48
5	-	O	0.127216	-1.134993	-0.043504	-
6	-	O	2.089064	-0.028869	-0.072118	-
7	C2	H	0.012392	1.522563	1.220723	2.50
8	C2	H	0.334092	2.042919	-0.436677	2.50
9	C3	H	-2.237210	1.144067	0.308940	2.27
10	C3	H	-1.574055	0.791455	-1.295294	2.27
11	C4	H	-1.545750	-1.029880	1.169152	4.35
12	C4	H	-1.839665	-1.486270	-0.526076	4.35

Compound 20: **Isobutyronitrile (2-Cyanopropane)**

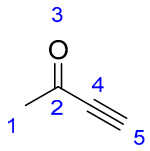


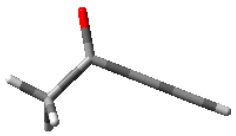
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	-0.405239	-2.185681	0.000000	-
2	-	C	-0.026629	-1.087975	0.000000	123.76
3	-	C	0.438658	0.309211	-0.000000	19.84
4	-	C	-0.026629	1.032249	1.279737	19.95
5	-	C	-0.026629	1.032249	-1.279737	19.95
6	C3	H	1.536699	0.274152	0.000000	2.70
7	C4	H	0.325365	0.517215	2.178429	1.33
8	C4	H	0.367828	2.053774	1.288429	1.33
9	C4	H	-1.119520	1.084616	1.320106	1.33
10	C5	H	0.325365	0.517215	-2.178429	1.33
11	C5	H	0.367828	2.053774	-1.288429	1.33
12	C5	H	-1.119520	1.084616	-1.320106	1.33

Compound 21: **Furan**

Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	-0.000000	0.000000	1.161192	-
2	-	C	-0.000000	1.094672	0.347334	142.54
3	-	C	-0.000000	-1.094672	0.347334	142.54
4	-	C	0.000000	0.717590	-0.960054	109.45
5	-	C	-0.000000	-0.717590	-0.960054	109.45
6	C2	H	-0.000000	2.049543	0.850322	7.45
7	C3	H	-0.000000	-2.049543	0.850322	7.45
8	C4	H	0.000000	1.374522	-1.818771	6.40
9	C5	H	-0.000000	-1.374522	-1.818771	6.40

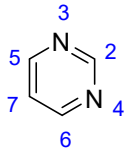
Compound 22: **3-Butyn-2-one**

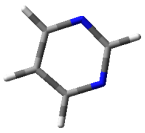




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	1.287423	-1.061063	0.000015	32.63
2	-	C	0.452063	0.202176	-0.000033	183.94
3	-	O	0.933957	1.320930	0.000034	-
4	-	C	-0.994215	0.005826	-0.000121	81.84
5	-	C	-2.191020	-0.168654	0.000038	78.10
6	C1	H	1.052982	-1.669866	-0.881556	2.38
7	C1	H	1.053211	-1.669598	0.881837	2.38
8	C1	H	2.346708	-0.795971	-0.000143	2.38
9	C5	H	-3.250066	-0.301720	0.000205	3.21

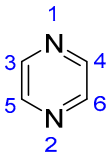
Compound 23: **Pyrimidine**

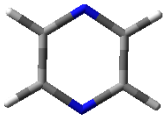




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	C2	H	-0.000000	-0.000000	-2.397628	9.21
2	-	C	-0.000000	-0.000000	-0.309221	159.10
3	-	N	0.000000	1.199170	-0.716460	-
4	-	N	-0.000000	-1.199170	-0.716460	-
5	-	C	0.000000	1.184371	0.622298	156.94
6	-	C	-0.000000	-1.184371	0.622298	156.94
7	-	C	0.000000	0.000000	1.356463	121.58
8	C5	H	0.000000	2.154249	1.117670	8.76
9	C6	H	-0.000000	-2.154249	1.117670	8.76
10	C7	H	0.000000	0.000000	2.441707	7.34

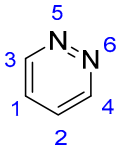
Compound 24: **1,4-Pyrazine**

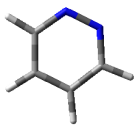




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	0.000000	0.000000	1.409502	-
2	-	N	0.000000	0.000000	-1.409502	-
3	-	C	0.000000	1.133170	0.698425	145.18
4	-	C	-0.000000	-1.133170	0.698425	145.18
5	-	C	0.000000	1.133170	-0.698425	145.18
6	-	C	-0.000000	-1.133170	-0.698425	145.18
7	C3	H	0.000000	2.067277	1.257022	8.60
8	C4	H	-0.000000	-2.067277	1.257022	8.60
9	C5	H	0.000000	2.067277	-1.257022	8.60
10	C6	H	-0.000000	-2.067277	-1.257022	8.60

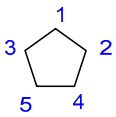
Compound 25: **1,2-Pyrazine (pyridazine)**

