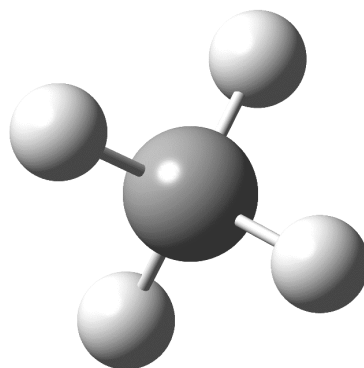
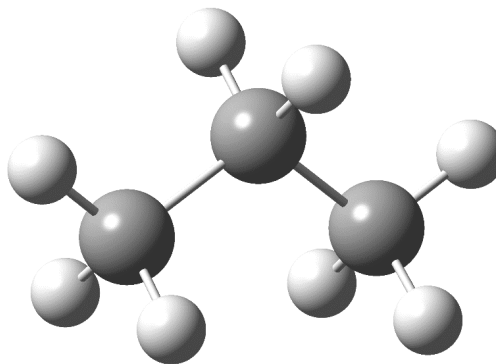


ALKANE

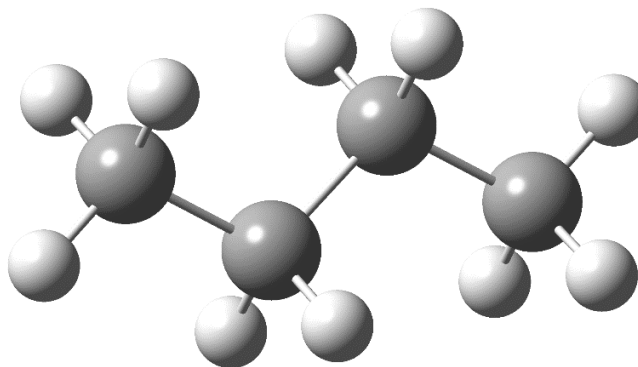
METHANE (no. 1)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0	0	0
2	No	Show	2	H	1			1.097869			0.633855	0.633855	0.633855
3	No	Show	3	H	1	2		1.097869	109.4712		-0.63386	-0.63386	0.633855
4	No	Show	4	H	1	2	3	1.097869	109.4712	-120	0.633855	-0.63386	-0.63386
5	No	Show	5	H	1	2	3	1.097869	109.4712	120	-0.63386	0.633855	-0.63386

PROPANE (no. 2)

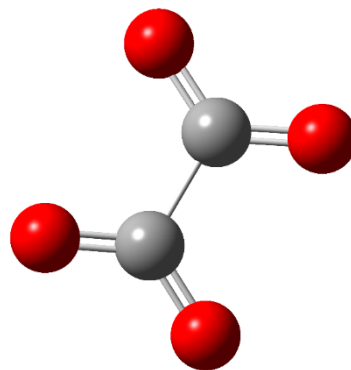
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0	0.590201	0
2	No	Show	2	C	1			1.524067			-1.26469	-0.26029	0
3	No	Show	3	C	1	2		1.524068	112.1588		1.26469	-0.2603	0
4	No	Show	4	H	1	2	3	1.102139	109.5435	-121.86	0.000001	1.250882	0.882162
5	No	Show	5	H	1	2	3	1.102139	109.5435	121.8599	0.000001	1.250882	-0.88216
6	No	Show	6	H	2	1	3	1.099891	111.7005	180	-2.17245	0.360775	0
7	No	Show	7	H	2	1	3	1.101569	110.8356	-59.6786	-1.29977	-0.91025	-0.8887
8	No	Show	8	H	2	1	3	1.101569	110.8356	59.67865	-1.29977	-0.91025	0.888699
9	No	Show	9	H	3	1	2	1.099889	111.7004	180	2.172451	0.360774	0
10	No	Show	10	H	3	1	2	1.101568	110.8355	-59.6786	1.299773	-0.91025	0.888699
11	No	Show	11	H	3	1	2	1.101568	110.8355	59.6786	1.299773	-0.91025	-0.8887

BUTANE (no. 3)

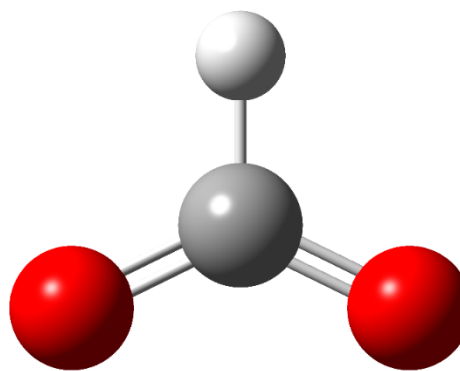
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0.561336	0.516295	-0.00023
2	No	Show	2	C	1			1.52533			-0.56134	-0.51629	-0.00023
3	No	Show	3	C	1	2		1.523524	112.7252		1.945823	-0.11957	0.000211
4	No	Show	4	C	2	1	3	1.523525	112.7252	179.9638	-1.94582	0.119568	0.000211
5	No	Show	5	H	1	3	2	1.103544	109.7559	121.786	0.450505	1.169331	0.882416
6	No	Show	6	H	1	3	2	1.10354	109.7555	-121.785	0.450883	1.168903	-0.88324
7	No	Show	7	H	2	1	3	1.10354	109.0669	-57.8625	-0.45088	-1.1689	-0.88324
8	No	Show	8	H	2	1	3	1.103544	109.0674	57.7892	-0.4505	-1.16933	0.882416
9	No	Show	9	H	3	1	2	1.101338	110.8806	-59.7428	2.085947	-0.75437	0.889217
10	No	Show	10	H	3	1	2	1.101346	110.8795	59.67707	2.085883	-0.75571	-0.88786
11	No	Show	11	H	3	1	2	1.099678	111.6822	179.9662	2.741522	0.63948	-0.0004
12	No	Show	12	H	4	2	1	1.101338	110.8805	-59.7426	-2.08595	0.754376	0.889216
13	No	Show	13	H	4	2	1	1.099677	111.6822	179.9663	-2.74152	-0.63948	-0.0004
14	No	Show	14	H	4	2	1	1.101345	110.8794	59.67717	-2.08588	0.755711	-0.88786

CARBOXYLATE

OXALATE (no. 4)

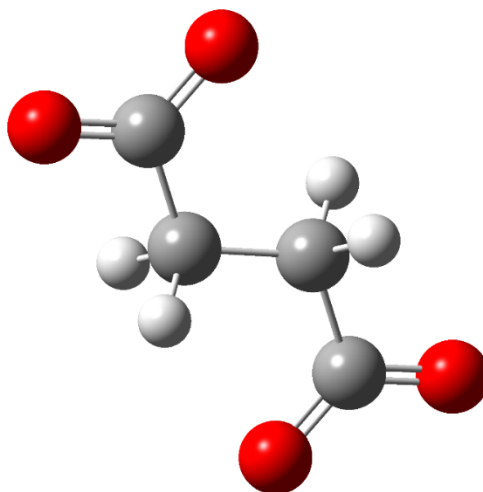


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.36355	1.718854	-0.09193
2	No	Show	2	O	1			3.513761			0.363551	-1.71885	-0.09193
3	No	Show	3	O	1	2		2.24386	50.61264		1.618182	0.682642	0.092203
4	No	Show	4	O	2	1	3	2.24386	50.61264	167.8101	-1.61818	-0.68264	0.092203
5	No	Show	5	C	1	3	2	1.257895	26.89821	3.827083	0.363551	0.696486	-0.00036
6	No	Show	6	C	2	1	5	1.257895	23.82527	159.2361	-0.36355	-0.69649	-0.00036

FORMATE (no. 5)

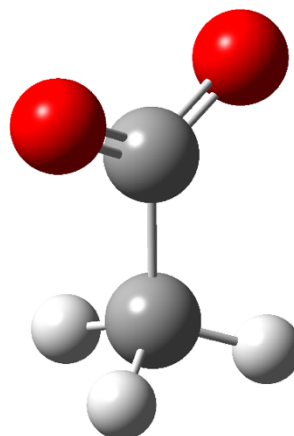
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.12596	-0.21714	0
2	No	Show	2	O	1			2.251922			1.125961	-0.21714	0
3	No	Show	3	C	1	2		1.254079	26.12459		0	0.335059	0
4	No	Show	4	H	3	1	2	1.128872	116.1246	180	0	1.463931	0

SUCCINATE (no. 6)

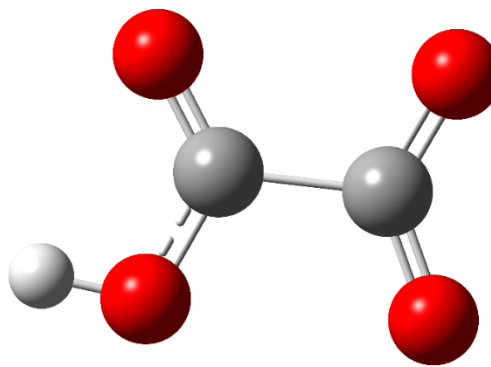


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.089187	-	-
2	No	Show	2	O	1			6.0471714			-	0.487533	2.982688
3	No	Show	3	O	1	2		2.2396411	54.2769186		1.721137	0.438099	-
4	No	Show	4	O	2	1	3	2.2396411	54.2769186	-180	1.721137	0.438099	1.759603
5	No	Show	5	C	1	3	4	2.3788433	62.6891967	1.5787742	-	-	-0.65843
6	No	Show	6	C	5	1	3	1.5157876	143.7735761	-8.6845439	0.322444	0.192101	0.65843
7	No	Show	7	C	3	1	5	1.2605595	27.4187618	0.3214765	0.575571	-	-
8	No	Show	8	C	4	2	1	1.2605595	27.4187618	1.2572976	-	0.070063	1.895471
9	No	Show	9	H	5	1	7	1.103211	92.7361401	122.2425018	0.575571	0.070063	1.895471
10	No	Show	10	H	5	1	7	1.1014372	88.7385725	-	1.215846	0.428653	-
11	No	Show	11	H	6	5	1	1.1014372	110.5890105	132.8406418	-	-1.22661	-
12	No	Show	12	H	6	5	1	1.103211	110.2552504	61.7720412	0.698406	1.22661	0.618336
										-53.8558268	0.698406	-	0.618336
											1.215846	0.428653	0.841656

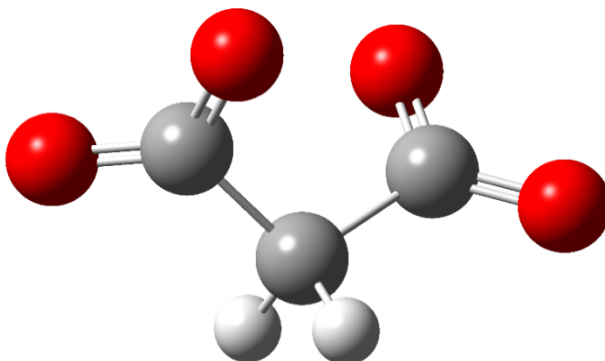
ACETATE (no. 7)



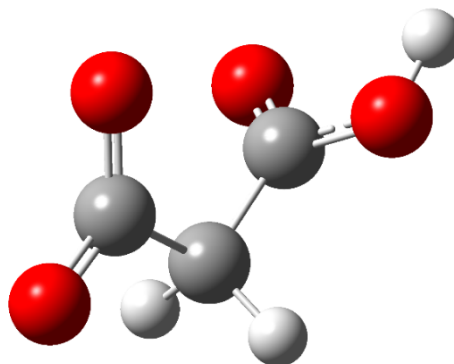
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.758534	-1.121734	0.002049
2	No	Show	2	O	1			2.2421744			0.761047	1.120439	0.002061
3	No	Show	3	C	1	2		2.3858457	61.9851142		-1.346483	0.00126	-0.004858
4	No	Show	4	C	2	1	3	1.26051	27.2058367	-1.0695365	0.183639	0.000026	-0.010593
5	No	Show	5	H	3	1	4	1.101887	105.6859453	-	-1.69341	-0.009688	1.040932
6	No	Show	6	H	3	1	4	1.0979298	86.3331683	100.1514768	-1.743407	-0.894984	-0.499477
7	No	Show	7	H	3	1	4	1.0978574	135.0877743	36.9803808	-1.742767	0.907316	-0.481631

HYDROGEN OXALATE (no. 8)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.35742	-1.01908	0.000065
2	No	Show	2	O	1			2.241368			-1.24353	1.219396	-0.00011
3	No	Show	3	O	2	1		2.740051	89.07274		1.490368	1.0359	0.000177
4	No	Show	4	O	3	2	1	2.258911	88.38203	0.008978	1.275516	-1.21277	-1.1E-05
5	No	Show	5	C	2	1	4	1.211125	30.04892	-0.0148	-0.69113	0.141587	0.00011
6	No	Show	6	C	3	2	1	1.24703	63.28165	0.025841	0.856361	-0.03793	-0.0003
7	No	Show	7	H	1	5	2	0.976185	107.4614	-0.02067	-2.31085	-0.8095	0.000169

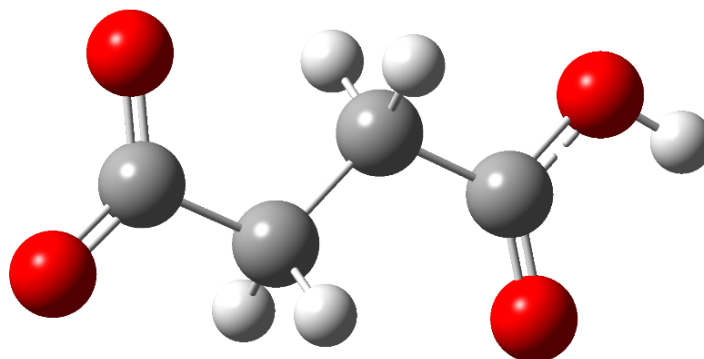
MALONATE (no. 9)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.226697	0.634403	0.219481
2	No	Show	2	O	1			3.650913			-1.2405	1.035434	-0.85145
3	No	Show	3	O	1	2		2.24159	61.28053		1.205021	-1.08694	-0.78943
4	No	Show	4	O	2	1	3	2.242038	100.1043	57.63899	-2.19729	-0.65146	0.273566
5	No	Show	5	C	2	1	3	2.377017	40.40813	79.02097	0.004782	0.055347	0.920246
6	No	Show	6	C	1	3	5	1.259291	27.26848	-0.19845	1.250899	-0.14252	0.046208
7	No	Show	7	C	4	2	1	1.259204	27.23775	15.3321	-1.25126	0.147503	0.044941
8	No	Show	8	H	5	2	1	1.099581	95.59766	82.96887	0.109318	0.981811	1.503182
9	No	Show	9	H	5	2	1	1.099732	138.0138	-150.194	-0.08731	-0.79531	1.611122

MALONATE(1-) (no. 10)

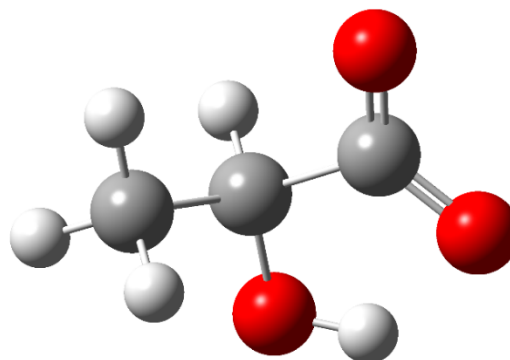
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.598859	0.503872	1.016327
2	No	Show	2	O	1			2.237402			1.804144	-0.33636	-1.04713
3	No	Show	3	O	1	2		4.226339	80.22141		-2.45662	-0.34039	0.178324
4	No	Show	4	O	3	1	2	2.248111	45.00892	-73.5455	-0.9849	1.218438	-0.49852
5	No	Show	5	C	1	2	4	2.362248	63.13126	53.36127	-0.145	-0.89613	0.255301
6	No	Show	6	C	2	1	5	1.214569	30.64824	-0.96874	1.172182	-0.2458	-0.01388
7	No	Show	7	C	3	1	6	1.251935	23.56749	-57.6538	-1.30326	0.089934	-0.04955
8	No	Show	8	H	5	1	6	1.097043	137.4731	32.7629	-0.25165	-1.77608	-0.39109
9	No	Show	9	H	5	1	6	1.097646	84.70585	145.6311	-0.21574	-1.20793	1.305351
10	No	Show	10	H	1	6	2	0.97571	107.485	1.759313	2.432032	0.931455	0.742457

SUCCINATE(1-) (no. 11)



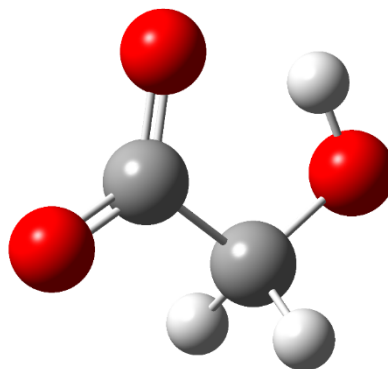
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.821305	0.844685	-0.00606
2	No	Show	2	O	1			2.23778			2.118203	-1.27972	0.008724
3	No	Show	3	O	2	1		5.111585	103.0479		-2.97181	-0.81082	-0.00587
4	No	Show	4	O	3	2	1	2.243676	74.30185	-0.76892	-2.1692	1.284341	0.008771
5	No	Show	5	C	1	2	4	2.364027	63.3531	-0.17709	0.482246	0.502027	-0.00245
6	No	Show	6	C	5	1	2	1.514882	144.6901	-0.53397	-0.61399	-0.54351	-0.00293
7	No	Show	7	C	2	1	5	1.21399	30.62801	0.017804	1.859261	-0.09369	0.000635
8	No	Show	8	C	4	3	2	1.259029	27.02594	0.212611	-2.03616	0.032392	-2.3E-05
9	No	Show	9	H	5	1	7	1.100682	88.89926	126.8686	0.407974	1.164127	0.873679
10	No	Show	10	H	5	1	7	1.100626	88.62345	-127.53	0.410738	1.163337	-0.87934
11	No	Show	11	H	6	5	1	1.101268	110.5015	-58.1853	-0.51945	-1.20107	-0.88125
12	No	Show	12	H	6	5	1	1.101318	110.4629	58.36686	-0.51744	-1.203	0.873804
13	No	Show	13	H	1	7	2	0.975601	107.6241	-0.02001	3.682	0.385348	-0.0028

LACTATE (no. 12)

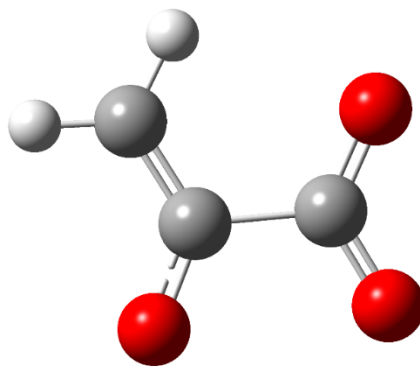


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.15116	-1.28357	-0.16318
2	No	Show	2	O	1			3.564554			1.458689	1.143935	-0.20694
3	No	Show	3	O	2	1		2.24987	45.68265		1.337817	-1.02354	0.384138
4	No	Show	4	C	1	3	2	1.417685	66.2296	0.130121	-0.6441	0.016669	-0.41235
5	No	Show	5	C	4	1	3	1.521323	110.9768	-122.446	-1.41841	1.06327	0.374734
6	No	Show	6	C	2	1	4	1.252873	18.99763	-179.397	0.852862	0.058588	-0.04982
7	No	Show	7	H	4	1	6	1.105574	109.6564	116.952	-0.72079	0.2453	-1.4913
8	No	Show	8	H	5	4	1	1.10135	109.8187	60.55319	-1.32763	0.861803	1.453688
9	No	Show	9	H	5	4	1	1.099543	110.6956	-59.2068	-2.48409	1.042713	0.104754
10	No	Show	10	H	5	4	1	1.098281	110.1821	-179.636	-1.01941	2.06526	0.167269
11	No	Show	11	H	1	4	5	0.981157	101.3962	-121.923	-0.35297	-1.74084	0.178071