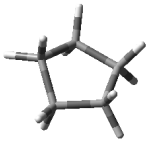




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	0.691979	1.180878	126.36
2	-	C	-0.000000	-0.691979	1.180878	126.36
3	-	C	0.000000	1.322940	-0.067711	151.72
4	-	C	-0.000000	-1.322940	-0.067711	151.72
5	-	N	0.000000	0.668403	-1.232308	-
6	-	N	-0.000000	-0.668403	-1.232308	-
7	C1	H	0.000000	1.272126	2.099037	7.49
8	C2	H	-0.000000	-1.272126	2.099037	7.49
9	C3		0.000000	2.407140	-0.151885	9.23
10	C4	H	-0.000000	-2.407140	-0.151885	9.23

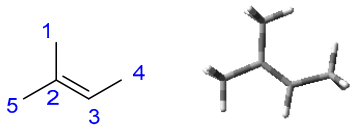
Compound 26: **Cyclopentane**





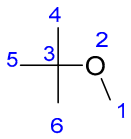
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-0.000000	0.000000	1.308322	25.84
2	-	C	-0.000000	1.243115	0.371790	25.84
3	-	C	-0.000000	-1.243115	0.371790	25.84
4	-	C	-0.328308	0.694836	-1.031133	25.84
5	-	C	0.328308	-0.694836	-1.031133	25.84
6	C1	H	0.877601	0.006551	1.963936	1.50
7	C1	H	-0.877601	-0.006551	1.963936	1.50
8	C2	H	-0.702811	2.017236	0.698224	1.50
9	C2	H	0.995910	1.703363	0.359696	1.50
10	C3	H	0.702811	-2.017236	0.698224	1.50
11	C3	H	-0.995910	-1.703363	0.359696	1.50
12	C4	H	-1.415293	0.589197	-1.152471	1.50
13	C4	H	0.027837	1.344896	-1.838294	1.50
14	C5	H	1.415293	-0.589197	-1.152471	1.50
15	C5	H	-0.027837	1.344896	-1.838294	1.50

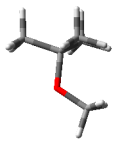
Compound 27: **2-Methyl-2-butene**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-1.508735	0.496709	0.000000	17.32
2	-	C	0.000000	0.450978	0.000000	132.10
3	-	C	0.735359	-0.671272	0.000000	118.44
4	-	C	0.267551	-2.099880	0.000000	13.41
5	-	C	0.663899	1.808386	0.000000	25.63
6	C1	H	-1.972994	-0.492122	0.000000	1.60
7	C1	H	-1.880102	1.041295	0.879589	1.60
8	C1	H	-1.880102	1.041295	-0.879589	1.60
9	C3	H	1.820291	-0.552712	0.000000	5.19
10	C4	H	-0.821428	-2.196887	0.000000	1.56
11	C4	H	0.649157	-2.636213	-0.879870	1.56
12	C4	H	0.649157	-2.636213	0.879870	1.56
13	C5	H	1.755677	1.729246	0.000000	1.68
14	C5	H	0.365948	2.396391	-0.879917	1.68
15	C5	H	0.365948	2.396391	0.879917	1.68

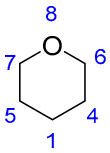
Compound 28: **Methyl t-butyl ether (MTBE)**





Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.635656	-1.945029	0.000000	49.47
2	-	O	-0.443936	-1.034131	0.000000	-
3	-	C	-0.139565	0.374999	-0.000000	72.79
4	-	C	-1.524158	1.033189	-0.000000	26.99
5	-	C	0.635656	0.773487	1.266946	26.99
6	-	C	0.635656	0.773487	-1.266946	26.99
7	C1	H	0.189192	-2.943662	0.000000	3.21
8	C1	H	1.272407	-1.853184	-0.892175	3.21
9	C1	H	1.272407	-1.853184	0.892175	3.21
10	C4	H	-1.438804	2.125188	-0.000000	1.19
11	C4	H	-2.088966	0.725958	-0.886242	1.19
12	C4	H	-2.088966	0.725958	0.886242	1.19
13	C5	H	0.737202	1.862898	1.324953	1.19
14	C5	H	0.104275	0.429520	2.160987	1.19
15	C5	H	1.645898	0.350169	1.281904	1.19
16	C6	H	0.737202	1.862898	-1.324953	1.19
17	C6	H	0.104275	0.429520	-2.160987	1.19
18	C6	H	1.645898	0.350169	-1.281904	1.19