GLYCOLATE (no. 13)

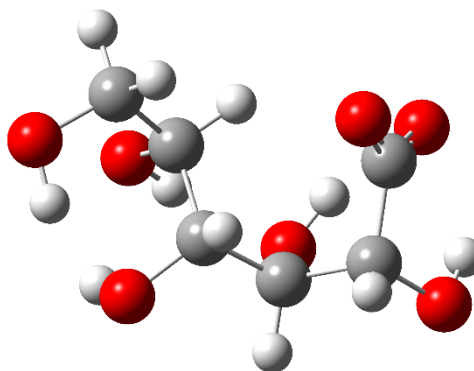


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.801717	0.058552	-0.00033
2	No	Show	2	O	1			3.570221			-1.71311	-0.5679	-0.00036
3	No	Show	3	O	2	1		2.25145	45.96167		-0.45632	1.300117	0.00023
4	No	Show	4	C	1	3	2	1.413455	65.30385	-0.04155	0.665501	-0.7822	0.000371
5	No	Show	5	C	2	1	4	1.252195	19.42394	179.8641	-0.62358	0.049275	0.000171
6	No	Show	6	H	4	1	5	1.10392	111.1661	120.3023	0.65387	-1.43733	-0.88806
7	No	Show	7	H	4	1	5	1.103915	111.1716	-120.306	0.654177	-1.43643	0.889462
8	No	Show	8	H	1	4	5	0.980881	101.175	-0.01679	1.382143	0.945166	-0.00102

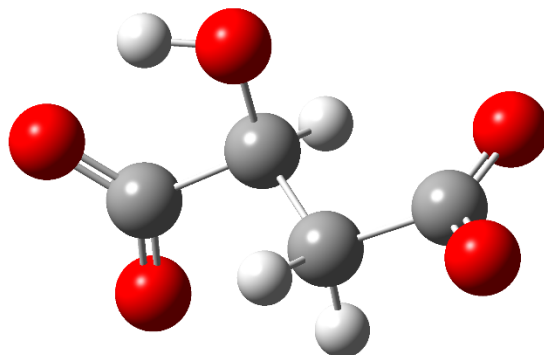
PYRUVATE (no. 14)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.21329	-1.31019	-0.00055
2	No	Show	2	O	1			2.6879			1.45913	-1.02213	0.000675
3	No	Show	3	O	2	1		2.237367	92.0525		1.299172	1.209514	-0.00057
4	No	Show	4	C	1	2	3	2.376315	90.72578	-0.06022	-1.49787	1.049019	0.000577
5	No	Show	5	C	1	4	3	1.289586	27.72786	0.01316	-0.7543	-0.10505	-9.8E-05
6	No	Show	6	C	2	1	5	1.261343	64.3612	-0.03469	0.794625	0.049982	-7.9E-05
7	No	Show	7	H	4	1	5	1.094471	93.79695	179.9958	-2.59076	0.990191	0.000694
8	No	Show	8	H	4	1	5	1.088132	147.3096	0.048627	-1.02407	2.028583	0.000425

CID_4134252 (no. 15)



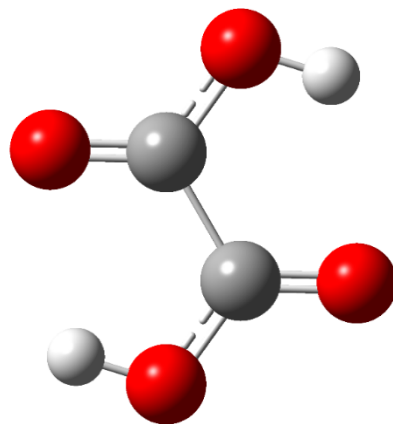
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.60767	-1.47327	1.029661
2	No	Show	2	O	1			3.252212			0.850514	-1.34164	-1.09563
3	No	Show	3	O	1	2		2.68595	54.26735		-1.76704	-0.58449	-1.49996
4	No	Show	4	O	2	1	3	2.790599	104.1042	148.2783	3.096929	-0.86962	0.491272
5	No	Show	5	O	1	3	2	2.805	62.8061	149.0179	-3.48491	0.541098	0.494556
6	No	Show	6	O	4	2	1	2.662006	63.75015	-109.708	2.304267	1.145861	-1.05656
7	No	Show	7	O	6	4	2	2.253495	90.88098	96.6922	1.171363	2.065063	0.66095
8	No	Show	8	C	1	3	2	1.429245	63.31376	52.79719	-0.67066	-0.46564	0.643113
9	No	Show	9	C	2	1	8	1.430152	44.5286	54.53475	0.697604	-1.08745	0.303417
10	No	Show	10	C	3	1	8	1.425357	63.45263	-28.4844	-1.26447	0.333787	-0.53258
11	No	Show	11	C	4	2	1	1.415891	60.42004	-38.5759	1.873031	-0.23036	0.804577
12	No	Show	12	C	5	1	8	1.41921	85.47447	11.32135	-2.39927	1.240578	-0.0939
13	No	Show	13	C	7	6	4	1.249212	26.68432	-12.8393	1.789639	1.134299	0.10243
14	No	Show	14	H	8	1	10	1.099752	106.0871	117.736	-0.55462	0.193479	1.515785
15	No	Show	15	H	9	2	1	1.100249	106.6337	81.74261	0.748897	-2.06365	0.808339
16	No	Show	16	H	10	3	1	1.102143	110.5332	145.126	-0.48674	0.976106	-0.97674
17	No	Show	17	H	11	4	2	1.098178	109.3495	147.0112	1.794283	-0.10874	1.893155
18	No	Show	18	H	12	5	1	1.105089	111.6438	-99.0759	-1.97914	1.995338	0.595343
19	No	Show	19	H	12	5	1	1.100178	107.0718	142.9912	-2.79455	1.768633	-0.97441
20	No	Show	20	H	1	8	10	0.974613	105.0412	42.97233	-1.9366	-1.84749	0.192021
21	No	Show	21	H	2	1	8	0.978575	129.1936	-17.5888	1.301023	-0.55889	-1.47239
22	No	Show	22	H	3	1	8	0.974729	93.19091	76.07233	-0.98403	-1.0904	-1.78465
23	No	Show	23	H	4	2	1	0.974895	75.04829	-154.133	3.326956	-0.50782	-0.38429
24	No	Show	24	H	5	1	8	0.972509	26.13046	-133.063	-3.09835	-0.17191	1.031176

MALATE (no. 16)

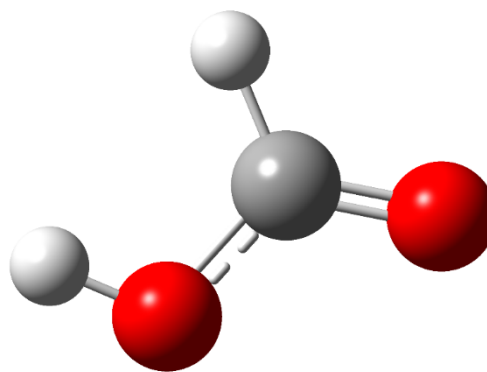
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.39002	1.605406	0.119612
2	No	Show	2	O	1			3.56625			-2.13891	-1.45892	-0.39944
3	No	Show	3	O	2	1		2.248929	45.66681		-2.68878	0.534	0.48576
4	No	Show	4	O	1	3	2	3.940792	120.3569	-42.4275	2.898941	-0.42939	0.876035
5	No	Show	5	O	4	1	3	2.240695	52.85042	117.0794	2.229367	0.372021	-1.10642
6	No	Show	6	C	1	3	2	1.419089	66.17697	0.110132	-0.47504	0.26269	-0.33172
7	No	Show	7	C	6	1	3	1.518836	110.8084	-123.165	0.582154	-0.59911	0.336498
8	No	Show	8	C	2	1	6	1.253521	18.87753	-179.628	-1.89051	-0.27743	-0.06227
9	No	Show	9	C	4	1	6	1.259558	35.08893	44.72444	2.020742	-0.17486	0.00974
10	No	Show	10	H	6	1	8	1.10443	109.5822	117.4918	-0.31031	0.227942	-1.42324
11	No	Show	11	H	7	6	1	1.101368	109.9422	59.9504	0.441899	-0.58624	1.428823
12	No	Show	12	H	7	6	1	1.102187	108.6872	177.1826	0.452513	-1.64087	0.000729
13	No	Show	13	H	1	6	7	0.980939	101.3294	-122.528	-1.29304	1.746517	0.475817

CARBOXYLIC ACID

OXALIC ACID (no. 17)

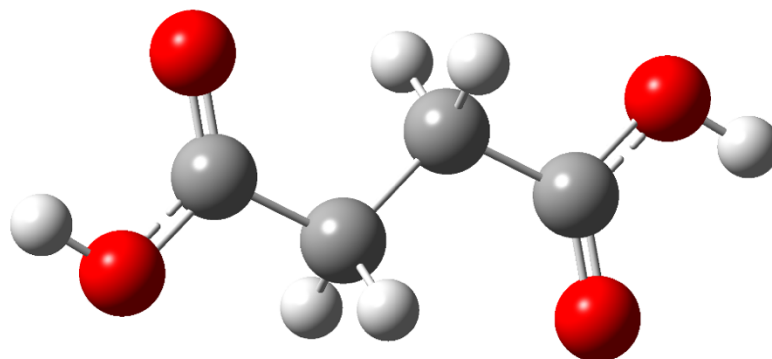


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.383977	1.737183	0
2	No	Show	2	O	1			3.558226			-0.38398	-1.73718	0
3	No	Show	3	O	1	2		2.230647	49.71966		-1.58891	0.696274	0
4	No	Show	4	O	2	1	3	2.230647	49.71966	180	1.588913	-0.69627	0
5	No	Show	5	C	3	1	4	1.205311	29.24549	0	-0.38398	0.666214	0
6	No	Show	6	C	4	2	1	1.205311	29.24549	0	0.383977	-0.66621	0
7	No	Show	7	H	1	5	3	0.979053	108.5653	180	1.319861	1.449666	0
8	No	Show	8	H	2	1	5	0.979053	85.38622	0	-1.31986	-1.44967	0

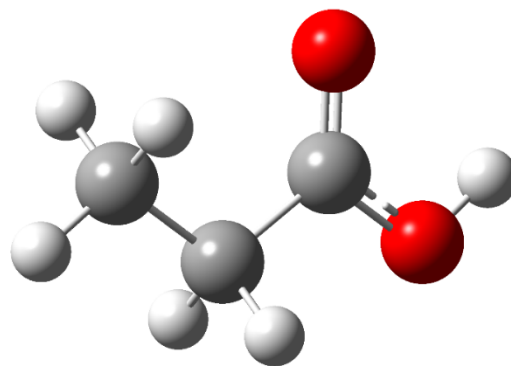
FORMIC ACID (no. 18)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.90391	-0.5931	0
2	No	Show	2	O	1			2.214199			1.181819	0.150151	0
3	No	Show	3	C	2	1		1.205966	31.09847		0	0.390272	0
4	No	Show	4	H	3	2	1	1.105619	124.1139	180	-0.4254	1.410776	0
5	No	Show	5	H	1	3	2	0.973055	109.3296	180	-1.79788	-0.20884	0

SUCCINIC ACID (no. 19)

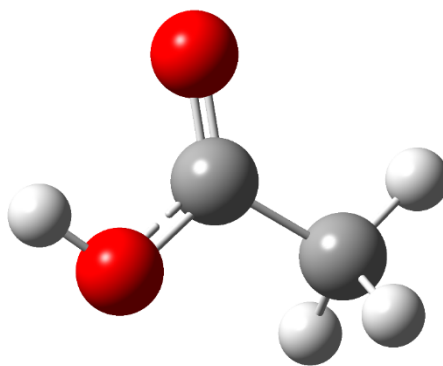


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.88656	-0.82477	-0.00251
2	No	Show	2	O	1			6.004157			2.886559	0.824772	-0.00247
3	No	Show	3	O	1	2		2.240329	54.68929		-2.14371	1.288808	0.003488
4	No	Show	4	O	2	1	3	2.240329	54.68933	179.6257	2.143714	-1.28881	0.003473
5	No	Show	5	C	1	3	4	2.358078	63.2772	-0.06519	-0.5479	-0.52277	-0.00091
6	No	Show	6	C	5	1	3	1.514577	143.7026	-0.21103	0.547901	0.522771	-0.001
7	No	Show	7	C	3	1	5	1.212905	30.26692	0.004363	-1.91431	0.097799	0.000276
8	No	Show	8	C	4	2	1	1.212905	30.26688	-0.06386	1.914312	-0.0978	0.000222
9	No	Show	9	H	5	1	7	1.100127	89.25788	126.7671	-0.47801	-1.17996	0.878575
10	No	Show	10	H	5	1	7	1.100097	89.14875	-127.028	-0.47898	-1.17948	-0.88079
11	No	Show	11	H	6	5	1	1.100126	111.4979	59.29047	0.478027	1.180099	0.878379
12	No	Show	12	H	6	5	1	1.100098	111.5127	-59.2226	0.478953	1.179343	-0.88099
13	No	Show	13	H	1	7	3	0.975795	107.7925	-0.00947	-3.7424	-0.35604	-0.00129
14	No	Show	14	H	2	1	7	0.975795	135.3447	179.6385	3.742399	0.356037	-0.00121

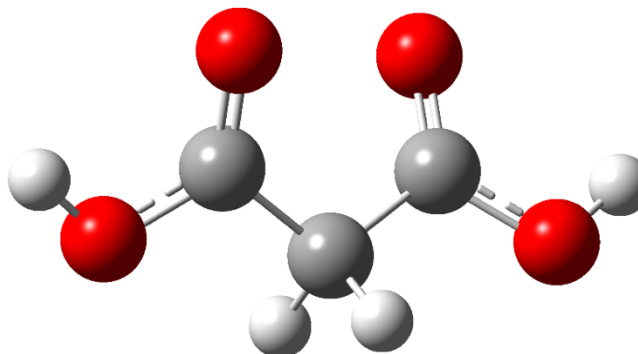
PROPIONIC ACID (no. 20)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.676426	-0.65028	-5.9E-05
2	No	Show	2	O	1			2.239159			0.589038	1.307123	0.000026
3	No	Show	3	C	1	2		2.365034	63.22829		-0.68673	-0.74443	0.00007
4	No	Show	4	C	3	1	2	1.517836	144.1514	0.013629	-1.95145	0.094796	-6.1E-05
5	No	Show	5	C	2	1	3	1.213402	30.48271	0.003061	0.55877	0.094099	0.000045
6	No	Show	6	H	3	1	5	1.100948	88.42277	-126.986	-0.63005	-1.40486	0.879113
7	No	Show	7	H	3	1	5	1.100945	88.41477	127.0066	-0.62998	-1.40506	-0.87881
8	No	Show	8	H	4	3	1	1.097821	110.3924	179.9918	-2.83915	-0.55112	-2.2E-05
9	No	Show	9	H	4	3	1	1.098981	110.8487	-59.9422	-1.99289	0.739882	0.888706
10	No	Show	10	H	4	3	1	1.098982	110.8488	59.9258	-1.99284	0.739695	-0.88897
11	No	Show	11	H	1	5	2	0.975647	107.6221	0.00379	2.437705	-0.04008	-8.3E-05

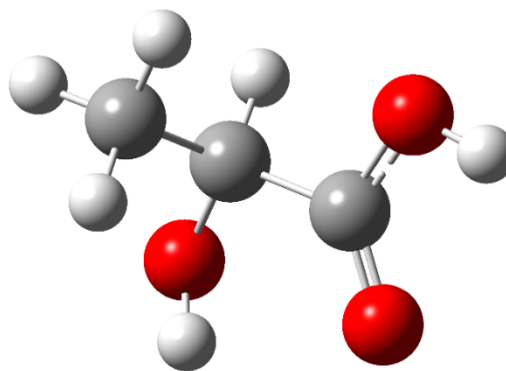
ACETIC ACID (no. 21)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-	-	-
2	No	Show	2	O	1			2.2381731			0.786652	1.029436	0.000012
3	No	Show	3	C	1	2		2.3586999	63.2730534		-	-	-
4	No	Show	4	C	2	1	3	1.2133273	30.5868769	-0.0118119	0.628789	1.203163	0.000026
5	No	Show	5	H	3	1	4	1.0985253	91.1701474	126.124638	1.389618	0.119868	0.000018
6	No	Show	6	H	3	1	4	1.0985261	91.1664619	-	-	-	-
7	No	Show	7	H	3	1	4	1.0936828	141.6668896	-0.0076388	0.086603	0.117715	0.000108
8	No	Show	8	H	1	4	2	0.9757	107.571	-0.00817	1.66006	0.708758	0.887015
											1.659933	0.708649	0.887163
											1.919587	0.836832	-
											-1.734	-0.796	0.000005
													-8E-05

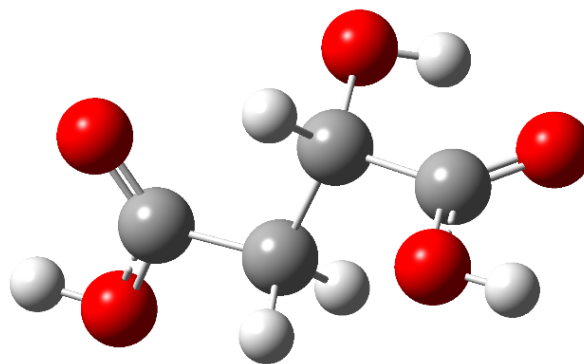
MALONIC ACID (no. 22)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.31859	-0.65971	-0.33312
2	No	Show	2	O	1			4.687334			2.322242	-0.65783	0.325462
3	No	Show	3	O	1	2		2.241005	60.31078		-1.32534	1.13846	0.562504
4	No	Show	4	O	2	1	3	2.241045	60.14643	-44.8614	1.320627	1.140117	-0.56135
5	No	Show	5	C	2	1	3	2.347915	3.549509	153.5159	0.00074	-0.80379	0.00604
6	No	Show	6	C	3	1	5	1.209481	29.97369	1.447938	-1.25418	0.020332	0.106905
7	No	Show	7	C	4	2	1	1.209452	29.97365	0.18667	1.253848	0.021808	-0.10561
8	No	Show	8	H	5	2	1	1.099477	82.80391	-131.076	0.058983	-1.45275	0.891649
9	No	Show	9	H	5	2	1	1.099399	101.3057	123.1629	-0.0551	-1.46601	-0.86976
10	No	Show	10	H	1	6	3	0.976489	107.7798	-1.21404	-3.10743	-0.10103	-0.19474
11	No	Show	11	H	2	1	6	0.976483	141.0566	-47.2469	3.109609	-0.09864	0.18095

LACTIC ACID (no. 23)

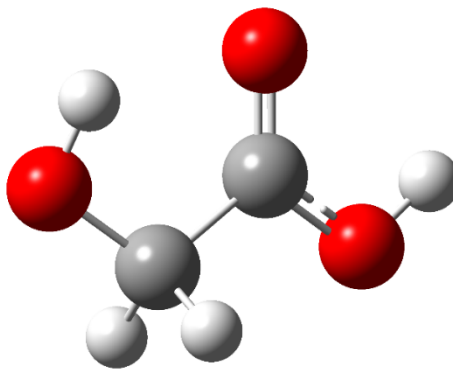
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.40448	-1.09738	-0.33366
2	No	Show	2	O	1			3.571311			1.567676	0.882659	-0.3378
3	No	Show	3	O	2	1		2.245953	48.94418		1.152745	-1.15335	0.514724
4	No	Show	4	C	1	3	2	1.410513	62.99391	-10.5825	-0.67579	0.107516	-0.41609
5	No	Show	5	C	4	1	3	1.525534	112.4199	-116.187	-1.25442	1.199742	0.478048
6	No	Show	6	C	3	2	1	1.211963	29.64176	-5.05184	0.769803	-0.14392	-0.03596
7	No	Show	7	H	4	1	6	1.099399	107.3973	116.8526	-0.69516	0.432197	-1.46627
8	No	Show	8	H	5	4	1	1.100578	109.8088	62.35326	-1.20129	0.886261	1.531698
9	No	Show	9	H	5	4	1	1.097831	109.174	-56.9423	-2.30584	1.366126	0.209582
10	No	Show	10	H	5	4	1	1.098114	110.9168	-177.178	-0.69989	2.139846	0.35741
11	No	Show	11	H	1	4	6	0.972001	106.4693	43.94931	-1.13154	-1.52843	0.493671
12	No	Show	12	H	2	1	4	0.97644	130.2353	163.0932	2.468619	0.668522	-0.02815

MALIC ACID (no. 24)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.373188	1.691954	-0.08163
2	No	Show	2	O	1			3.57253			2.12955	-1.34685	0.584593
3	No	Show	3	O	1	2		4.077589	85.38453		-2.85563	-0.70671	-0.7509
4	No	Show	4	O	2	1	3	2.247834	48.63174	133.7833	2.677439	0.443684	-0.65902
5	No	Show	5	O	3	1	4	2.240992	46.89051	130.3878	-2.22041	0.556578	0.987684
6	No	Show	6	C	1	4	2	1.408061	63.13261	-8.51784	0.491663	0.351281	0.332131
7	No	Show	7	C	6	1	4	1.524873	111.8767	-117.231	-0.53797	-0.54583	-0.34631
8	No	Show	8	C	4	2	1	1.211097	29.34243	-4.38337	1.885998	-0.16085	0.030118
9	No	Show	9	C	5	3	1	1.211834	30.09477	-33.5348	-1.93531	-0.1547	0.048884
10	No	Show	10	H	6	1	8	1.099596	108.2086	117.8371	0.342142	0.313198	1.420848
11	No	Show	11	H	7	6	1	1.100833	111.0882	176.7166	-0.39661	-1.59894	-0.05854
12	No	Show	12	H	7	6	1	1.099647	110.5964	57.3617	-0.44284	-0.48531	-1.44016
13	No	Show	13	H	1	6	8	0.972948	106.3034	32.45913	0.943023	1.787581	-0.86443
14	No	Show	14	H	2	1	6	0.976715	130.3866	166.9548	3.030773	-1.62549	0.331356
15	No	Show	15	H	3	1	6	0.976246	119.8765	126.2956	-3.73588	-0.43974	-0.42387

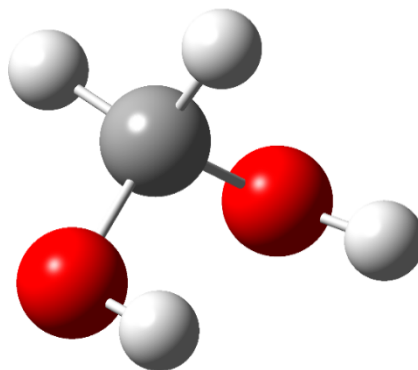
GLYCOLIC ACID (no. 25)



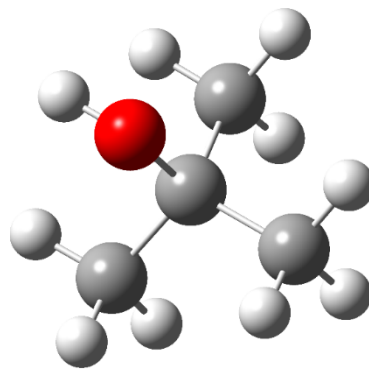
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.88589	0.055734	-0.08058
2	No	Show	2	O	1			3.581723			1.62675	-0.64206	-0.0242
3	No	Show	3	O	2	1		2.248384	48.9103		0.506723	1.307274	0.00541
4	No	Show	4	C	1	3	2	1.406928	62.29036	5.942946	-0.7346	-0.74213	0.051259
5	No	Show	5	C	3	2	1	1.212018	29.43136	2.491022	0.516251	0.095315	-0.00188
6	No	Show	6	H	4	1	5	1.104805	112.7544	120.0059	-0.70761	-1.29911	1.005008
7	No	Show	7	H	4	1	5	1.099236	109.6022	-120.23	-0.70117	-1.47888	-0.76385
8	No	Show	8	H	1	4	5	0.971883	106.2637	-28.7982	-1.65498	0.928395	0.279559
9	No	Show	9	H	2	1	4	0.976426	130.4768	-169.298	2.393193	-0.0371	-0.02203

ALCOHOL

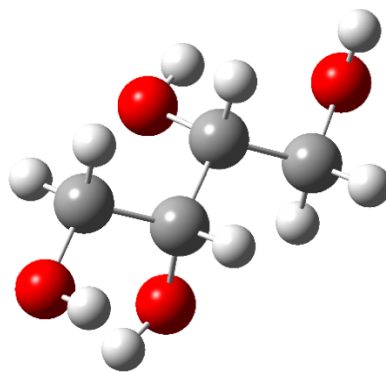
METHANEDIOL (no. 26)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.06555	-0.26149	1.171396
2	No	Show	2	O	1			2.342792			-0.06555	-0.26149	-1.1714
3	No	Show	3	C	1	2		1.407212	33.65153		-0.06555	0.518302	0
4	No	Show	4	H	3	1	2	1.097126	106.4334	116.3	-1.00893	1.07841	0
5	No	Show	5	H	3	1	2	1.102471	110.5634	-124.301	0.787161	1.217105	0
6	No	Show	6	H	1	3	2	0.969827	107.3272	75.7897	0.831937	-0.61074	1.285894
7	No	Show	7	H	2	1	3	0.969827	96.78017	111.2628	0.831937	-0.61074	-1.28589

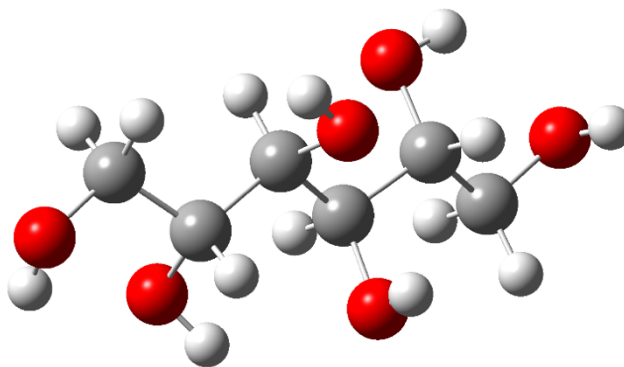
TERT-BUTANOL (no. 27)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.486	1.366227	0
2	No	Show	2	C	1			1.435412			0.003978	0.017032	0
3	No	Show	3	C	2	1		1.525513	109.3554		-0.486	-0.69882	1.254858
4	No	Show	4	C	2	1	3	1.525513	109.3554	121.3505	-0.486	-0.69882	-1.25486
5	No	Show	5	C	2	1	4	1.521648	105.5346	119.3248	1.521091	0.134424	0
6	No	Show	6	H	3	2	1	1.101607	110.1358	61.77277	-1.58677	-0.74127	1.261846
7	No	Show	7	H	3	2	1	1.09989	111.0325	-178.336	-0.1013	-1.72835	1.297652
8	No	Show	8	H	3	2	1	1.100111	110.2199	-57.8175	-0.1531	-0.16008	2.154406
9	No	Show	9	H	4	2	1	1.100111	110.2199	57.81752	-0.1531	-0.16008	-2.15441
10	No	Show	10	H	4	2	1	1.101607	110.1358	-61.7728	-1.58677	-0.74127	-1.26185
11	No	Show	11	H	4	2	1	1.09989	111.0325	178.3355	-0.1013	-1.72835	-1.29765
12	No	Show	12	H	5	2	1	1.100182	110.257	59.90122	1.860941	0.679876	0.892964
13	No	Show	13	H	5	2	1	1.099113	110.5094	180	1.984449	-0.86225	0
14	No	Show	14	H	5	2	1	1.100182	110.257	-59.9012	1.860941	0.679876	-0.89296
15	No	Show	15	H	1	2	5	0.970023	106.585	180	-1.45434	1.309134	0

BUTANE-1,2,3,4 (no. 28)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.79291	1.18084	0.818217
2	No	Show	2	O	1			2.844703			0.792906	-1.18084	0.818224
3	No	Show	3	O	1	2		2.755231	95.12515		-3.06268	-0.0468	-0.14738
4	No	Show	4	O	2	1	3	2.755242	95.12521	138.7967	3.06268	0.046795	-0.14739
5	No	Show	5	C	1	3	2	1.420708	61.03938	47.82719	-0.68507	0.326059	-0.31144
6	No	Show	6	C	2	1	5	1.420708	57.19307	37.81891	0.685069	-0.32606	-0.31144
7	No	Show	7	C	3	1	5	1.42076	60.5413	30.98369	-1.80715	-0.69938	-0.27525
8	No	Show	8	C	4	2	1	1.42076	60.54088	-16.8429	1.807152	0.699375	-0.27524
9	No	Show	9	H	5	1	6	1.107791	110.1922	-117.979	-0.77728	0.913843	-1.2459
10	No	Show	10	H	6	2	1	1.10779	110.1923	-148.684	0.77728	-0.91385	-1.24589
11	No	Show	11	H	7	3	1	1.102551	111.892	-149.733	-1.76724	-1.34228	-1.17007
12	No	Show	12	H	7	3	1	1.098454	106.3481	91.53537	-1.69282	-1.32767	0.618495
13	No	Show	13	H	8	4	2	1.102552	111.8918	-149.734	1.767241	1.342281	-1.17006
14	No	Show	14	H	8	4	2	1.098454	106.3482	91.53518	1.692823	1.32766	0.618506
15	No	Show	15	H	1	5	6	0.971815	105.0755	-163.362	-1.74471	1.35042	0.916919
16	No	Show	16	H	2	1	5	0.971815	133.6972	116.9854	1.744707	-1.35041	0.916935
17	No	Show	17	H	3	1	5	0.97023	101.1138	-72.6201	-3.21136	0.452275	-0.96602
18	No	Show	18	H	4	2	1	0.970231	101.1132	-120.447	3.211355	-0.45228	-0.96602

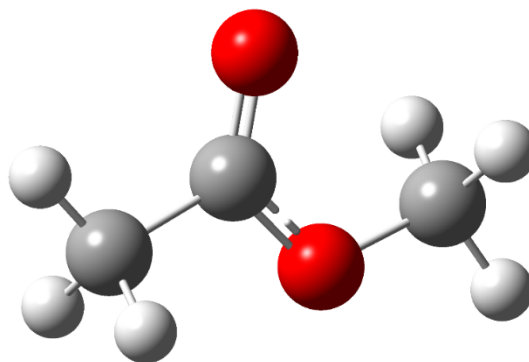
MANNITOL (no. 29)



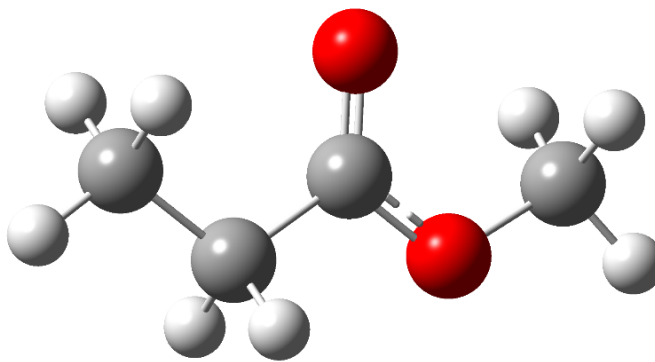
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.40647	1.301918	1.255324
2	No	Show	2	O	1			2.881013			0.44382	-1.43544	0.965256
3	No	Show	3	O	2	1		2.961952	77.28534		-1.97868	-1.3216	-0.73525
4	No	Show	4	O	1	2	3	3.235167	72.73261	-98.8099	1.961443	1.260305	-0.94866
5	No	Show	5	O	3	2	1	2.775095	126.6718	-39.487	-4.33404	0.035046	-0.17586
6	No	Show	6	O	4	1	2	2.756082	116.5584	-51.5835	4.294974	-0.01594	-0.22629
7	No	Show	7	C	1	2	3	1.422975	57.07605	-32.3374	-0.59733	0.555386	0.059029
8	No	Show	8	C	2	1	7	1.422253	54.84794	40.34719	0.560217	-0.43141	-0.03534
9	No	Show	9	C	3	2	1	1.422336	70.50205	-15.3773	-1.9432	-0.18364	0.117296
10	No	Show	10	C	4	1	7	1.418829	60.32523	-88.5052	1.91674	0.256769	0.053333
11	No	Show	11	C	5	3	2	1.415942	57.52751	62.06767	-3.09236	0.698398	-0.32776
12	No	Show	12	C	6	4	1	1.421409	60.54127	55.34448	3.062188	-0.71986	-0.15466
13	No	Show	13	H	7	1	8	1.103767	110.7943	-117.776	-0.56276	1.215785	-0.8247
14	No	Show	14	H	8	2	1	1.099653	106.3936	-150.155	0.493803	-0.94882	-1.00339
15	No	Show	15	H	9	3	2	1.103535	110.1499	-68.995	-2.10971	-0.48812	1.164846
16	No	Show	16	H	10	4	1	1.107304	110.3152	-61.8224	2.017571	0.711693	1.057823
17	No	Show	17	H	11	5	3	1.10601	111.1959	89.94252	-2.92076	0.989595	-1.38086
18	No	Show	18	H	11	5	3	1.099736	107.5582	-151.865	-3.12955	1.615044	0.278699
19	No	Show	19	H	12	6	4	1.100752	106.2343	91.55358	2.938297	-1.2231	-1.12576
20	No	Show	20	H	12	6	4	1.10048	111.9656	-149.804	3.068062	-1.48041	0.640698
21	No	Show	21	H	1	7	8	0.96877	108.2533	-178.9	-1.1426	1.925339	1.344663
22	No	Show	22	H	2	1	7	0.972051	54.88118	-163.206	0.341729	-0.96828	1.81156
23	No	Show	23	H	3	2	1	0.970774	42.26474	-162.201	-1.43014	-2.00084	-0.31081
24	No	Show	24	H	4	1	7	0.972112	140.9503	-165.511	2.90363	1.477756	-1.04866
25	No	Show	25	H	5	3	2	0.970855	51.39269	-142.352	-4.2194	-0.82777	-0.60594
26	No	Show	26	H	6	4	1	0.970207	102.1527	-47.7178	4.465943	0.353961	0.654196

ESTER

METHYL ACETATE (no. 30)

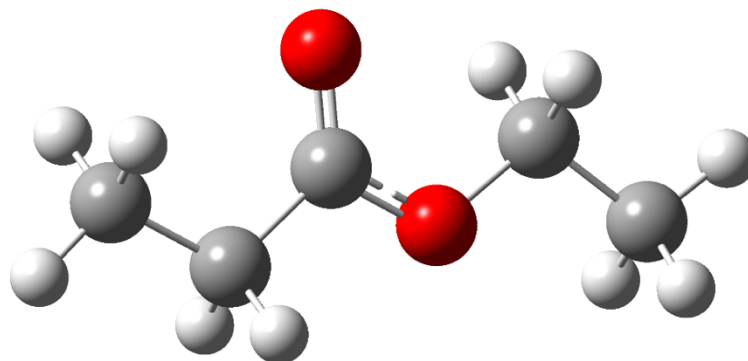


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.542494	-0.72283	0.00041
2	No	Show	2	O	1			2.240972			-0.2701	1.365628	0.000057
3	No	Show	3	C	1	2		2.351633	63.40768		-1.79896	-0.50431	-9.1E-05
4	No	Show	4	C	2	1	3	1.213581	30.34335	0.009695	-0.46168	0.167264	0.000228
5	No	Show	5	C	1	4	2	1.432536	115.3784	-0.02837	1.860483	-0.16152	-0.00025
6	No	Show	6	H	3	1	4	1.098322	91.02521	-126.433	-1.87932	-1.15186	0.883382
7	No	Show	7	H	3	1	4	1.098397	91.29832	125.7898	-1.88322	-1.14137	-0.89089
8	No	Show	8	H	3	1	4	1.09383	141.7548	-0.50183	-2.59139	0.249676	0.005698
9	No	Show	9	H	5	1	4	1.094195	105.7855	-179.994	2.546909	-1.01363	-0.0001
10	No	Show	10	H	5	1	4	1.097924	110.3866	60.61174	2.014733	0.453455	0.896101
11	No	Show	11	H	5	1	4	1.097925	110.3865	-60.6001	2.014156	0.452689	-0.89723

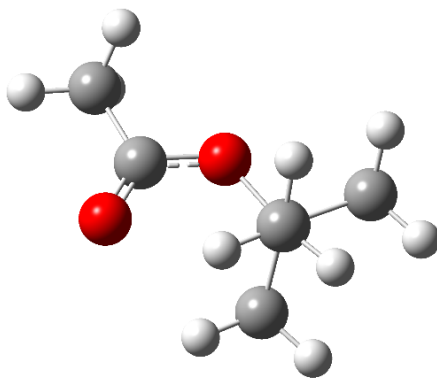
METHYL PROPIONATE (no. 31)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.143012	-0.70428	-4E-06
2	No	Show	2	O	1			2.241885			0.104067	1.282339	-3.3E-05
3	No	Show	3	C	1	2		2.358573	63.3551		-1.21523	-0.74393	-3.4E-05
4	No	Show	4	C	3	1	2	1.518129	144.1889	-0.00812	-2.46112	0.123519	0.000069
5	No	Show	5	C	2	1	3	1.213799	30.24331	-0.00786	0.048265	0.069823	-0.00011
6	No	Show	6	C	1	5	2	1.432774	115.4452	-0.00646	2.392606	-0.00331	0.000057
7	No	Show	7	H	3	1	5	1.100734	88.44357	126.9483	-1.1742	-1.40484	-0.87932
8	No	Show	8	H	3	1	5	1.100734	88.43646	-126.965	-1.17409	-1.40489	0.879204
9	No	Show	9	H	4	3	1	1.098975	110.8765	59.95947	-2.48878	0.769273	-0.88874
10	No	Show	10	H	4	3	1	1.097848	110.3586	-179.992	-3.36268	-0.50294	0.000114
11	No	Show	11	H	4	3	1	1.098975	110.8765	-59.9441	-2.48867	0.769231	0.888913
12	No	Show	12	H	6	1	5	1.094177	105.806	-180	3.167608	-0.77571	0.00013
13	No	Show	13	H	6	1	5	1.097895	110.3623	60.59152	2.478453	0.624419	0.896696
14	No	Show	14	H	6	1	5	1.097895	110.3622	-60.5906	2.478568	0.624366	-0.89661