Compound 29: **Tetrahydropyran (THP)**

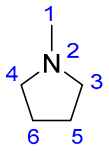


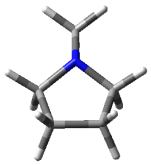
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	-	C	-0.626248	1.328824	0.000000	23.46
2	C1	H	-1.701325	1.095140	0.000000	1.64
3	C1	H	-0.541876	2.422329	0.000000	1.64
4	-	C	0.020517	0.731339	1.259702	26.60
5	-	C	0.020517	0.731339	-1.259702	26.60
6	-	C	0.020517	-0.797942	1.179649	68.71
7	-	C	0.020517	-0.797942	-1.179649	68.71
8	-	O	0.663440	-1.265666	-0.000000	-
9	C4	H	1.058694	1.078846	1.344361	1.57
10	C4	H	-0.507657	1.055870	2.165785	1.57
11	C5	H	1.058694	1.078846	-1.344361	1.57
12	C5	H	-0.507657	1.055870	-2.165785	1.57
13	C6	H	0.567381	-1.242901	2.016957	3.65
14	C6	H	-1.018037	-1.174735	1.213826	3.65
15	C7	H	0.567381	-1.242901	-2.016957	3.65
16	C7	H	-1.018037	-1.174735	-1.213826	3.65

[a:] Atomic coordinates for chair conformation.

The chair conformation of THP was found to comprise 99.98% of the Boltzmann population. Thus, the boat and twisted boat conformations can be neglected.

Compound 30: **N-Methylpyrrolidine**

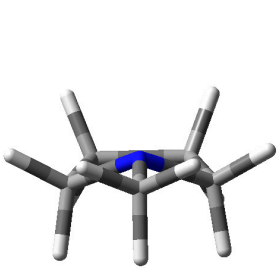




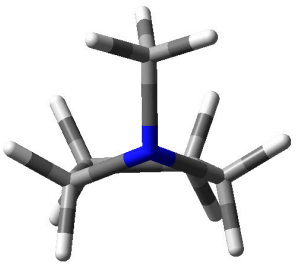
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	-	C	0.337276	2.099453	-0.000000	42.14
2	-	N	0.446990	0.654778	-0.000000	-
3	-	C	-0.163353	0.003840	-1.157016	56.27
4	-	C	-0.163353	0.003840	0.778520	56.27
5	-	C	-0.163353	-1.489826	-0.778520	24.06
6	-	C	-0.163353	-1.489826	-0.000000	24.06
7	C1	H	-0.713743	2.454949	-0.886306	2.38
8	C1	H	0.833530	2.510891	0.886306	2.38
9	C1	H	0.833530	2.510891	0.886306	2.38
10	C3	H	0.405145	0.224036	2.068209	2.50
11	C3	H	-1.202898	0.357961	1.320962	2.50
12	C4	H	0.405145	0.224036	-2.068209	2.50
13	C4	H	-1.202898	0.357961	-1.320962	2.50
14	C5	H	0.734195	-1.983997	1.162545	1.81
15	C5	H	-1.029164	-2.010529	1.199099	1.81
16	C6	H	0.734195	-1.983997	-1.162545	1.81
17	C6	H	-1.029164	-2.010529	-1.199099	1.81

[a:] Atomic coordinates for equatorial methyl conformation.

N-Methylpyrrolidine exhibits two conformations with the methyl group either equatorial or axial. The equatorial configuration comprises 98.96% of the Boltzmann population, allowing for the axial configuration to effectively be ignored in chemical shift calculations.

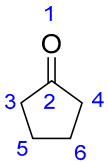


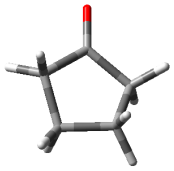
Conformer 1 (98.96%)



Conformer 2 (1.04%)

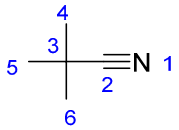
Compound 31: **Cyclopentanone**

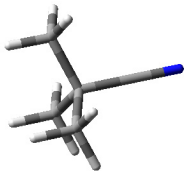




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	-0.000000	-0.000000	2.138951	-
2	-	C	-0.000000	-0.000000	0.927928	220.72
3	-	C	-0.000000	1.244707	0.029822	38.37
4	-	C	-0.000000	-1.244707	0.029822	38.37
5	-	C	0.298048	0.713931	-1.382020	23.25
6	-	C	-0.298048	-0.713931	-1.382020	23.25
7	C3	H	-1.005695	1.686525	0.083726	2.17
8	C3	H	0.699264	1.997654	0.405732	2.17
9	C4	H	1.005695	-1.686525	0.083726	2.17
10	C4	H	-0.699264	-1.997654	0.405732	2.17
11	C5	H	-0.115120	1.343317	-2.176147	1.96
12	C5	H	1.383118	0.661440	-1.539712	1.96
13	C6	H	0.115120	-1.343317	-2.176147	1.96
14	C6	H	-1.383118	-0.661440	-1.539712	1.96