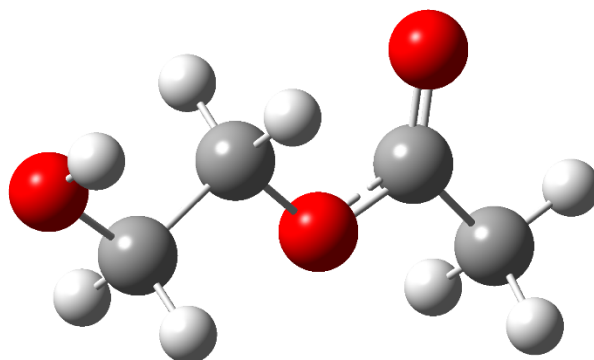
ETHYL PROPIONATE (no. 32)



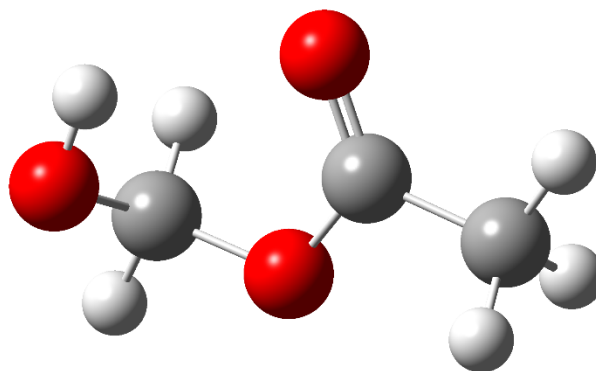
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.693454	-0.439	-0.00029
2	No	Show	2	O	1			2.242086			-0.62339	1.375621	-0.00096
3	No	Show	3	C	1	2		2.359025	63.31978		-1.63465	-0.81973	-0.00213
4	No	Show	4	C	1	2	3	1.442534	88.79476	179.9761	1.842885	0.432611	0.000147
5	No	Show	5	C	2	1	4	1.214357	30.17143	179.9876	-0.50075	0.167473	-0.00096
6	No	Show	6	C	3	1	5	1.518234	144.1624	-0.35134	-2.99278	-0.14113	0.002547
7	No	Show	7	C	4	1	5	1.508209	107.3188	179.99	3.070617	-0.44338	0.001133
8	No	Show	8	H	3	1	5	1.100761	88.54471	126.7272	-1.5002	-1.46435	-0.88421
9	No	Show	9	H	3	1	5	1.100696	88.36492	-127.169	-1.49702	-1.47097	0.8745
10	No	Show	10	H	4	1	5	1.099275	108.6051	-58.7646	1.796348	1.074863	-0.89078
11	No	Show	11	H	4	1	5	1.099273	108.6045	58.74675	1.795297	1.075347	0.890667
12	No	Show	12	H	6	3	1	1.098963	110.8784	60.12247	-3.11473	0.497162	-0.8837
13	No	Show	13	H	6	3	1	1.097819	110.3527	-179.827	-3.79439	-0.89121	0.001068
14	No	Show	14	H	6	3	1	1.098975	110.8804	-59.7761	-3.11191	0.490634	0.893853
15	No	Show	15	H	7	4	1	1.098396	109.534	179.9996	3.970833	0.185969	0.001479
16	No	Show	16	H	7	4	1	1.098998	110.6986	-60.3736	3.09111	-1.08244	0.894991
17	No	Show	17	H	7	4	1	1.098997	110.6993	60.37197	3.092172	-1.08299	-0.89231

TERT-BUTYL ACETATE (no. 34)

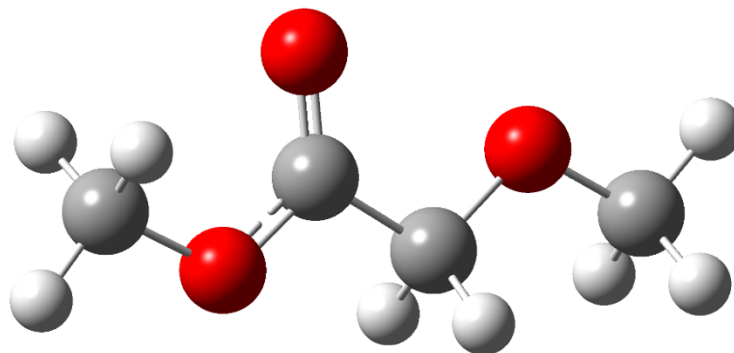
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.308219	-0.66691	0.000061
2	No	Show	2	O	1			2.26005			1.422618	1.299289	0
3	No	Show	3	C	1	2		1.469054	95.19704		-1.03019	-0.06129	0.000001
4	No	Show	4	C	3	1	2	1.523422	110.2045	62.46452	-1.23704	0.757723	-1.26777
5	No	Show	5	C	3	1	2	1.521764	102.5418	179.99	-1.94364	-1.2784	-0.00023
6	No	Show	6	C	3	1	2	1.523423	110.205	-62.4844	-1.2373	0.757441	1.267917
7	No	Show	7	C	2	1	3	1.214773	29.18623	-179.999	1.415041	0.08454	0.000047
8	No	Show	8	C	7	2	1	1.500182	124.4742	179.9964	2.646442	-0.77231	0.000019
9	No	Show	9	H	4	3	1	1.099939	110.0425	51.63941	-0.99388	0.150962	-2.15241
10	No	Show	10	H	4	3	1	1.099571	108.7661	170.1319	-2.29481	1.051391	-1.33054
11	No	Show	11	H	4	3	1	1.096075	111.8776	-69.8643	-0.62098	1.664268	-1.27342
12	No	Show	12	H	5	3	1	1.099449	110.3727	60.14269	-1.76308	-1.89263	0.893595
13	No	Show	13	H	5	3	1	1.099449	110.3728	-60.1448	-1.76294	-1.89241	-0.89417
14	No	Show	14	H	5	3	1	1.098504	109.77	179.9989	-2.99348	-0.95506	-0.00027
15	No	Show	15	H	6	3	1	1.096073	111.8776	69.86093	-0.6212	1.663956	1.27392
16	No	Show	16	H	6	3	1	1.099571	108.7661	-170.135	-2.29507	1.051142	1.330509
17	No	Show	17	H	6	3	1	1.099939	110.0424	-51.6427	-0.99437	0.150465	2.15247
18	No	Show	18	H	8	7	2	1.098365	109.2856	-121.129	2.63805	-1.41948	-0.8874
19	No	Show	19	H	8	7	2	1.098358	109.2903	121.1944	2.637636	-1.42027	0.886847
20	No	Show	20	H	8	7	2	1.094049	109.7051	0.029228	3.537531	-0.13757	0.000476

2-HYDROXYETHYL ACETATE (no. 35)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.38639	-0.48958	-0.00025
2	No	Show	2	O	1			3.627912			-3.18592	0.139114	-0.07175
3	No	Show	3	O	1	2		2.240553	113.6977		1.62929	1.374568	-0.01571
4	No	Show	4	C	1	3		1.434064	88.56166	-0.39882	-0.78635	0.33539	-0.02572
5	No	Show	5	C	2	1	4	1.41551	21.48915	-175.339	-1.97939	-0.598	-0.00376
6	No	Show	6	C	3	1	4	1.212825	30.40782	-179.844	1.559781	0.163847	0.000633
7	No	Show	7	C	6	3	1	1.495843	125.7577	179.8909	2.721533	-0.7782	0.021426
8	No	Show	8	H	4	1	6	1.100784	109.563	-58.9931	-0.7892	0.999182	0.852402
9	No	Show	9	H	4	1	6	1.09946	109.8814	60.35375	-0.78882	0.95378	-0.93479
10	No	Show	10	H	5	2	1	1.102923	111.9619	124.5067	-1.93528	-1.23497	0.89555
11	No	Show	11	H	5	2	1	1.099008	107.0178	-117.264	-1.95202	-1.25227	-0.88637
12	No	Show	12	H	7	6	3	1.098433	109.1712	-120.055	2.680349	-1.42139	-0.86805
13	No	Show	13	H	7	6	3	1.098182	109.3179	122.277	2.649265	-1.42465	0.906235
14	No	Show	14	H	7	6	3	1.093764	109.6795	0.992651	3.656098	-0.21018	0.037592
15	No	Show	15	H	2	1	6	0.969471	98.24963	-59.8547	-3.25195	0.659382	0.743627

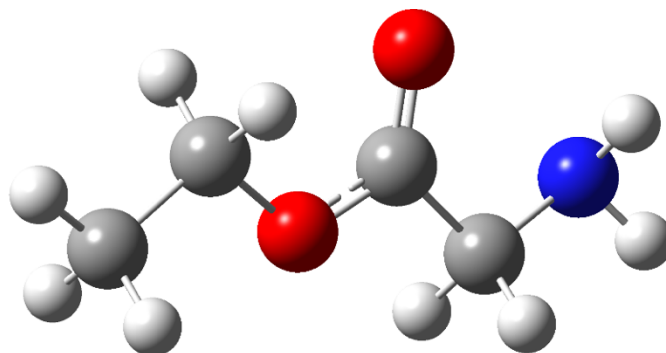
METHYLENE GLYCOL MONOACETATE (no. 37)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.05509	-0.87497	-0.04262
2	No	Show	2	O	1			2.343233			-1.99192	0.290461	0.574821
3	No	Show	3	O	1	2		2.242082	75.60641		0.482202	1.284329	-0.31775
4	No	Show	4	C	2	1	3	1.391882	34.78901	107.4595	-1.40278	-0.5145	-0.3959
5	No	Show	5	C	3	1	4	1.214854	30.58191	-177.459	0.823053	0.145417	-0.06761
6	No	Show	6	C	5	3	1	1.493935	125.6944	-179.943	2.214917	-0.29956	0.243119
7	No	Show	7	H	4	2	1	1.098785	112.4317	-121.745	-1.37949	-0.0322	-1.3829
8	No	Show	8	H	4	2	1	1.093522	108.3751	114.7132	-1.94241	-1.46501	-0.42947
9	No	Show	9	H	6	5	3	1.098339	109.1168	122.4703	2.225506	-0.78671	1.227455
10	No	Show	10	H	6	5	3	1.098431	109.1034	-120.029	2.529511	-1.04277	-0.50201
11	No	Show	11	H	6	5	3	1.093794	109.7651	1.20846	2.889258	0.561584	0.234033
12	No	Show	12	H	2	1	5	0.971441	95.89263	10.26722	-1.61505	1.17837	0.459567

METHYL METHOXYACETATE (no. 38)

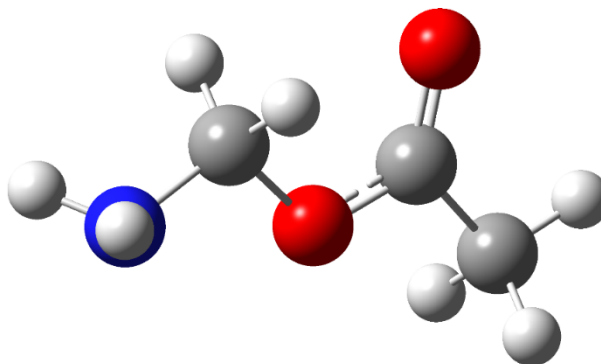
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.77622	0.417856	-0.00036
2	No	Show	2	O	1			3.541178			-1.57086	-0.73844	-8.5E-05
3	No	Show	3	O	2	1		2.248006	49.11055		-0.73488	1.348344	0.000084
4	No	Show	4	C	1	3	2	1.402648	63.93982	-0.01417	0.760591	-0.54957	-4.8E-05
5	No	Show	5	C	3	2	1	1.209833	29.49788	-0.01044	-0.57348	0.149326	0.000013
6	No	Show	6	C	1	4	5	1.415643	110.8432	179.9728	3.053435	-0.19269	0.000197
7	No	Show	7	C	2	1	4	1.434563	137.9477	179.9748	-2.89144	-0.17805	0.000067
8	No	Show	8	H	4	1	6	1.105285	112.0725	-60.4198	0.808756	-1.20262	-0.89048
9	No	Show	9	H	4	1	6	1.105289	112.0708	60.37111	0.808968	-1.20223	0.890665
10	No	Show	10	H	6	1	4	1.103666	111.0714	-60.5452	3.192854	-0.82026	0.897302
11	No	Show	11	H	6	1	4	1.096554	107.3241	179.9964	3.799507	0.610932	-0.00015
12	No	Show	12	H	6	1	4	1.103665	111.0722	60.53808	3.193158	-0.8213	-0.89613
13	No	Show	13	H	7	2	1	1.097638	110.2201	-60.6125	-3.04314	0.43538	0.897561
14	No	Show	14	H	7	2	1	1.093811	105.7096	179.9947	-3.57539	-1.03165	0.000001
15	No	Show	15	H	7	2	1	1.097636	110.2203	60.60188	-3.04325	0.435608	-0.89725

ETHYL GLYCINATE (no. 40)



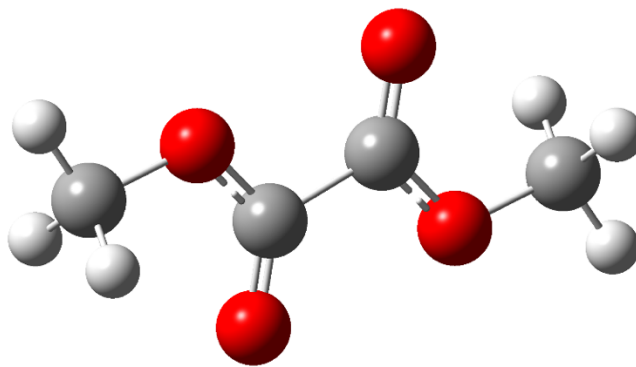
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.67084	-0.432	-0.00568
2	No	Show	2	O	1			2.245268			0.639802	1.391022	0.000356
3	No	Show	3	N	2	1		2.741164	92.18013		2.921374	-0.12034	-0.15518
4	No	Show	4	C	1	2	3	1.443291	89.04514	-176.722	-1.82851	0.429912	-0.00604
5	No	Show	5	C	3	2	1	1.454153	61.49605	-7.85333	1.652191	-0.79906	0.052381
6	No	Show	6	C	4	1	2	1.50804	107.2961	-179.823	-3.04799	-0.45724	-0.00557
7	No	Show	7	C	2	1	4	1.213032	29.83664	179.5125	0.515568	0.184371	0.002841
8	No	Show	8	H	4	1	7	1.099221	108.5529	-58.3117	-1.78601	1.073029	0.884403
9	No	Show	9	H	4	1	7	1.099161	108.5331	59.20139	-1.78618	1.071415	-0.89757
10	No	Show	10	H	5	3	2	1.0989	110.6174	123.3384	1.479081	-1.54532	-0.73546
11	No	Show	11	H	5	3	2	1.10564	115.6444	-115.76	1.546968	-1.3332	1.014702
12	No	Show	12	H	6	4	1	1.098361	109.5134	-179.916	-3.9537	0.164106	-0.00734
13	No	Show	13	H	6	4	1	1.098972	110.6948	-60.3012	-3.06244	-1.09802	-0.89828
14	No	Show	14	H	6	4	1	1.098967	110.6992	60.45909	-3.06389	-1.09521	0.889124
15	No	Show	15	H	3	2	1	1.021108	163.5178	-58.2511	3.663128	-0.79598	0.034478
16	No	Show	16	H	3	2	1	1.022819	69.89112	-131.77	3.014124	0.581493	0.583051

ACETOXYMETHYLAMINE (no. 41)

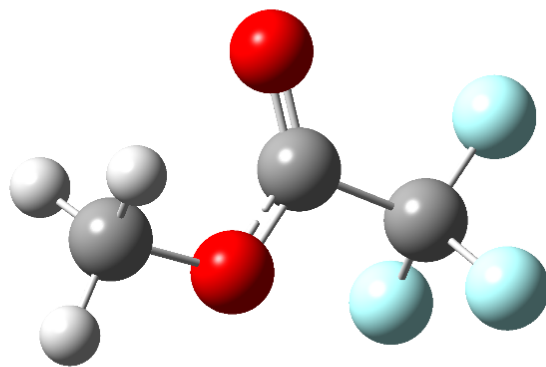


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.16197	-0.49039	0.000077
2	No	Show	2	O	1			2.241046			1.118929	1.348515	-4.4E-05
3	No	Show	3	N	1	2		2.326502	124.1634		-2.4883	-0.46213	-0.00013
4	No	Show	4	C	3	1	2	1.426225	36.67727	-0.01636	-1.33419	0.375805	0.000111
5	No	Show	5	C	2	1	4	1.21714	30.07394	-180	1.01739	0.135618	-3E-06
6	No	Show	6	C	5	2	1	1.498032	125.0734	-180	2.167318	-0.82447	-2.6E-05
7	No	Show	7	H	4	3	1	1.09687	112.9118	117.7871	-1.26528	1.007975	-0.89361
8	No	Show	8	H	4	3	1	1.096876	112.9144	-117.786	-1.26539	1.007698	0.894043
9	No	Show	9	H	6	5	2	1.098373	109.2899	121.1685	2.10201	-1.46886	0.887056
10	No	Show	10	H	6	5	2	1.094019	109.7329	0.015421	3.110845	-0.27072	0.000192
11	No	Show	11	H	6	5	2	1.098376	109.2879	-121.135	2.102231	-1.4685	-0.88739
12	No	Show	12	H	3	1	5	1.017222	124.513	-77.9491	-3.06255	-0.27991	0.819491
13	No	Show	13	H	3	1	5	1.017215	124.5215	77.88393	-3.06253	-0.27947	-0.81966

DIMETHYL OXALATE (no. 33)



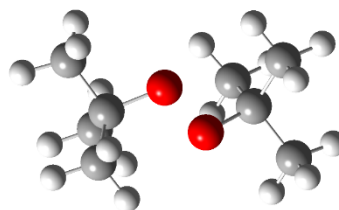
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.62177	0.636021	0.000001
2	No	Show	2	O	1			3.484059			1.621772	-0.63602	-2E-06
3	No	Show	3	O	1	2		2.252582	49.97255		-0.90279	-1.49874	0.000002
4	No	Show	4	O	2	1	3	2.252582	49.97255	-180	0.902787	1.498736	0
5	No	Show	5	C	3	1	4	1.205619	28.23632	0	-0.70125	-0.31008	0
6	No	Show	6	C	4	2	1	1.205619	28.23632	0.000575	0.701254	0.310081	0.000005
7	No	Show	7	C	1	5	3	1.438379	114.9014	-0.00035	-2.97921	0.1603	-3E-06
8	No	Show	8	C	2	1	5	1.438379	139.2727	-180	2.979205	-0.1603	-2E-06
9	No	Show	9	H	7	1	5	1.097213	109.7933	60.49791	-3.1617	-0.44238	0.898523
10	No	Show	10	H	7	1	5	1.097213	109.7934	-60.4956	-3.16168	-0.44241	-0.89851
11	No	Show	11	H	7	1	5	1.093012	105.5815	-179.999	-3.60449	1.056792	-2.2E-05
12	No	Show	12	H	8	2	1	1.093011	105.5815	179.9991	3.604486	-1.05679	0.000013
13	No	Show	13	H	8	2	1	1.097213	109.7934	60.49584	3.161687	0.442408	0.898508
14	No	Show	14	H	8	2	1	1.097213	109.7934	-60.4977	3.161695	0.442383	-0.89853

METHYL TRIFLUOROACETATE (no. 39)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							1.236745	-0.8329	-1.07758
2	No	Show	2	F	1			2.154822			1.818775	0.940131	-0.00016
3	No	Show	3	F	2	1		2.154819	60.01586		1.236839	-0.83264	1.077753
4	No	Show	4	O	1	2	3	2.751573	89.52321	63.42337	-1.28704	-0.63138	-0.00006
5	No	Show	5	O	4	1	2	2.25103	81.87656	29.19172	-0.76538	1.558368	-1.5E-05
6	No	Show	6	C	4	1	5	2.337275	28.91864	-46.9087	0.986695	-0.0901	0.000007
7	No	Show	7	C	5	4	1	1.198484	27.31667	-23.3072	-0.47712	0.395065	0.000015
8	No	Show	8	C	4	1	6	1.444066	155.7294	121.0761	-2.69753	-0.32178	0.000034
9	No	Show	9	H	8	4	1	1.086891	109.3143	-132.865	-2.9406	0.247323	0.893548
10	No	Show	10	H	8	4	1	1.083215	105.4182	107.7521	-3.20269	-1.27999	0.000634
11	No	Show	11	H	8	4	1	1.086896	109.3121	-11.6298	-2.94089	0.246362	-0.89402

PEROXIDE

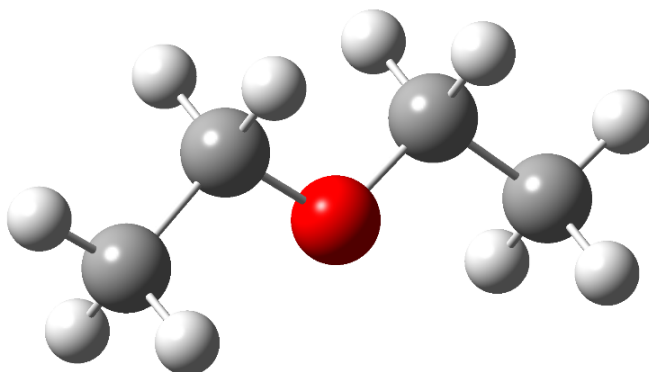
DI-TERT-BUTYL PEROXIDE (no. 36)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.519239	0.492753	0.455136
2	No	Show	2	O	1			1.431663			-0.51924	-0.49275	0.455136
3	No	Show	3	C	1	2		1.445154	108.4259		-0.04126	1.746956	0.00649
4	No	Show	4	C	2	1	3	1.445154	108.4259	141.7992	0.041262	-1.74696	0.00649
5	No	Show	5	C	3	1	2	1.524074	109.7479	60.48115	-1.15384	2.181702	0.953044
6	No	Show	6	C	3	1	2	1.522595	102.2069	178.3624	1.153842	2.685661	0.100586
7	No	Show	7	C	3	1	2	1.522643	110.8061	-63.1976	-0.5385	1.634697	-1.42829
8	No	Show	8	C	4	2	1	1.524074	109.7479	60.48115	1.153842	-2.1817	0.953044
9	No	Show	9	C	4	2	1	1.522595	102.2069	178.3624	-1.15384	-2.68566	0.100586
10	No	Show	10	C	4	2	1	1.522643	110.8061	-63.1976	0.5385	-1.6347	-1.42829
11	No	Show	11	H	5	3	1	1.099985	110.2026	54.35738	-0.78153	2.213682	1.987611
12	No	Show	12	H	5	3	1	1.099409	109.7783	173.9419	-1.50695	3.185337	0.676038
13	No	Show	13	H	5	3	1	1.098504	111.0222	-66.2846	-2.00561	1.489741	0.904182
14	No	Show	14	H	6	3	1	1.099579	110.5487	60.78266	1.966842	2.342376	-0.55536
15	No	Show	15	H	6	3	1	1.09939	110.5792	-59.9074	1.526321	2.734681	1.133792
16	No	Show	16	H	6	3	1	1.098786	109.4704	-179.598	0.852514	3.69477	-0.21283
17	No	Show	17	H	7	3	1	1.09847	110.9623	63.39921	-1.35811	0.907312	-1.50438
18	No	Show	18	H	7	3	1	1.099723	109.4299	-177.112	-0.9122	2.613129	-1.76356
19	No	Show	19	H	7	3	1	1.099724	110.6022	-57.6754	0.2775	1.325467	-2.09755
20	No	Show	20	H	8	4	2	1.099985	110.2026	54.35738	0.781531	-2.21368	1.987611
21	No	Show	21	H	8	4	2	1.099409	109.7783	173.9419	1.50695	-3.18534	0.676038
22	No	Show	22	H	8	4	2	1.098504	111.0222	-66.2846	2.005613	-1.48974	0.904182
23	No	Show	23	H	9	4	2	1.099579	110.5487	60.78266	-1.96684	-2.34238	-0.55536
24	No	Show	24	H	9	4	2	1.09939	110.5792	-59.9074	-1.52632	-2.73468	1.133792
25	No	Show	25	H	9	4	2	1.098786	109.4704	-179.598	-0.85251	-3.69477	-0.21283
26	No	Show	26	H	10	4	2	1.09847	110.9623	63.39921	1.358108	-0.90731	-1.50438
27	No	Show	27	H	10	4	2	1.099723	109.4299	-177.112	0.912202	-2.61313	-1.76356
28	No	Show	28	H	10	4	2	1.099724	110.6022	-57.6754	-0.2775	-1.32547	-2.09755

ETHER

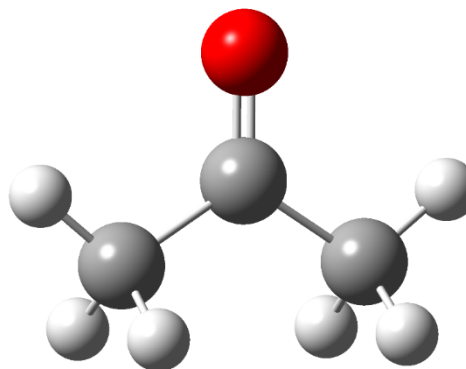
DIETHYL ETHER (no. 42)



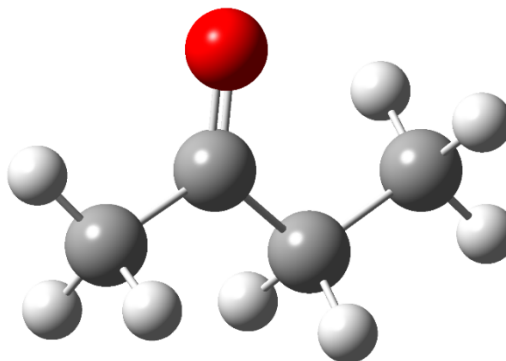
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0	0	-0.27913
2	No	Show	2	C	1			1.417224			0	1.174173	0.514493
3	No	Show	3	C	1	2		1.417224	111.8904		0	-1.17417	0.514493
4	No	Show	4	C	2	1	3	1.511807	108.6414	180	0	2.376715	-0.40172
5	No	Show	5	C	3	1	2	1.511807	108.6414	180	0	-2.37672	-0.40172
6	No	Show	6	H	2	1	3	1.106281	109.6737	58.76219	0.890678	1.18023	1.170628
7	No	Show	7	H	2	1	3	1.106281	109.6737	-58.7622	-0.89068	1.18023	1.170628
8	No	Show	8	H	3	1	2	1.106281	109.6737	58.76219	-0.89068	-1.18023	1.170628
9	No	Show	9	H	3	1	2	1.106281	109.6737	-58.7622	0.890678	-1.18023	1.170628
10	No	Show	10	H	4	2	1	1.098625	110.3044	180	0	3.304399	0.186817
11	No	Show	11	H	4	2	1	1.099624	110.4456	60.01773	-0.89247	2.370205	-1.04408
12	No	Show	12	H	4	2	1	1.099624	110.4456	-60.0177	0.892471	2.370205	-1.04408
13	No	Show	13	H	5	3	1	1.098625	110.3044	180	0	-3.3044	0.186817
14	No	Show	14	H	5	3	1	1.099624	110.4456	-60.0177	-0.89247	-2.37021	-1.04408
15	No	Show	15	H	5	3	1	1.099624	110.4456	60.01773	0.892471	-2.37021	-1.04408

KETONE

ACETONE (no. 43)

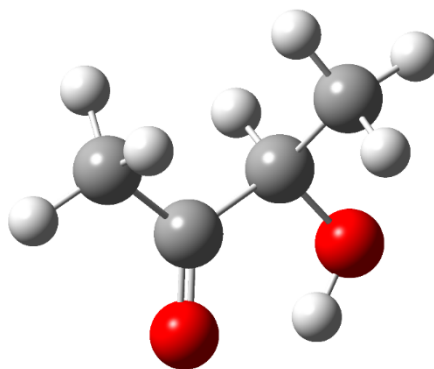


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2E-06	1.398333	0
2	No	Show	2	C	1			1.220097			0	0.178236	-2E-06
3	No	Show	3	C	2	1		1.503502	121.644		1.279969	-0.61056	-0.00018
4	No	Show	4	C	2	1	3	1.503501	121.6439	180	-1.27997	-0.61056	0.00018
5	No	Show	5	H	3	2	1	1.095937	110.3926	-0.49592	2.143988	0.063585	-0.00919
6	No	Show	6	H	3	2	1	1.100341	109.3841	120.9351	1.311059	-1.25641	0.890131
7	No	Show	7	H	3	2	1	1.100248	109.4821	-122.065	1.303343	-1.27186	-0.87921
8	No	Show	8	H	4	2	1	1.100248	109.4815	-122.063	-1.30334	-1.27184	0.879218
9	No	Show	9	H	4	2	1	1.100341	109.3846	120.9361	-1.31106	-1.25643	-0.89012
10	No	Show	10	H	4	2	1	1.095939	110.3926	-0.49581	-2.14399	0.063583	0.009194

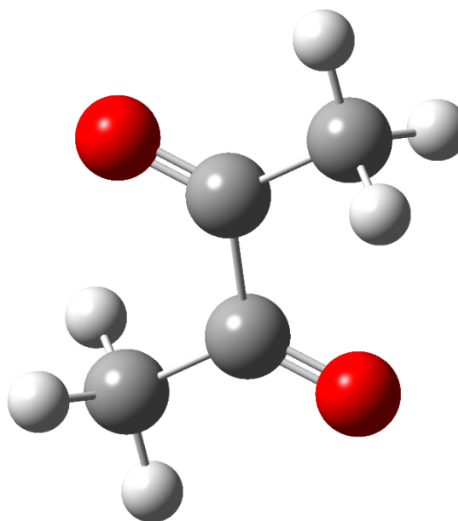
METHYL ETHYL KETONE (no. 44)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.39806	1.375028	-0.01296
2	No	Show	2	C	1			2.3861			0.673386	-0.75689	-0.03342
3	No	Show	3	C	1	2		1.220375	32.62749		-0.52435	0.161207	-0.01138
4	No	Show	4	C	2	1	3	1.518314	87.7119	-176.81	2.000862	-0.02247	0.027587
5	No	Show	5	C	3	1	2	1.50357	121.701	179.7064	-1.87815	-0.49227	0.019119
6	No	Show	6	H	2	1	3	1.102518	121.5196	-62.3557	0.557595	-1.46819	0.80096
7	No	Show	7	H	2	1	3	1.103195	117.8029	69.9287	0.588809	-1.36652	-0.94896
8	No	Show	8	H	4	2	1	1.098147	110.7113	-178.123	2.838711	-0.73191	0.002412
9	No	Show	9	H	4	2	1	1.099407	110.8863	61.66254	2.078686	0.570556	0.95006
10	No	Show	10	H	4	2	1	1.099142	110.8384	-57.912	2.106078	0.666303	-0.82249
11	No	Show	11	H	5	3	1	1.100802	108.8393	-113.86	-1.99314	-1.02735	0.974226
12	No	Show	12	H	5	3	1	1.095881	110.4341	6.686728	-2.66854	0.260151	-0.08144
13	No	Show	13	H	5	3	1	1.099414	110.0839	129.0043	-1.95422	-1.24075	-0.78256

ACETOIN (no. 46)



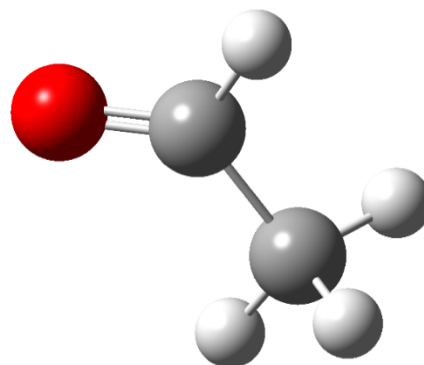
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.553529	-0.971	-0.16483
2	No	Show	2	O	1			2.604424			-0.96245	-1.38448	0.366106
3	No	Show	3	C	1	2		1.412034	64.39673		0.692056	0.122255	-0.40254
4	No	Show	4	C	2	1	3	1.220048	66.7371	-1.02873	-0.73342	-0.25417	-0.03195
5	No	Show	5	C	3	1	4	1.524053	110.5584	123.4002	1.161948	1.351064	0.366858
6	No	Show	6	C	4	2	1	1.496863	122.7262	-178.644	-1.79922	0.788383	-0.16514
7	No	Show	7	H	3	1	4	1.106549	109.9732	-116.067	0.670389	0.35836	-1.48339
8	No	Show	8	H	5	3	1	1.100153	110.1063	-64.4216	1.096675	1.167166	1.449566
9	No	Show	9	H	5	3	1	1.098349	111.3238	174.2816	0.561343	2.23496	0.11314
10	No	Show	10	H	5	3	1	1.098395	109.0451	54.73917	2.209127	1.557541	0.107524
11	No	Show	11	H	6	4	2	1.1016	108.3243	100.9171	-1.73426	1.462999	0.703308
12	No	Show	12	H	6	4	2	1.095726	109.9427	-18.1341	-2.78685	0.313937	-0.17594
13	No	Show	13	H	6	4	2	1.098393	110.8555	-141.267	-1.64316	1.394029	-1.06808
14	No	Show	14	H	1	3	4	0.975279	104.9913	2.509649	0.969926	-1.69038	0.140242

2,3-BUTANEDIONE (no. 45)

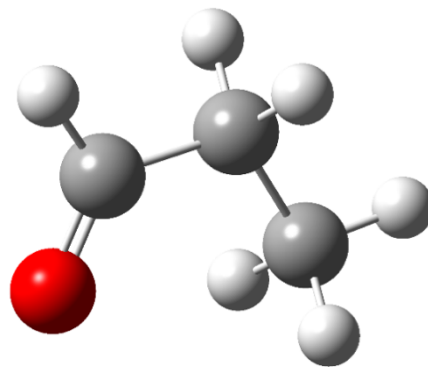
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							-0.07461	0.768166	0.000005
2	No	Show	2	O	1			1.213341			-1.1905	1.244606	0.000182
3	No	Show	3	C	1	2		1.543562	118.6683		0.074611	-0.76817	0.000005
4	No	Show	4	O	3	1	2	1.213341	118.6683	-179.981	1.190497	-1.24461	0.000182
5	No	Show	5	C	3	1	2	1.493539	116.5597	0.01626	-1.1905	-1.56199	-0.00015
6	No	Show	6	H	5	3	1	1.099805	109.2456	-58.3264	-1.78745	-1.29286	0.883465
7	No	Show	7	H	5	3	1	1.099806	109.2464	58.33208	-1.78721	-1.29292	-0.88395
8	No	Show	8	H	5	3	1	1.094862	110.0043	-179.997	-0.96094	-2.63252	-8.2E-05
9	No	Show	9	C	1	2	3	1.493539	124.7721	-179.997	1.190497	1.561992	-0.00015
10	No	Show	10	H	9	1	2	1.099805	109.2456	121.6706	1.787454	1.292857	0.883465
11	No	Show	11	H	9	1	2	1.099806	109.2464	-121.671	1.787212	1.292921	-0.88395
12	No	Show	12	H	9	1	2	1.094862	110.0043	0	0.960938	2.632518	-8.2E-05

ALDEHYDE

ACETALDEHYDE (no. 47)



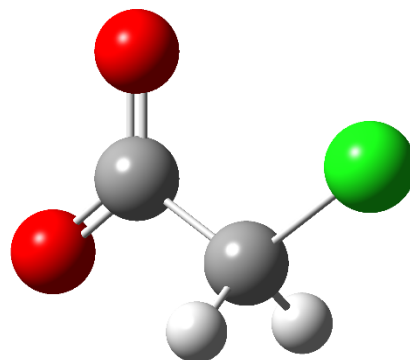
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.21031	0.359932	0
2	No	Show	2	C	1			2.396477			0.939374	-0.6993	0
3	No	Show	3	C	1	2		1.214395	30.93336		0	0.459483	0
4	No	Show	4	H	2	1	3	1.100804	120.2074	68.37038	1.591178	-0.62955	0.884339
5	No	Show	5	H	2	1	3	1.100804	120.2074	-68.3704	1.591178	-0.62955	-0.88434
6	No	Show	6	H	2	1	3	1.096528	86.03547	180	0.387869	-1.64704	0
7	No	Show	7	H	3	1	2	1.113001	120.022	180	0.475999	1.465563	0

PROPIONALDEHYDE (no. 48)

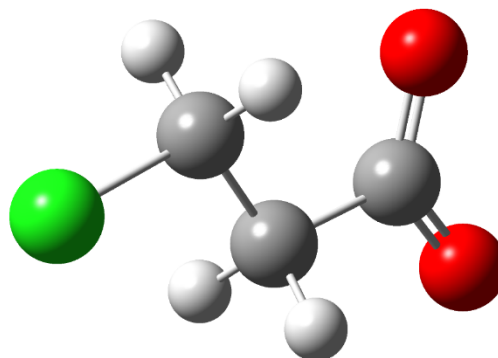
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.38098	-0.69506	-1.7E-05
2	No	Show	2	C	1			2.396895			0.543071	0.73432	-8E-06
3	No	Show	3	C	2	1		1.517881	88.71677		1.420743	-0.50409	-5E-06
4	No	Show	4	C	1	2	3	1.215225	31.15719	179.9917	-0.92115	0.429804	0.000077
5	No	Show	5	H	2	1	4	1.103832	118.9782	65.03801	0.729405	1.380256	0.875487
6	No	Show	6	H	2	1	4	1.103829	118.9742	-65.0548	0.72935	1.380226	-0.87553
7	No	Show	7	H	3	2	1	1.099412	110.8157	59.78347	1.224692	-1.12189	-0.88803
8	No	Show	8	H	3	2	1	1.099412	110.8155	-59.7895	1.224758	-1.12184	0.888074
9	No	Show	9	H	3	2	1	1.09794	110.7642	179.9971	2.483416	-0.22805	-5.3E-05
10	No	Show	10	H	4	1	2	1.112697	120.1839	179.9745	-1.59978	1.311595	-0.00019

HALOCARBOXYLATE

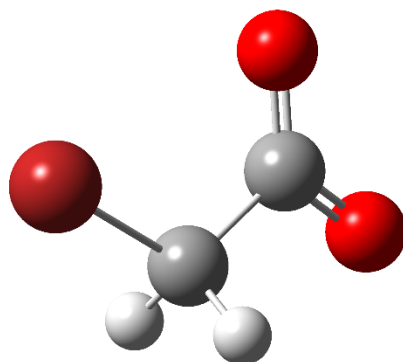
CHLOROACETATE (no. 49)



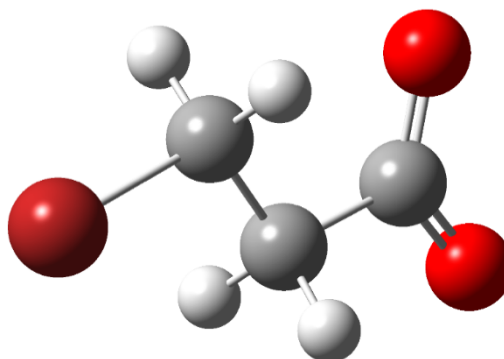
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.74743	0.073665	0.000061
2	No	Show	2	O	1			3.932364			-2.12921	-0.586	0.000096
3	No	Show	3	O	2	1		2.237259	49.0403		-0.96683	1.325595	-8.4E-05
4	No	Show	4	C	2	1	3	2.323797	14.98209	179.973	0.18456	-0.80166	-0.00015
5	No	Show	5	C	3	2	1	1.245493	26.7843	-0.00439	-1.06494	0.083973	0.000081
6	No	Show	6	H	4	2	1	1.08576	92.42795	125.3899	0.172118	-1.43178	0.883972
7	No	Show	7	H	4	2	1	1.085764	92.43592	-125.393	0.172138	-1.43119	-0.88469