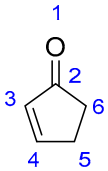
Compound 32: **Pivalonitrile**

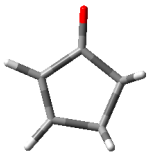




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	0.000000	0.000000	2.360404	-
2	-	C	0.000000	0.000000	1.199078	125.94
3	-	C	0.000000	0.000000	-0.279922	28.09
4	-	C	0.000000	1.464540	-0.772873	28.43
5	-	C	1.268329	-0.732270	-0.772873	28.43
6	-	C	-1.268329	-0.732270	-0.772873	28.43
7	C4	H	0.000000	1.481013	-1.868679	1.37
8	C4	H	-0.887101	2.000032	-0.420003	1.37
9	C4	H	0.887101	2.000032	-0.420003	1.37
10	C5	H	1.282595	-0.740506	-1.868679	1.37
11	C5	H	2.175629	-0.231764	-0.420003	1.37
12	C5	H	1.288528	-1.768268	-0.420003	1.37
13	C6	H	-1.282595	-0.740506	-1.868679	1.37
14	C6	H	-1.288528	-1.768268	-0.420003	1.37
15	C6	H	-2.175629	-0.231764	-0.420003	1.37

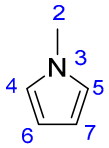
Compound 33: **Cyclopent-2-en-1-one**

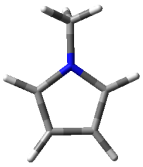




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	0.062874	2.101042	0.000000	-
2	-	C	-0.000000	0.886527	0.000000	210.57
3	-	C	-1.226581	0.053604	0.000000	134.63
4	-	C	-0.904837	-1.248423	0.000000	164.76
5	-	C	0.586361	-1.494497	0.000000	28.97
6	-	C	1.199661	-0.079145	0.000000	34.01
7	C3	H	-2.222203	0.482809	0.000000	6.22
8	C4	H	-1.619092	-2.067869	0.000000	7.73
9	C5	H	0.883541	-2.084946	0.876941	2.70
10	C5	H	0.883541	-2.084946	-0.876941	2.70
11	C6	H	1.821800	0.119109	0.879224	2.37
12	C6	H	1.821800	0.119109	-0.879224	2.37

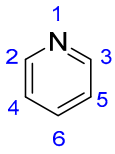
Compound 34: **N-Methylpyrrole**

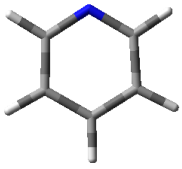




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	C2	H	1.122656	2.408002	0.000000	3.67
2	-	C	0.077753	2.072793	0.000000	36.08
3	-	N	-0.025623	0.626404	0.000000	-
4	-	C	-0.019442	-0.174768	1.119668	121.66
5	-	C	-0.019442	-0.174768	-1.119668	121.66
6	-	C	-0.019442	-1.491662	0.711854	108.18
7	-	C	-0.019442	-1.491662	-0.711854	108.18
8	C2	H	-0.419796	2.475976	-0.886418	3.67
9	C2	H	-0.419796	2.475976	0.886418	3.67
10	C4	H	-0.018103	0.263657	2.108051	6.61
11	C5	H	-0.018103	0.263657	-2.108051	6.61
12	C6	H	-0.033705	-2.355849	1.362526	6.14
13	C7	H	-0.033705	-2.355849	-1.362526	6.14

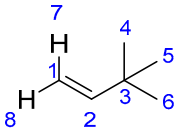
Compound 35: **Pyridine**

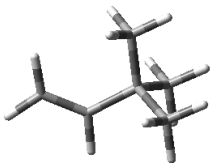




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	0.000000	0.000000	1.420887	-
2	-	C	0.000000	1.142176	0.721977	149.74
3	-	C	-0.000000	-1.142176	0.721977	149.74
4	-	C	-0.000000	1.198645	-0.673027	123.78
5	-	C	-0.000000	-1.198645	-0.673027	123.78
6	-	C	-0.000000	0.000000	-1.385530	136.09
7	C2	H	0.000000	2.059822	1.308640	8.62
8	C3	H	-0.000000	-2.059822	1.308640	8.62
9	C4	H	-0.000000	2.157868	-1.182641	7.30
10	C5	H	-0.000000	-2.157868	-1.182641	7.30
11	C6	H	-0.000000	0.000000	-2.472431	7.69

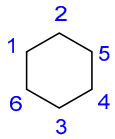
Compound 36: **t-Butylethylene (3,3-Dimethyl-1-butene)**

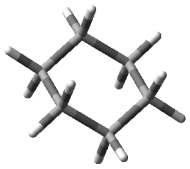




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	-0.126415	-2.206499	0.000000	108.86
2	-	C	0.568530	-1.068294	0.000000	149.88
3	-	C	0.032129	0.351659	0.000000	33.66
4	-	C	-1.504297	0.399969	0.000000	29.16
5	-	C	0.568530	1.072457	1.258635	29.16
6	-	C	0.568530	1.072457	-1.258635	29.16
7	C1	H	-1.212586	-2.231006	0.000000	4.91
8	C1	H	0.374902	-3.170922	0.000000	4.83
9	C2	H	1.659520	-1.129168	0.000000	5.86
10	C4	H	-1.851348	1.439804	0.000000	1.01
11	C4	H	-1.920343	-0.091428	-0.886937	1.01
12	C4	H	-1.920343	-0.091428	0.886937	1.01
13	C5	H	0.250199	2.122321	1.268782	1.01
14	C5	H	0.199058	0.594541	2.172973	1.01
15	C5	H	1.664817	1.054964	1.289888	1.01
16	C6	H	0.250199	2.122321	-1.268782	1.01
17	C6	H	0.199058	0.594541	-2.172973	1.01
18	C6	H	1.664817	1.054964	-1.289888	1.01

Compound 37: **Cyclohexane**

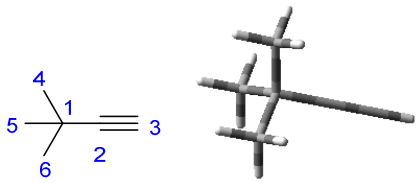




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	-	C	-1.270575	0.733567	0.229404	26.93
2	-	C	-0.000000	1.467134	-0.229404	26.93
3	-	C	-0.000000	-1.467134	0.229404	26.93
4	-	C	1.270575	-0.733567	-0.229404	26.93
5	-	C	1.270575	0.733567	0.229404	26.93
6	-	C	-1.270575	-0.733567	-0.229404	26.93
7	C1	H	-1.329754	0.767734	1.327713	1.43
8	C2	H	-0.000000	1.535468	-1.327713	1.43
9	C3	H	-0.000000	-1.535468	1.327713	1.43
10	C4	H	1.329754	-0.767734	-1.327713	1.43
11	C5	H	1.329754	0.767734	1.327713	1.43
12	C6	H	-1.329754	-0.767734	-1.327713	1.43
13	C1	H	-2.163615	1.249164	-0.146953	1.43
14	C2	H	-0.000000	2.498328	0.146953	1.43
15	C3	H	-0.000000	-2.498328	-0.146953	1.43
16	C4	H	2.163615	-1.249164	0.146953	1.43
17	C5	H	2.163615	1.249164	-0146953	1.43
18	C6	H	-2.163615	-1.249164	0.146953	1.43

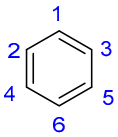
[a:] Atomic coordinates for chair form of cyclohexane (> 99.9% of Boltzmann distribution).

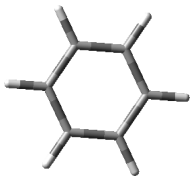
Compound 38: **t-Butylacetylene**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.299144	0.000020	0.000000	27.23
2	-	C	-1.174913	0.000162	0.000000	93.21
3	-	C	-2.383181	0.000246	0.000000	66.36
4	-	C	0.808400	1.460302	0.000000	30.88
5	-	C	0.808400	-0.730286	1.264506	30.88
6	-	C	0.808400	-0.730286	-1.264506	30.88
7	C3	H	-3.449350	0.000284	0.000000	2.07
8	C4	H	1.904911	1.475745	0.000000	1.25
9	C4	H	0.456098	1.998231	-0.886296	1.25
10	C4	H	0.456098	1.998231	0.886296	1.25
11	C5	H	1.904875	-0.739966	1.276783	1.25
12	C5	H	0.457933	-0.230491	2.173519	1.25
13	C5	H	0.457933	-1.766265	1.287910	1.25
14	C6	H	1.904875	-0.739966	-1.276783	1.25
15	C6	H	0.454561	-1.766265	-1.287910	1.25
16	C6	H	0.457933	-0.230491	-2.173519	1.25

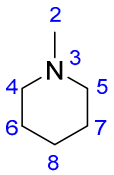
Compound 39: **Benzene**

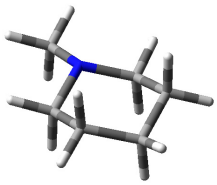




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	1.396612	0.000000	128.34
2	-	C	1.209501	0.698306	0.000000	128.34
3	-	C	-1.209501	0.698306	0.000000	128.34
4	-	C	1.209501	-0.698306	0.000000	128.34
5	-	C	-1.209501	-0.698306	0.000000	128.34
6	-	C	-0.000000	-1.396612	0.000000	128.34
7	C1	H	0.000000	2.483624	0.000000	7.36
8	C2	H	2.150881	1.241812	0.000000	7.36
9	C3	H	-2.150881	1.241812	0.000000	7.36
10	C4	H	2.150881	-1.241812	0.000000	7.36
11	C5	H	-2.150881	-1.241812	0.000000	7.36
12	C6	H	-0.000000	-2.483624	0.000000	7.36