3-CHLOROPROPANOATE (no. 50)

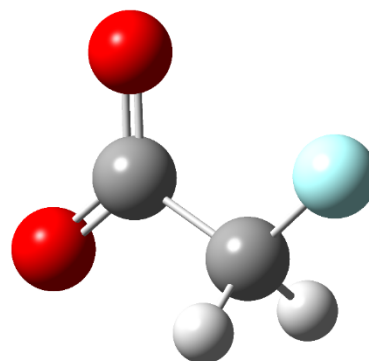
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-2.44688	-0.14401	-9.1E-05
2	No	Show	2	O	1			5.0995			2.596957	-0.89541	0.000644
3	No	Show	3	O	2	1		2.232883	62.65879		1.874871	1.217489	-0.00051
4	No	Show	4	C	2	1	3	2.369986	0.052822	-151.565	0.252558	-0.5481	-0.00074
5	No	Show	5	C	4	2	1	1.508257	141.4667	28.2628	-0.77684	0.55425	0.000921
6	No	Show	6	C	3	2	1	1.255697	27.34808	-0.02086	1.689697	-0.02448	-8.3E-05
7	No	Show	7	H	4	2	1	1.09066	91.53534	154.7851	0.12939	-1.18358	-0.87854
8	No	Show	8	H	4	2	1	1.090601	91.46772	-98.1768	0.1292	-1.18668	0.87471
9	No	Show	9	H	5	4	2	1.084525	112.3107	-61.9954	-0.71435	1.174587	0.888317
10	No	Show	10	H	5	4	2	1.0845	112.3099	62.14741	-0.71439	1.177185	-0.88463

BROMOACETATE (no. 51)

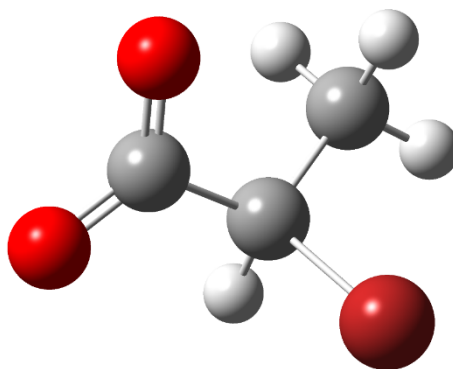
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.33979	0.032831	0.000231
2	No	Show	2	O	1			3.126299			1.50208	1.335712	-0.00053
3	No	Show	3	O	2	1		2.24871	97.96183		2.713332	-0.5589	0.001054
4	No	Show	4	C	3	2	1	2.318686	64.24587	0.062342	0.411137	-0.83494	-0.00121
5	No	Show	5	C	2	1	4	1.244023	71.62334	-0.05879	1.637574	0.09909	-0.00011
6	No	Show	6	H	4	3	2	1.096082	92.50807	-125.742	0.438768	-1.47558	0.887731
7	No	Show	7	H	4	3	2	1.09611	92.59738	125.5353	0.438478	-1.47291	-0.89211

3-BROMOPROPANOATE (no. 52)

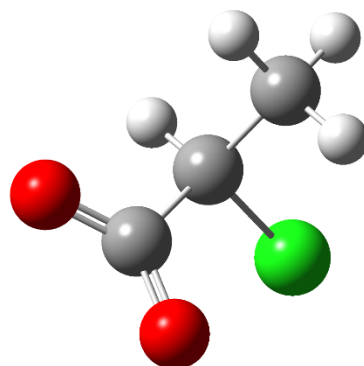
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.92376	-0.07376	-2.9E-05
2	No	Show	2	O	1			4.682012			2.582095	1.19844	0.000029
3	No	Show	3	O	2	1		2.232216	91.56995		3.247264	-0.93237	-0.0002
4	No	Show	4	C	3	2	1	2.371243	62.71887	-0.01118	0.911648	-0.52287	0.000293
5	No	Show	5	C	4	3	2	1.508165	141.1528	0.035002	-0.08193	0.611752	-3.6E-05
6	No	Show	6	C	2	1	5	1.25525	64.21904	-179.987	2.363816	-0.03769	-6E-06
7	No	Show	7	H	4	3	2	1.090463	91.3693	126.5572	0.773671	-1.1579	-0.87539
8	No	Show	8	H	4	3	2	1.090474	91.38429	-126.506	0.773879	-1.15715	0.876559
9	No	Show	9	H	5	4	3	1.083941	112.5377	62.31129	-0.00593	1.230295	-0.88692
10	No	Show	10	H	5	4	3	1.083942	112.5375	-62.3708	-0.00607	1.230678	0.88659

FLUOROACETATE (no. 53)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							1.790105	0.15984	0.000187
2	No	Show	2	O	1			3.532608			-1.64081	-0.68166	0.000184
3	No	Show	3	O	2	1		2.240555	48.87977		-0.61182	1.308632	-4.4E-05
4	No	Show	4	C	2	1	3	2.335412	14.12259	179.9554	0.694556	-0.69559	-0.00018
5	No	Show	5	C	3	2	1	1.248494	26.61775	0.029695	-0.62754	0.060237	-0.00017
6	No	Show	6	H	4	2	1	1.089203	93.31229	125.0751	0.753895	-1.32137	0.889335
7	No	Show	7	H	4	2	1	1.089217	93.33709	-125.116	0.754092	-1.3209	-0.89003

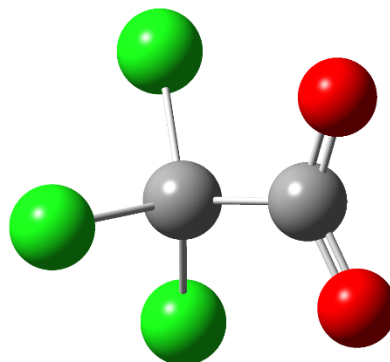
2-BROMOPROPANOATE (no. 54)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							1.321301	-0.28793	0.103596
2	No	Show	2	O	1			3.480852			-1.99936	0.040152	1.094512
3	No	Show	3	O	2	1		2.234449	70.57645		-1.88357	-1.31342	-0.67952
4	No	Show	4	C	3	2	1	2.377886	62.34598	-35.2251	-0.3575	0.507387	-0.5791
5	No	Show	5	C	4	3	2	1.506277	137.416	-43.8136	-0.40003	1.972181	-0.23062
6	No	Show	6	C	2	1	4	1.252188	49.60449	48.08101	-1.51118	-0.32879	0.00202
7	No	Show	7	H	4	3	2	1.084241	82.83593	-159.062	-0.30037	0.341934	-1.64912
8	No	Show	8	H	5	4	3	1.09193	108.6378	-38.5034	-1.33226	2.394517	-0.61127
9	No	Show	9	H	5	4	3	1.08775	111.0487	80.69396	-0.37033	2.118453	0.846842
10	No	Show	10	H	5	4	3	1.088386	110.9135	-157.763	0.433083	2.504235	-0.68606

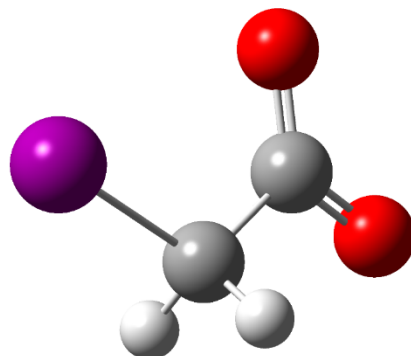
2-CHLOROPROPANOATE (no. 55)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.652862	-0.56615	-0.17753
2	No	Show	2	O	1			2.991385			-1.08978	-1.16568	0.855358
3	No	Show	3	O	2	1		2.235749	94.0459		-2.11414	0.114171	-0.66491
4	No	Show	4	C	3	2	1	2.34686	63.42415	-16.763	0.186227	0.472651	-0.36905
5	No	Show	5	C	4	3	2	1.516296	106.1907	-100.098	0.31286	1.695965	0.517868
6	No	Show	6	C	2	1	4	1.247797	68.0423	17.62323	-1.10657	-0.28708	-0.03052
7	No	Show	7	H	4	3	2	1.084549	84.42367	149.427	0.170568	0.748721	-1.41776
8	No	Show	8	H	5	4	3	1.090467	108.9661	-28.3621	-0.55547	2.337233	0.363263
9	No	Show	9	H	5	4	3	1.089716	110.3704	91.13997	0.351642	1.401888	1.566436
10	No	Show	10	H	5	4	3	1.08818	110.7901	-147.908	1.210869	2.259523	0.272677

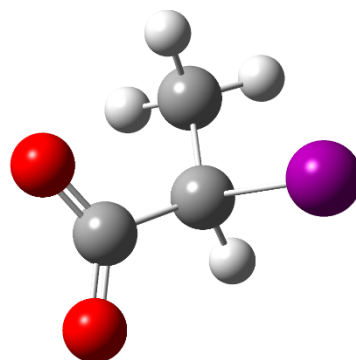
TRICHLOROACETATE (no. 56)



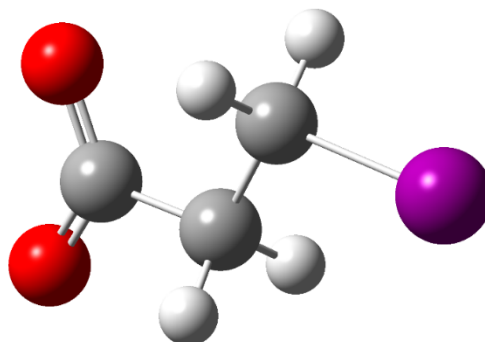
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.4169	0.012241	1.752817
2	No	Show	2	Cl	1			2.898255			-0.92096	1.436513	-0.72049
3	No	Show	3	Cl	2	1		2.875536	60.25196		-0.93255	-1.43894	-0.70203
4	No	Show	4	O	2	1	3	2.919483	68.92775	-95.0024	1.943873	1.113315	-0.26043
5	No	Show	5	O	4	2	1	2.242861	96.14987	60.86713	1.935968	-1.12953	-0.26207
6	No	Show	6	C	4	2	1	2.390281	37.35098	37.53746	-0.15726	0.000147	-0.01641
7	No	Show	7	C	5	4	2	1.237941	25.06171	-13.3326	1.416953	-0.00633	-0.22276

2-iodoacetate (no. 57)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							-1.10787	0.020252	-0.0001
2	No	Show	2	O	1			3.232558			1.848643	1.327336	0.000401
3	No	Show	3	O	2	1		2.234316	101.1717		3.130901	-0.50241	-0.00077
4	No	Show	4	C	3	2	1	2.327584	64.09188	-0.04439	0.832703	-0.8711	0.00084
5	No	Show	5	C	2	1	4	1.247186	74.15913	0.040022	2.022423	0.092316	0.000051
6	No	Show	6	H	4	3	2	1.085159	93.08431	-125.327	0.87494	-1.49914	0.884782
7	No	Show	7	H	4	3	2	1.085151	93.03007	125.4658	0.875023	-1.50088	-0.88185

2-IODOPROPANOATE (no. 58)

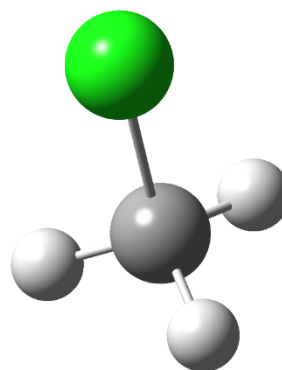
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							1.149319	-0.14771	0.060257
2	No	Show	2	O	1			3.624925			-2.31709	-0.13244	1.120368
3	No	Show	3	O	2	1		2.23431	70.62747		-2.09979	-1.43128	-0.6846
4	No	Show	4	C	3	2	1	2.377125	62.26858	-37.4696	-0.79775	0.5552	-0.58805
5	No	Show	5	C	4	3	2	1.509144	137.8325	-43.2407	-0.9895	2.000455	-0.1982
6	No	Show	6	C	2	1	4	1.253094	50.39867	47.32219	-1.82442	-0.41796	0.004126
7	No	Show	7	H	4	3	2	1.084242	83.04746	-158.868	-0.75585	0.422949	-1.66338
8	No	Show	8	H	5	4	3	1.08794	111.4439	80.93822	-0.92891	2.132992	0.879941
9	No	Show	9	H	5	4	3	1.088331	110.9314	-157.443	-0.24405	2.633987	-0.67507
10	No	Show	10	H	5	4	3	1.092573	108.6027	-38.2987	-1.98003	2.322081	-0.52851

3-iodanylPROPANOATE (no. 59)

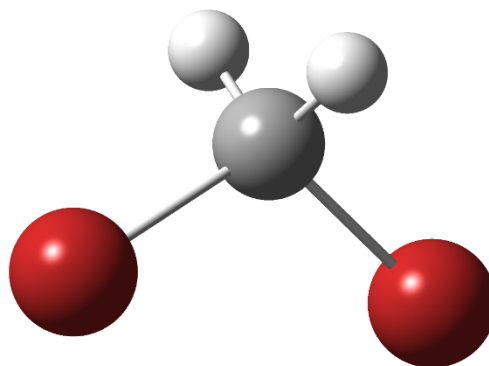
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							1.62301	-0.04903	0.000034
2	No	Show	2	O	1			5.421118			-	-0.95921	-0.00018
3	No	Show	3	O	2	1		2.231479	64.14808		3.72115	1.183814	0.000325
4	No	Show	4	C	2	1	3	2.372574	135.9135	-0.27536	-3.0991	-0.5055	0.000195
5	No	Show	5	C	4	2	1	1.509406	141.3471	179.6556	-	0.645293	-0.00054
6	No	Show	6	C	3	2	1	1.255271	27.43096	0.006519	0.41565	-0.04736	-3.3E-05
7	No	Show	7	H	4	2	1	1.090526	91.16343	53.07347	2.85433	-1.13988	-0.87468
8	No	Show	8	H	4	2	1	1.090532	91.18959	-53.7245	1.24607	-1.13872	0.875915
9	No	Show	9	H	5	4	2	1.083723	112.7438	-62.5378	-	1.262159	-0.88797
10	No	Show	10	H	5	4	2	1.083721	112.7449	62.58123	0.49563	1.263377	0.886039

HALOALKANE

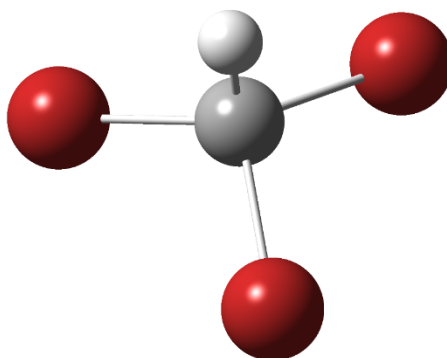
CHLOROMETHANE (no. 60)



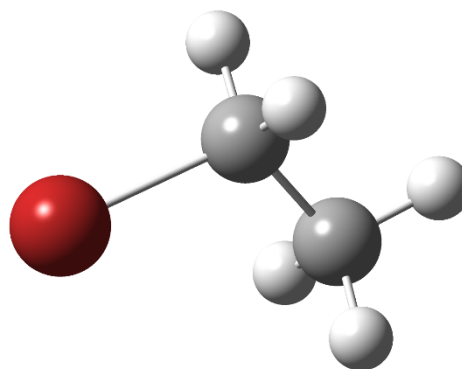
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0.000003	0.661446	0
2	No	Show	2	C	1			1.798189			0.000003	-1.13674	0
3	No	Show	3	H	2	1		1.094261	108.0034		-1.04068	-1.47495	0
4	No	Show	4	H	2	1	3	1.094317	107.9826	-	0.520307	-1.47459	0.901484
5	No	Show	5	H	2	1	4	1.094317	107.9826	-	0.520307	-1.47459	-0.90148
										119.992			
										120.016			

DIBROMOMETHANE (no. 61)

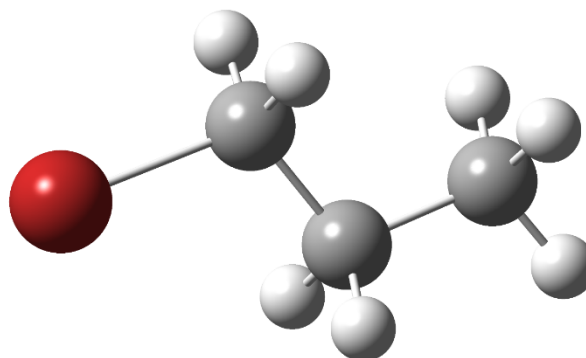
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.61474	-0.12496	0
2	No	Show	2	Br	1			3.229476			1.614738	-0.12496	0
3	No	Show	3	C	2	1		1.934731	33.42522		0	0.940783	0
4	No	Show	4	H	3	2	1	1.09248	107.9271	119.3514	-1E-06	1.551246	0.906006
5	No	Show	5	H	3	2	1	1.09248	107.9271	-119.351	-1E-06	1.551246	-0.90601

BROMOFORM (no. 62)

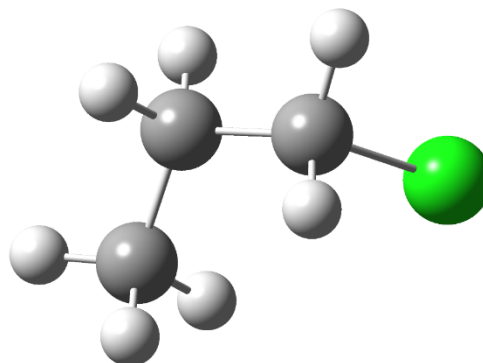
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							-0.00034	0.000343	0.532111
2	No	Show	2	Br	1			1.933516			0.355344	-1.81017	-0.04585
3	No	Show	3	Br	1	2		1.933222	111.4648		-1.74582	0.597443	-0.04592
4	No	Show	4	Br	1	3	2	1.933482	111.4988	125.2322	1.390572	1.212637	-0.04587
5	No	Show	5	H	1	3	2	1.09261	107.3348	-117.385	-0.0014	0.000925	1.62472

BROMOETHANE (no. 63)

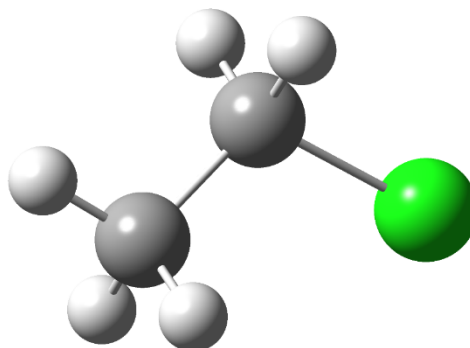
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-0.79346	-0.06675	0
2	No	Show	2	C	1			1.969746			1.026355	0.687036	0
3	No	Show	3	C	2	1		1.509585	111.2878		2.070968	-0.40275	0
4	No	Show	4	H	2	1	3	1.09521	105.0617	122.2297	1.073451	1.31704	-0.89463
5	No	Show	5	H	2	1	3	1.09521	105.0617	-122.23	1.073451	1.31704	0.89463
6	No	Show	6	H	3	2	1	1.100907	108.4483	180	3.065956	0.068416	0
7	No	Show	7	H	3	2	1	1.098474	111.305	-60.8304	1.987057	-1.03604	0.893617
8	No	Show	8	H	3	2	1	1.098475	111.305	60.83048	1.987058	-1.03604	-0.89362

BROMOPROPANE (no. 64)

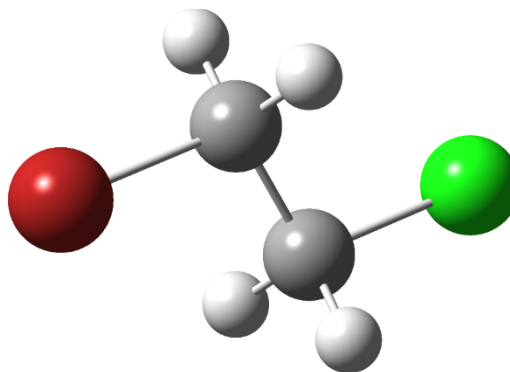
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.284	-0.04776	-1.5E-05
2	No	Show	2	C	1			2.892976			1.571028	-0.5148	0.000073
3	No	Show	3	C	2	1		1.514518	39.12217		0.56575	0.617978	0.000066
4	No	Show	4	C	2	1	3	1.525573	149.0982	-0.01502	2.989359	0.047083	-6.9E-05
5	No	Show	5	H	2	1	3	1.100382	87.06629	126.2139	1.410602	-1.14647	0.886695
6	No	Show	6	H	2	1	3	1.100382	87.05834	-126.227	1.410482	-1.14659	-0.88644
7	No	Show	7	H	3	2	1	1.096451	112.1863	-118.156	0.649283	1.245676	-0.89504
8	No	Show	8	H	3	2	1	1.096449	112.1862	118.1552	0.649212	1.245619	0.89522
9	No	Show	9	H	4	2	1	1.098986	110.6348	179.9973	3.728225	-0.76646	0.000164
10	No	Show	10	H	4	2	1	1.10046	111.0268	-60.0675	3.167673	0.668815	-0.89039
11	No	Show	11	H	4	2	1	1.100464	111.0269	60.0632	3.167663	0.669296	0.88992

CHLOROPROPANE (no. 65)

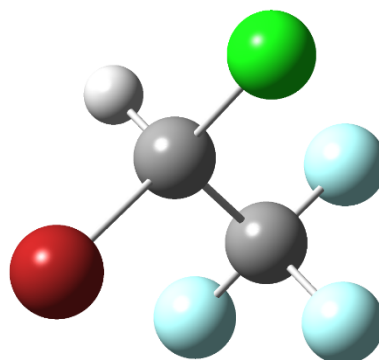
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.444525	-0.34593	-0.06796
2	No	Show	2	C	1			2.763732			-1.1497	0.561996	-0.35755
3	No	Show	3	C	2	1		1.514413	37.64434		0.169895	0.894295	0.307042
4	No	Show	4	C	2	1	3	1.522048	94.34363	-124.201	-1.78039	-0.7289	0.144901
5	No	Show	5	H	2	1	3	1.100952	88.43533	125.1213	-1.00792	0.527547	-1.44879
6	No	Show	6	H	2	1	3	1.10246	143.388	8.37425	-1.81772	1.413724	-0.14843
7	No	Show	7	H	3	2	1	1.0972	111.8732	-118.226	0.084435	0.909039	1.400809
8	No	Show	8	H	3	2	1	1.095573	112.0882	118.3132	0.577407	1.849812	-0.0411
9	No	Show	9	H	4	2	1	1.101099	110.7492	90.51898	-1.9303	-0.69126	1.235098
10	No	Show	10	H	4	2	1	1.09906	110.8257	-149.574	-2.75849	-0.89573	-0.32778
11	No	Show	11	H	4	2	1	1.100012	111.1776	-29.5624	-1.14318	-1.59666	-0.08091

CHLOROETHANE (no. 66)

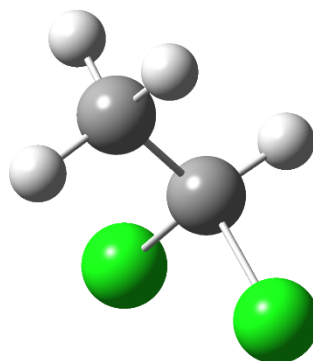
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.133915	-0.14996	0
2	No	Show	2	C	1			1.816075			-0.49185	0.659363	0
3	No	Show	3	C	2	1		1.509737	111.0128		-1.60455	-0.36104	0
4	No	Show	4	H	2	1	3	1.095696	105.6803	122.0656	-0.50737	1.292692	0.893982
5	No	Show	5	H	2	1	3	1.095696	105.6802	-122.066	-0.50737	1.292692	-0.89398
6	No	Show	6	H	3	2	1	1.100365	108.6746	180	-2.56878	0.169113	0
7	No	Show	7	H	3	2	1	1.098616	111.0941	-60.7381	-1.55732	-0.99754	-0.8942
8	No	Show	8	H	3	2	1	1.098616	111.0941	60.73813	-1.55732	-0.99754	0.894203

1-BROMO-2-CHLOROETHANE (no. 67)

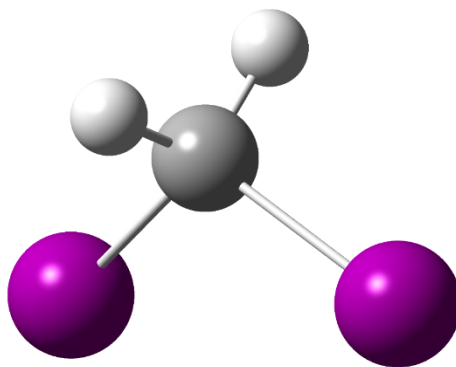
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.66447	-0.03802	-8E-06
2	No	Show	2	Cl	1			4.481064			2.815658	0.053435	-1.8E-05
3	No	Show	3	C	1	2		1.958188	18.40852		0.180505	0.618148	0.000032
4	No	Show	4	C	3	1	2	1.509845	108.8333	-0.00356	1.118574	-0.56492	0.000033
5	No	Show	5	H	3	1	4	1.095075	106.5396	121.0015	0.293062	1.232054	-0.89977
6	No	Show	6	H	3	1	4	1.095077	106.5414	-121.001	0.293064	1.232035	0.899847
7	No	Show	7	H	4	3	1	1.095295	112.0831	-62.3157	1.004909	-1.18056	0.898777
8	No	Show	8	H	4	3	1	1.095294	112.0841	62.30926	1.004874	-1.18061	-0.89867

HALOTHANE (no. 68)

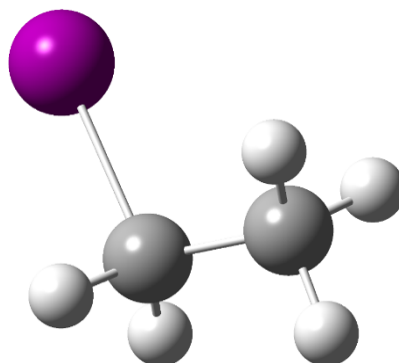
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.62375	-0.2832	0.012922
2	No	Show	2	Cl	1			3.071901			0.422107	2.008252	0.030407
3	No	Show	3	F	2	1		2.967809	84.16135		2.399803	-0.15879	-0.4174
4	No	Show	4	F	3	2	1	2.157377	70.62084	-53.7099	1.213026	-0.62131	1.323839
5	No	Show	5	F	3	2	1	2.157905	97.66446	0.751784	1.011206	-1.8098	-0.4678
6	No	Show	6	C	4	3	2	1.331731	36.01468	74.22773	1.199804	-0.57291	-0.00695
7	No	Show	7	C	6	4	3	1.526869	112.2224	-121.401	0.115643	0.360727	-0.5401
8	No	Show	8	H	7	6	4	1.095009	108.9841	-179.518	0.146341	0.353882	-1.63465

1,1-DICHLOROETHANE (no. 69)

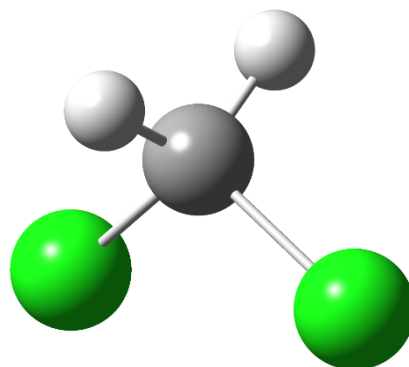
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0.211349	-0.52516	-1.46758
2	No	Show	2	Cl	1			2.935162			0.211349	-0.52516	1.467581
3	No	Show	3	C	1	2		1.800123	35.38621		0.211349	0.517262	0
4	No	Show	4	C	3	1	2	1.505872	110.9086	-122.537	-0.97457	1.445299	0
5	No	Show	5	H	3	1	4	1.093076	106.1497	-123.404	1.170076	1.042292	0
6	No	Show	6	H	4	3	1	1.097895	110.623	60.77814	-1.91235	0.874396	0
7	No	Show	7	H	4	3	1	1.098429	109.0654	-178.694	-0.93214	2.081721	0.894267
8	No	Show	8	H	4	3	1	1.098429	109.0654	-59.7497	-0.93214	2.081721	-0.89427

DIIODOMETHANE (no. 70)

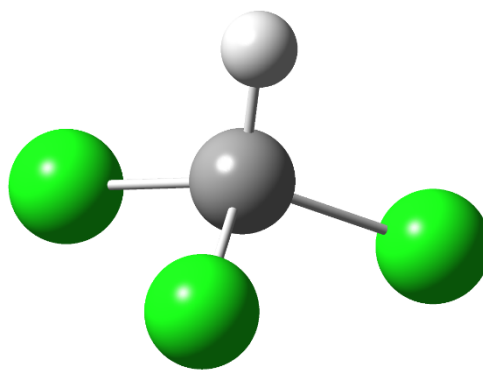
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							0	1.800602	-0.09096
2	No	Show	2	I	1			3.601204			0	-1.8006	-0.09096
3	No	Show	3	C	1	2		2.132714	32.40543		0	0	1.051979
4	No	Show	4	H	3	1	2	1.093164	107.4827	-	-	0	1.664784
5	No	Show	5	H	3	1	4	1.093164	107.4827	-	-	0	1.664784
										119.749	0.90525		
										120.502			

IDOETHANE (no. 71)

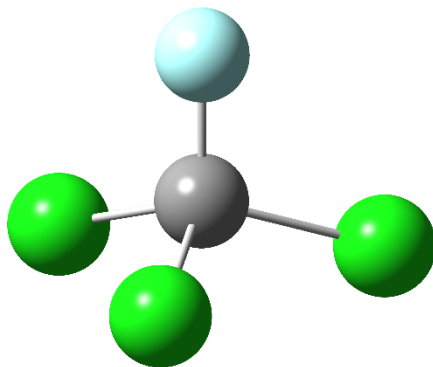
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z	
1	No	Show	1	I							0	0.639602	0	
2	No	Show	2	C		1		2.16807			-0.60653	-1.4419	0	
3	No	Show	3	C		2	1	1.511959	112.0357		0.580319	-2.37859	0	
4	No	Show	4	H		2	1	3	1.095255	104.3121	122.421	-1.22854	-1.54266	0.895844
										-				
5	No	Show	5	H		2	1	3	1.095255	104.3121	122.421	-1.22854	-1.54266	-0.89584
6	No	Show	6	H		3	2	1	1.101713	108.4252	180	0.206109	-3.41481	0
										-				
7	No	Show	7	H		3	2	1	1.098453	111.4965	60.9099	1.204132	-2.23791	-0.89312
8	No	Show	8	H		3	2	1	1.098453	111.4965	60.9099	1.204132	-2.23791	0.89312

DICHLOROMETHANE (no. 72)

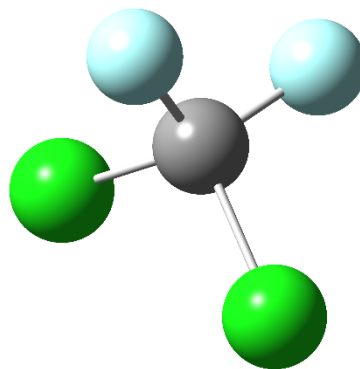
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0	1.475644	-0.21944
2	No	Show	2	Cl	1			2.951288			0	-1.47564	-0.21944
3	No	Show	3	C	1	2		1.782466	34.1198		0	0	0.780391
4	No	Show	4	H	3	1	2	1.092566	108.2166	-119.06	-0.90716	0	1.38929
5	No	Show	5	H	3	1	4	1.092566	108.2166	-121.88	0.907162	0	1.38929

CHLOROFORM (no. 73)

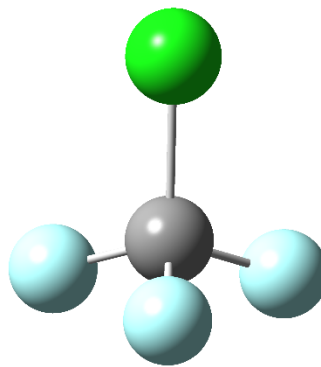
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0.8439	-1.45995	-0.08596
2	No	Show	2	Cl	1			2.920655			0.842563	1.460706	-0.08598
3	No	Show	3	Cl	2	1		2.920908	60.00287		-1.68642	-0.00078	-0.08598
4	No	Show	4	C	3	2	1	1.775682	34.6677	33.41867	-0.00013	0.000031	0.470308
5	No	Show	5	H	4	3	2	1.092444	108.2663	118.4801	0.000049	0.000193	1.562752

TRICHLOROFLUOROMETHANE (no. 74)

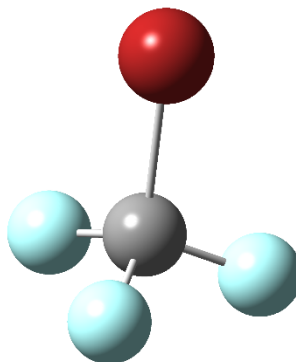
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.58269	1.577938	-0.30899
2	No	Show	2	Cl	1			2.913447			-1.07524	-1.29357	-0.30896
3	No	Show	3	Cl	1	2		2.913459	60.00026		1.657857	-0.28438	-0.30907
4	No	Show	4	F	3	1	2	2.532257	54.88362	-66.047	0.000179	0.000036	1.583957
5	No	Show	5	C	4	3	1	1.333345	41.63083	37.68405	-8.3E-05	-2.9E-05	0.250612

DICHLORODIFLUOROMETHANE (no. 75)

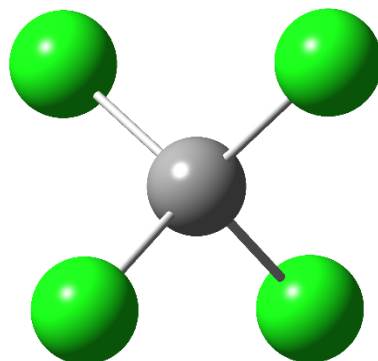
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0	-1.46336	-0.65272
2	No	Show	2	Cl	1			2.926728			0	1.463364	-0.65272
3	No	Show	3	F	1	2		2.537114	54.77542		1.074959	0	1.119277
4	No	Show	4	F	3	1	2	2.149918	64.932	70.71518	-1.07496	0	1.119277
5	No	Show	5	C	3	1	4	1.327168	41.16723	-34.564	0	0	0.340921

CHLOROTRIFLUOROMETHANE (no. 76)

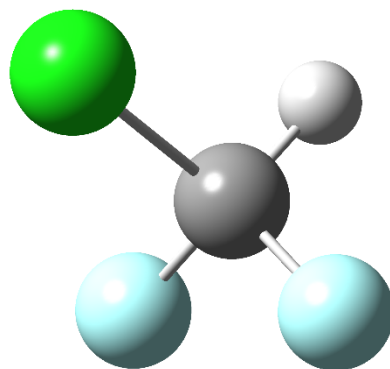
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.41134	-0.00002	0.000085
2	No	Show	2	F	1			2.54464			0.809738	-0.81263	-0.93888
3	No	Show	3	F	2	1		2.150716	65.00223		0.809767	1.219426	-0.23438
4	No	Show	4	F	2	1	3	2.150633	65.00685	66.9635	0.810047	-0.40675	1.173104
5	No	Show	5	C	2	1	3	1.322533	40.65595	33.48356	0.354474	-1.4E-05	-8E-06

BROMOTRIFLUOROMETHANE (no. 77)

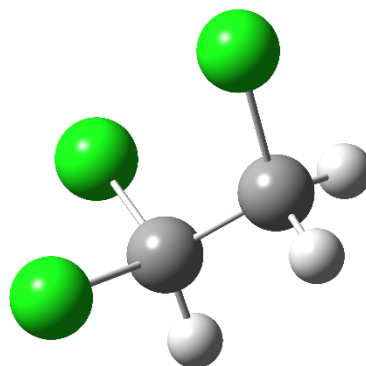
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							1.117802	-0.00013	0.000025
2	No	Show	2	F	1			2.689657			-1.26796	-0.71255	-1.01725
3	No	Show	3	F	2	1		2.150977	66.43181		-1.26808	-0.52483	1.125525
4	No	Show	4	F	3	2	1	2.151575	60.01334	75.38391	-1.26711	1.237782	-0.10836
5	No	Show	5	C	3	2	1	1.321738	35.54341	39.35648	-0.81579	0.000118	-2.3E-05

CARBON TETRACHLORIDE (no. 78)

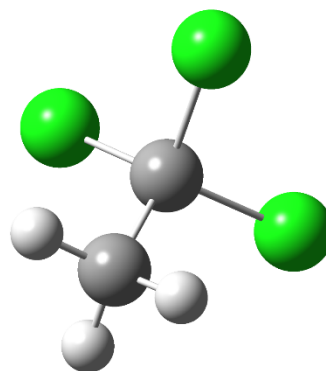
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.025944	1.025944	1.025944
2	No	Show	2	Cl	1			2.901808			-1.02594	-1.02594	1.025944
3	No	Show	3	Cl	1	2		2.901808	60		1.025944	-1.02594	-1.02594
4	No	Show	4	Cl	1	2	3	2.901808	60	70.52878	-1.02594	1.025944	-1.02594
5	No	Show	5	C	1	2	3	1.776987	35.26439	35.26439	0	0	0

CHLORODIFLUOROMETHANE (no. 79)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.9106	0.90096	0
2	No	Show	2	F	1			2.550637			0.58452	-0.8599	1.08154
3	No	Show	3	F	2	1		2.16308	64.91088		0.58452	-0.8599	-
4	No	Show	4	C	2	1	3	1.338038	41.47844	35.12403	0.58452	-0.07211	0
5	No	Show	5	H	4	2	1	1.093838	111.0299	120.3944	1.451698	0.594586	0

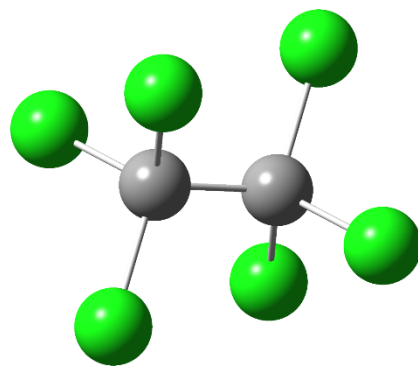
1,1,2-TRICHLOROETHANE (no. 80)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.2975	1.040045	1.467549
2	No	Show	2	Cl	1			2.935098			-0.2975	1.040045	-1.46755
3	No	Show	3	Cl	1	2		3.346754	63.99183		-0.2975	-1.96779	0
4	No	Show	4	C	1	2	3	1.789861	34.92285	66.26821	0.640504	0.62767	0
5	No	Show	5	C	4	1	2	1.511128	111.8074	-124.965	1.075457	-0.81951	0
6	No	Show	6	H	4	1	5	1.095296	106.8346	-119.354	1.527991	1.269574	0
7	No	Show	7	H	5	4	1	1.096203	109.0882	-178.003	1.674325	-1.01384	-0.89736
8	No	Show	8	H	5	4	1	1.096203	109.0882	-57.9547	1.674325	-1.01384	0.897359