Compound 40: **N-Methylpiperidine**

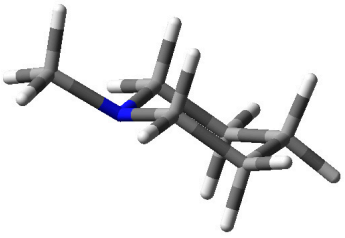




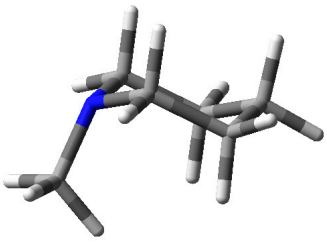
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	C2	H	0.306115	2.814503	0.000000	2.25
2	-	C	-0.674985	2.297496	0.000000	46.87
3	-	N	-0.562141	0.848381	0.000000	-
4	-	C	0.097724	0.358034	1.209700	56.53
5	-	C	0.097724	0.358034	-1.209700	56.53
6	-	C	0.097724	-1.173280	1.258284	25.96
7	-	C	0.097724	-1.173280	-1.258284	25.96
8	-	C	0.751697	-1.759410	-0.000000	23.73
9	C2	H	-1.228316	2.626094	-0.887079	2.25
10	C2	H	-1.228316	2.626094	0.887079	2.25
11	C4	H	1.144244	0.727945	1.275961	2.35
12	C4	H	-0.436303	0.763048	2.078205	2.35
13	C5	H	1.144244	0.727945	-1.275961	2.35
14	C5	H	-0.436303	0.763048	-2.078205	2.35
15	C6	H	0.620496	-1.510648	2.162182	1.60
16	C6	H	-0.940512	-1.522536	1.331180	1.60
17	C7	H	0.620496	-1.510648	-2.162182	1.60
18	C7	H	-0.940512	-1.522536	-1.331180	1.60
19	C8	H	1.823705	-1.512325	-0.000000	1.42
20	C8	H	0.680300	-2.854217	-0.000000	1.42

[a:] Atomic coordinates are for conformer 1, which represents > 99% of the Boltzmann population.

N-Methylpiperidine exhibits two conformations with the methyl group either equatorial or axial. The equatorial configuration comprises 99.60% of the Boltzmann population, allowing for the axial configuration to be ignored in chemical shift calculations.

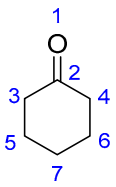


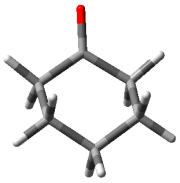
Conformer 1 (99.60%)



Conformer 2 (0.39%)

Compound 41: **Cyclohexanone**

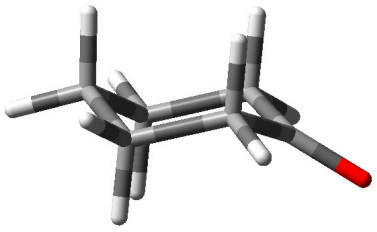




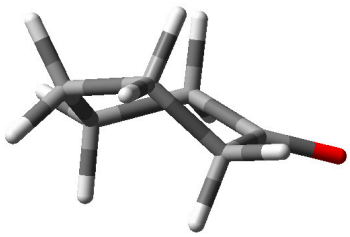
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates[a] x	y	z	Experimental δ (ppm)
1	-	O	-1.263609	1.956120	-0.000000	-
2	-	C	-0.413572	1.085927	-0.000000	212.15
3	-	C	0.158071	0.501362	1.286793	42.00
4	-	C	0.158071	0.501362	-1.286793	42.00
5	-	C	0.158071	-1.042001	1.267030	27.03
6	-	C	0.158071	-1.042001	-1.267030	27.03
7	-	C	0.829137	-1.591400	0.000000	25.02
8	C3	H	1.196136	0.856697	1.380658	2.34
9	C3	H	-0.407459	0.903074	2.132693	2.34
10	C4	H	1.196136	0.856697	-1.380658	2.34
11	C4	H	-0.407459	0.903074	-2.132693	2.34
12	C5	H	0.658987	-1.421571	2.165729	1.87
13	C5	H	-0.879451	-1.401316	1.312464	1.87
14	C6	H	0.658987	-1.421571	-2.165729	1.87
15	C6	H	-0.879451	-1.421571	-1.312464	1.87
16	C7	H	1.893839	-1.314426	0.000000	1.72
17	C7	H	0.791517	-2.687790	0.000000	1.72

[a:] Atomic coordinates are for conformer 1, which represents 98.91% of the Boltzmann population.

Cyclohexanone exhibits two conformations, chair and twist-boat. The chair configuration comprises 98.91% of the Boltzmann population, allowing for the twist-boat conformation to be ignored in chemical shift calculations.

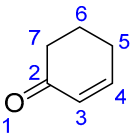


Conformer 1 (98.91%)



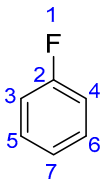
Conformer 2 (1.09%)

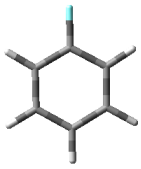
Compound 42: **Cyclohex-2-en-1-one (2-Cyclohexenone)**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	-2.361295	0.001724	-0.080774	-
2	-	C	-1.143351	0.022365	0.018018	199.74
3	-	C	-0.380622	1.289614	-0.051625	129.99
4	-	C	0.960739	1.326104	0.025453	150.61
5	-	C	1.819221	0.093708	0.131664	25.69
6	-	C	1.075885	-1.163703	-0.342437	22.75
7	-	C	-0.328663	-1.243271	0.271587	38.13
8	C3	H	-0.974066	2.195379	-0.146979	6.03
9	C4	H	1.470878	2.288967	0.014595	7.00
10	C5	H	2.743146	0.236151	-0.443511	2.35
11	C5	H	2.140602	-0.025522	1.179610	2.35
12	C6	H	0.988069	-1.130692	-1.436432	2.03
13	C6	H	1.652501	-2.063136	-0.097731	2.03
14	C7	H	-0.898731	-2.099010	-0.102835	2.44
15	C7	H	-0.251295	-1.364837	1.363507	2.44

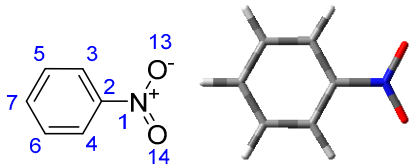
Compound 43: **Fluorobenzene**





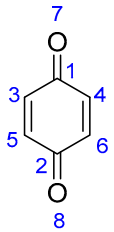
Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	F	0.000000	0.000000	2.282591	-
2	-	C	0.000000	0.000000	0.931458	162.86
3	-	C	-0.000000	1.217551	0.260430	115.32
4	-	C	-0.000000	-1.217551	0.260430	115.32
5	-	C	-0.000000	1.208664	-1.135566	129.96
6	-	C	-0.000000	-1.208664	-1.135566	129.96
7	-	C	-0.000000	-0.000000	-1.835837	123.98
8	C3	H	-0.000000	2.142010	0.828608	7.06
9	C4	H	-0.000000	-2.142010	0.828608	7.06
10	C5	H	-0.000000	2.151613	-1.675360	7.34
11	C6	H	-0.000000	-2.151613	-1.675360	7.34
12	C7	H	-0.000000	-0.000000	-2.921902	7.13

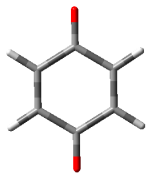
Compound 44: **Nitrobenzene**



Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	N	-0.000000	-0.000000	1.717815	-
2	-	C	-0.000000	-0.000000	0.245092	148.25
3	-	C	0.000000	1.220735	-0.427765	123.52
4	-	C	-0.000000	-1.220735	-0.427765	123.52
5	-	C	0.000000	1.212318	-1.821048	129.31
6	-	C	-0.000000	-1.212318	-1.821048	129.31
7	-	C	0.000000	0.000000	-2.516503	134.56
8	C3	H	0.000000	2.142803	0.140191	8.24
9	C4	H	-0.000000	-2.142803	0.140191	8.24
10	C5	H	0.000000	2.153082	-2.363343	7.56
11	C6	H	-0.000000	-2.153082	-2.363343	7.56
12	C7	H	0.000000	0.000000	-3.602893	7.70
13	-	O	0.000000	1.089518	2.289919	-
14	-	O	-0.000000	-1.089518	2.289919	-

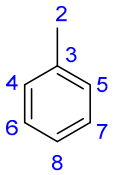
Compound 45: **1,4-Benzoquinone (p-Benzoquinone)**

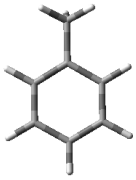




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	-0.000000	1.445285	187.21
2	-	C	0.000000	-0.000000	-1.445285	187.21
3	-	C	0.000000	1.269144	0.671532	136.56
4	-	C	-0.000000	-1.269144	0.671532	136.56
5	-	C	0.000000	1.269144	-0.671532	136.56
6	-	C	-0.000000	-1.269144	-0.671532	136.56
7	-	O	0.000000	-0.000000	2.670223	-
8	-	O	0.000000	-0.000000	-2.670223	-
9	C3	H	0.000000	2.182717	1.259654	6.79
10	C4	H	-0.000000	-2.182717	1.259654	6.79
11	C5	H	0.000000	2.182717	-1.259654	6.79
12	C6	H	-0.000000	-2.182717	-1.259654	6.79

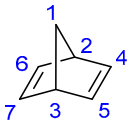
Compound 46: **Toluene**

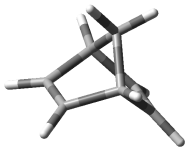




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	C2	H	1.060485	2.801442	-0.000000	2.36
2	-	C	0.028512	2.425416	-0.000000	21.46
3	-	C	-0.004238	0.913882	-0.000000	137.89
4	-	C	-0.007351	0.194294	1.202312	129.05
5	-	C	-0.007351	0.194294	-1.202312	129.05
6	-	C	-0.007351	-1.201161	1.205396	128.24
7	-	C	-0.007351	-1.201161	-1.205396	128.24
8	-	C	-0.006588	-1.905024	0.000000	125.31
9	C4	H	-0.011732	0.734438	2.146855	7.17
10	C5	H	-0.011732	0.734438	-2.146855	7.17
11	C6	H	-0.012171	-1.738466	2.150420	7.25
12	C7	H	-0.012171	-1.738466	-2.150420	7.25
13	C8	H	-0.009692	-2.991785	0.000000	7.16
14	C2	H	-0.466342	2.837579	-0.886013	2.36
15	C2	H	-0.466342	2.837579	0.886013	2.36

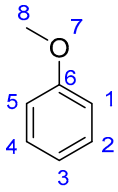
Compound 47: **Norbornadiene (2,5-Norbornadiene)**

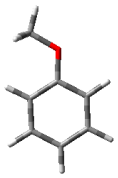




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	0.000000	1.355167	75.32
2	-	C	0.000000	1.122368	0.271791	50.26
3	-	C	-0.000000	-1.122368	0.271791	50.26
4	-	C	1.245986	0.667933	-0.520792	143.43
5	-	C	1.245986	-0.667933	-0.520792	143.43
6	-	C	-1.245986	0.667933	-0.520792	143.43
7	-	C	-1.245986	-0.667933	-0.520792	143.43
8	C1	H	0.899910	-0.000000	1.979632	1.99
9	C1	H	-0.899910	0.000000	1.979632	1.99
10	C2	H	0.000000	2.159751	0.612341	3.58
11	C3	H	-0.000000	-2.159751	0.612341	3.58
12	C4	H	1.937013	1.338860	-1.019357	6.76
13	C5	H	1.937013	-1.338860	-1.019357	6.76
14	C6	H	-1.937013	1.338860	-1.019357	6.76
15	C7	H	-1.937013	-1.338860	-1.019357	6.76

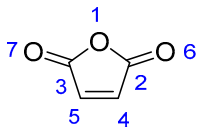
Compound 48: **Anisole**

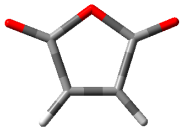




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	C	0.000000	0.529515	0.000000	113.90
2	-	C	-1.373336	0.242655	0.000000	129.45
3	-	C	-1.808034	-1.077795	0.000000	120.65
4	-	C	-0.886000	-2.130483	0.000000	129.45
5	-	C	0.476156	-1.839995	0.000000	113.90
6	-	C	0.930030	-0.516890	0.000000	159.55
7	-	O	0.325395	1.857237	0.000000	-
8	-	C	1.698003	2.211176	0.000000	55.14
9	C1	H	-2.074585	1.071481	0.000000	6.91
10	C2	H	-2.874609	-1.287350	0.000000	7.29
11	C3	H	-1.228212	-3.161259	0.000000	6.95
12	C4	H	1.204690	-2.646844	0.000000	7.29
13	C5	H	1.995503	-0.316937	0.000000	6.91
14	C8	H	1.726725	3.302499	0.000000	3.81
15	C8	H	2.213204	1.835708	0.894422	3.81
16	C8	H	2.213204	1.835708	-0.894422	3.81

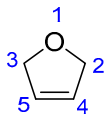
Compound 49: **Maleic anhydride**

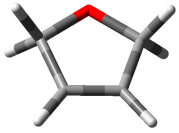




Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	-0.000730	-0.971804	0.000000	-
2	-	C	-0.000164	-0.158714	1.131991	164.07
3	-	C	-0.000164	-0.158714	-1.131991	164.07
4	-	C	0.000754	1.258255	0.667804	136.49
5	-	C	0.000754	1.258255	-0.667804	136.49
6	-	O	-0.000164	-0.600004	2.245452	-
7	-	O	-0.000164	-0.600004	-2.245452	-
8	C4	H	0.000693	2.089998	1.360223	7.03
9	C5	H	0.000693	2.089998	-1.360223	7.03

Compound 50: **2,5-Dihydrofuran**





Atom #	Carbon Attachment	Atom	Calculated Atomic Coordinates x	y	z	Experimental δ (ppm)
1	-	O	0.000642	-1.189607	-0.000000	-
2	-	C	-0.000207	-0.371239	1.172196	75.41
3	-	C	-0.000207	-0.371239	-1.172196	75.41
4	-	C	-0.000207	1.045499	0.665433	126.19
5	-	C	-0.000207	1.045499	-0.665433	126.19
6	C2	H	-0.886896	-0.600210	1.785570	4.65
7	C2	H	0.886347	-0.599315	1.786304	4.65
8	C3	H	-0.886896	-0.600210	-1.785570	4.65
9	C3	H	0.886347	-0.599315	-1.786304	4.65
10	C4	H	0.000462	1.912389	1.317664	5.89
11	C5	H	0.000462	1.912389	-1.317664	5.89