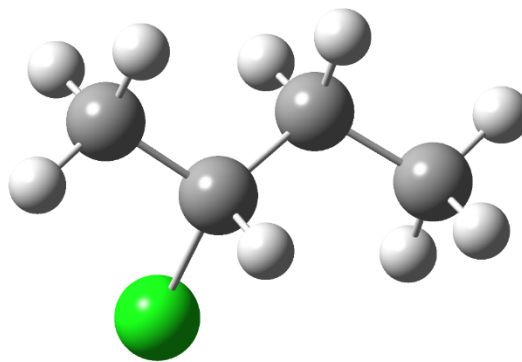
1,1,1-TRICHLOROETHANE (no. 81)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.088471	-1.2793	-0.36528
2	No	Show	2	Cl	1			2.909899			-1.65259	-0.30251	-0.36514
3	No	Show	3	Cl	1	2		2.909073	60.00262		0.564142	1.582131	-0.36483
4	No	Show	4	C	3	1	2	1.79359	35.81029	36.80872	-0.00016	-0.00012	0.263684
5	No	Show	5	C	4	3	1	1.509258	110.525	121.243	0.000015	-0.00051	1.772942
6	No	Show	6	H	5	4	3	1.097549	109.162	60.05845	-0.67223	0.788609	2.133486
7	No	Show	7	H	5	4	3	1.097634	109.1898	-179.941	-0.34724	-0.97734	2.133516
8	No	Show	8	H	5	4	3	1.097516	109.1181	-59.9396	1.019913	0.187082	2.132329

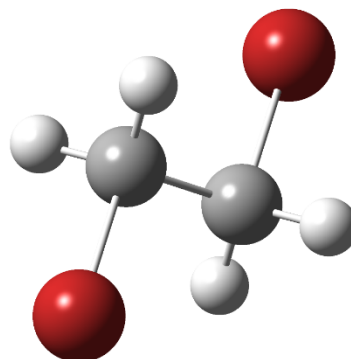
HEXACHLOROETHANE (no. 82)



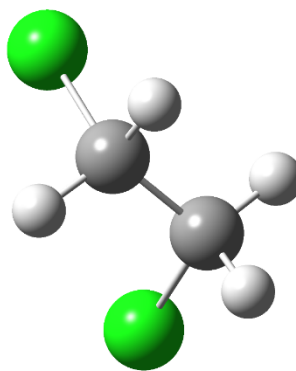
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.388146	-1.05091	-1.30293
2	No	Show	2	Cl	1			2.898425			1.389021	1.653201	-0.25955
3	No	Show	3	Cl	1	2		2.898132	59.99764		1.39037	-0.60237	1.560284
4	No	Show	4	Cl	1	3	2	3.243033	63.47403	-106.759	-1.38907	-1.65327	0.259609
5	No	Show	5	Cl	4	1	3	2.898383	63.46626	112.0374	-1.39029	0.602556	-1.56025
6	No	Show	6	Cl	5	4	1	2.897972	60.00371	-106.751	-1.38817	1.050806	1.302848
7	No	Show	7	C	1	3	2	1.776794	35.36	-35.5514	0.79132	-0.00013	-0.00037
8	No	Show	8	C	7	1	3	1.582679	109.6525	-120.253	-0.79136	0.000113	0.000327

2-CHLOROBUTANE (no. 83)

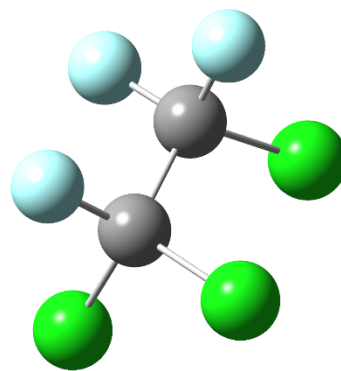
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.862	-1.23084	-0.06959
2	No	Show	2	C	1			1.837079			-0.26558	0.451676	0.364327
3	No	Show	3	C	2	1		1.518806	109.5766		1.066098	0.711324	-0.31831
4	No	Show	4	C	2	1	3	1.51362	108.4221	124.0768	-1.33681	1.451499	-0.01497
5	No	Show	5	C	3	2	1	1.521523	114.4041	-62.5621	2.18633	-0.22375	0.112669
6	No	Show	6	H	2	1	4	1.098231	103.7659	118.044	-0.13496	0.409699	1.453955
7	No	Show	7	H	3	2	1	1.102135	108.7144	61.97394	0.918006	0.670068	-1.40967
8	No	Show	8	H	3	2	1	1.102967	105.9387	176.4462	1.334811	1.752325	-0.07204
9	No	Show	9	H	4	2	1	1.097674	111.3489	57.27667	-2.28852	1.225757	0.483195
10	No	Show	10	H	4	2	1	1.100542	108.8389	176.8427	-1.01058	2.456183	0.293862
11	No	Show	11	H	4	2	1	1.099745	110.582	-64.0582	-1.49451	1.454934	-1.10335
12	No	Show	12	H	5	3	2	1.09894	110.7089	-176.228	3.134297	0.058994	-0.36596
13	No	Show	13	H	5	3	2	1.099332	111.2242	63.68767	1.963949	-1.26459	-0.16254
14	No	Show	14	H	5	3	2	1.100983	110.8006	-56.4643	2.331271	-0.18361	1.203331

1,2-DIBROMOETHANE (no. 84)

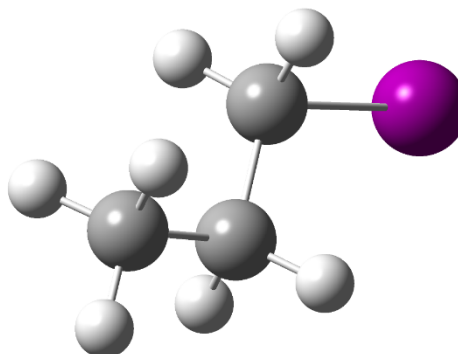
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							0.714789	2.201564	0
2	No	Show	2	Br	1			4.629388			-0.71479	-2.20156	0
3	No	Show	3	C	1	2		1.960923	17.98723		0.714789	0.240641	0
4	No	Show	4	C	3	1	2	1.508418	108.6063	0	-0.71479	-0.24064	0
5	No	Show	5	H	3	1	4	1.095064	106.3054	-121.173	1.25882	-0.06681	0.899262
6	No	Show	6	H	3	1	4	1.095064	106.3054	121.1729	1.25882	-0.06681	-0.89926
7	No	Show	7	H	4	3	1	1.095064	112.4115	62.65898	-1.25882	0.066807	-0.89926
8	No	Show	8	H	4	3	1	1.095064	112.4115	-62.659	-1.25882	0.066807	0.899262

1,2-DICHLOROETHANE (no. 85)

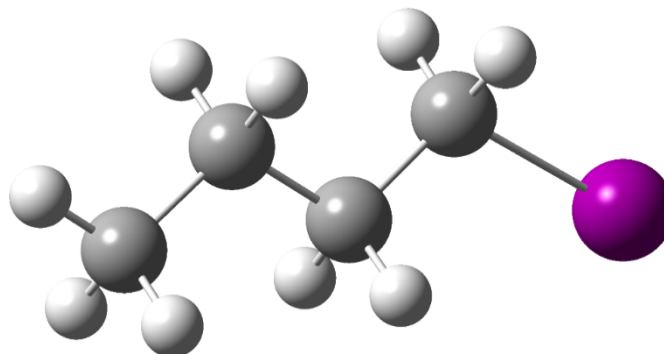
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.60404	1.58429	-0.48234
2	No	Show	2	Cl	1			3.391069			0.604038	-1.58429	-0.48234
3	No	Show	3	C	1	2		1.802609	53.95147		-0.60404	0.449023	0.917864
4	No	Show	4	C	3	1	2	1.505302	112.0692	33.85323	0.604038	-0.44902	0.917864
5	No	Show	5	H	3	1	4	1.095541	106.9982	-123.068	-1.53812	-0.12124	0.867816
6	No	Show	6	H	3	1	4	1.096877	106.7401	119.3989	-0.59296	1.065913	1.824762
7	No	Show	7	H	4	3	1	1.096877	109.1123	175.8993	0.592961	-1.06591	1.824762
8	No	Show	8	H	4	3	1	1.095541	111.9454	54.12506	1.538117	0.121242	0.867816

1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (no. 86)

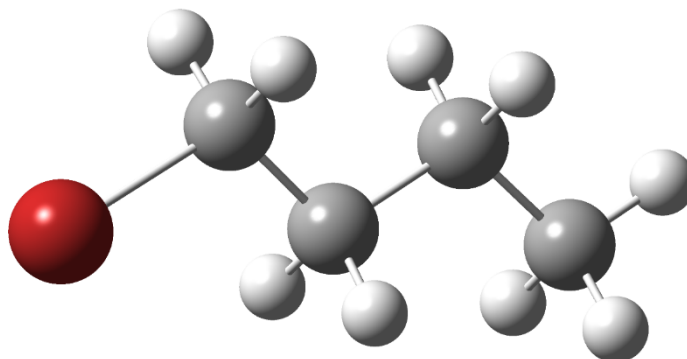
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-0.60404	1.58429	-0.48234
2	No	Show	2	Cl	1			3.391069			0.604038	-1.58429	-0.48234
3	No	Show	3	C	1	2		1.802609	53.95147		-0.60404	0.449023	0.917864
4	No	Show	4	C	3	1	2	1.505302	112.0692	33.85323	0.604038	-0.44902	0.917864
5	No	Show	5	H	3	1	4	1.095541	106.9982	-123.068	-1.53812	-0.12124	0.867816
6	No	Show	6	H	3	1	4	1.096877	106.7401	119.3989	-0.59296	1.065913	1.824762
7	No	Show	7	H	4	3	1	1.096877	109.1123	175.8993	0.592961	-1.06591	1.824762
8	No	Show	8	H	4	3	1	1.095541	111.9454	54.12506	1.538117	0.121242	0.867816

1-IODOPROPANE (no. 87)

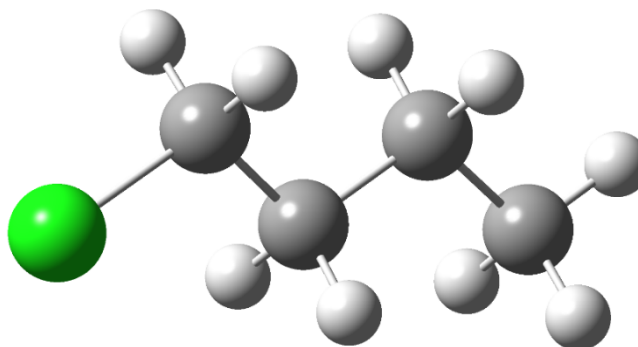
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							0	-1.05163	0
2	No	Show	2	C	1			3.080189			0.570345	1.975295	0
3	No	Show	3	C	2	1		1.516706	40.5293		-0.61168	1.024923	0
4	No	Show	4	C	2	1	3	1.526395	150.5126	0	0.078021	3.420113	0
5	No	Show	5	H	2	1	3	1.100363	86.42982	126.1917	1.194934	1.787881	0.88632
6	No	Show	6	H	2	1	3	1.100363	86.42982	-126.192	1.194934	1.787881	-0.88632
7	No	Show	7	H	3	2	1	1.096548	112.4293	-117.837	-1.23432	1.131637	-0.8963
8	No	Show	8	H	3	2	1	1.096548	112.4293	117.8375	-1.23432	1.131637	0.896298
9	No	Show	9	H	4	2	1	1.099404	110.6076	180	0.927272	4.118298	0
10	No	Show	10	H	4	2	1	1.100482	111.0213	-60.0803	-0.5343	3.628513	-0.89034
11	No	Show	11	H	4	2	1	1.100482	111.0213	60.08028	-0.5343	3.628513	0.890336

1-IODOBUTANE (no. 88)

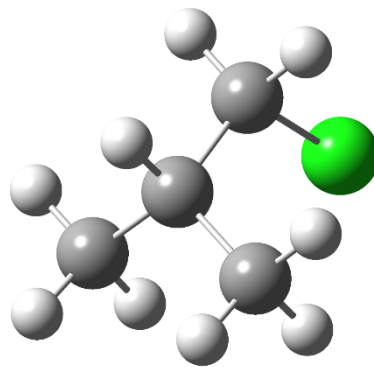
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							1.477663	-0.09023	0.000002
2	No	Show	2	C	1			3.081492			-1.60181	-0.20175	0.000002
3	No	Show	3	C	2	1		1.528945	150.9977		-2.96498	0.490679	0.000042
4	No	Show	4	C	2	1	3	1.515722	40.49263	0.005362	-0.48549	0.823557	-3.7E-05
5	No	Show	5	C	3	2	1	1.523961	111.932	179.9996	-4.11269	-0.51193	-1.9E-05
6	No	Show	6	H	2	1	4	1.101667	86.73215	-126.239	-1.51553	-0.84921	0.887144
7	No	Show	7	H	2	1	4	1.101667	86.73487	126.2345	-1.51558	-0.84921	-0.88714
8	No	Show	8	H	3	2	1	1.102395	109.186	-58.1219	-3.03896	1.144937	0.884207
9	No	Show	9	H	3	2	1	1.102396	109.1861	58.1212	-3.03897	1.145043	-0.88405
10	No	Show	10	H	4	2	1	1.096343	112.4715	-117.816	-0.49665	1.455225	0.895976
11	No	Show	11	H	4	2	1	1.096343	112.4715	117.8158	-0.49665	1.455156	-0.8961
12	No	Show	12	H	5	3	2	1.100897	110.8901	59.81718	-4.06812	-1.15968	0.889031
13	No	Show	13	H	5	3	2	1.099458	111.3341	179.9962	-5.08768	-0.00381	0.000079
14	No	Show	14	H	5	3	2	1.100897	110.8901	-59.8245	-4.0682	-1.15948	-0.88921

1-BROMOBUTANE (no. 89)

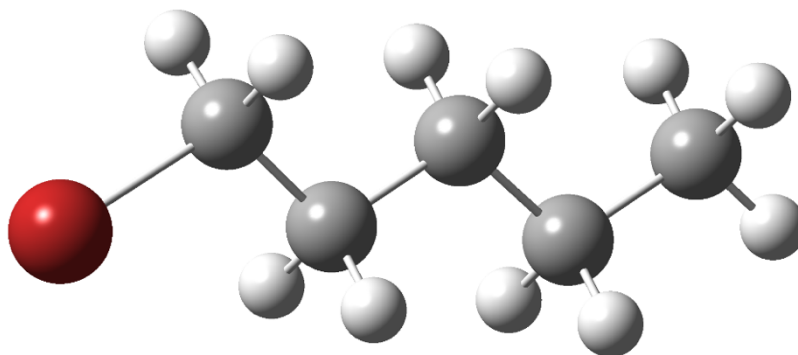
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.77251	-0.1336	-1E-06
2	No	Show	2	C	1			2.892015			1.118136	-0.2227	-3E-06
3	No	Show	3	C	2	1		1.528418	149.8789		2.463172	0.503201	-0.00001
4	No	Show	4	C	2	1	3	1.513574	39.19184	0.001125	-0.02491	0.769443	0.000009
5	No	Show	5	C	3	2	1	1.523867	111.9069	179.9997	3.634993	-0.47097	0.000005
6	No	Show	6	H	2	1	4	1.101544	87.21593	-126.252	1.04461	-0.87136	-0.88727
7	No	Show	7	H	2	1	4	1.101544	87.21651	126.2513	1.044622	-0.87136	0.887261
8	No	Show	8	H	3	2	1	1.102384	109.2107	-58.126	2.521307	1.159218	-0.88404
9	No	Show	9	H	3	2	1	1.102384	109.2108	58.12522	2.521305	1.159243	0.884004
10	No	Show	10	H	4	2	1	1.096178	112.2874	-118.069	-0.02602	1.40239	-0.89497
11	No	Show	11	H	4	2	1	1.096179	112.2874	118.0694	-0.02602	1.402369	0.895001
12	No	Show	12	H	5	3	2	1.100873	110.8856	59.81166	3.606162	-1.11959	-0.88903
13	No	Show	13	H	5	3	2	1.09931	111.3436	179.9992	4.597227	0.060622	-1.4E-05
14	No	Show	14	H	5	3	2	1.100874	110.8855	-59.8132	3.606173	-1.11954	0.889074

1-CHLOROBUTANE (no. 90)

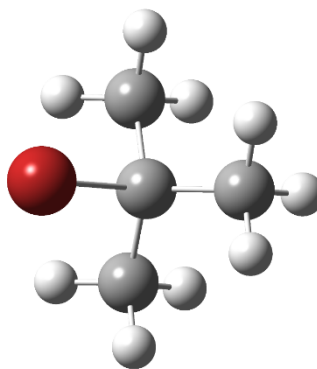
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-2.30888	-0.24717	-8E-06
2	No	Show	2	C	1			2.754			0.445032	-0.26911	-2.6E-05
3	No	Show	3	C	2	1		1.527159	148.6961		1.756153	0.513948	-6.1E-05
4	No	Show	4	C	2	1	3	1.51386	37.81002	0.006491	-0.74356	0.668457	0.000056
5	No	Show	5	C	3	2	1	1.52367	111.9647	179.9969	2.969995	-0.40701	0.000038
6	No	Show	6	H	2	1	4	1.101882	87.82027	-126.255	0.397931	-0.91984	-0.88798
7	No	Show	7	H	2	1	4	1.101882	87.82375	126.2492	0.398009	-0.9199	0.887897
8	No	Show	8	H	3	2	1	1.102406	109.2227	-58.1207	1.785871	1.17201	-0.88401
9	No	Show	9	H	3	2	1	1.102408	109.2229	58.11477	1.785839	1.17215	0.88379
10	No	Show	10	H	4	2	1	1.09679	111.94	-118.467	-0.76499	1.303057	-0.89424
11	No	Show	11	H	4	2	1	1.09679	111.9399	118.4664	-0.76498	1.302908	0.894461
12	No	Show	12	H	5	3	2	1.100944	110.8731	59.79627	2.969716	-1.05645	-0.88895
13	No	Show	13	H	5	3	2	1.099428	111.3797	179.9954	3.908089	0.166337	-0.00007
14	No	Show	14	H	5	3	2	1.100942	110.8731	-59.8052	2.969761	-1.0562	0.889207

1-CHLORO-2-METHYLPROPANE (no. 91)

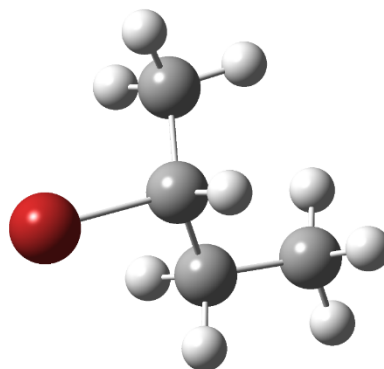
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.670048	0.301432	0
2	No	Show	2	C	1			2.785063			-1.1034	0.047358	0
3	No	Show	3	C	2	1		1.520682	37.09961		0.020738	1.07146	0
4	No	Show	4	C	2	1	3	1.525187	92.93721	-124.062	-1.1034	-0.80933	1.261859
5	No	Show	5	C	2	1	3	1.525187	92.93721	124.0616	-1.1034	-0.80933	-1.26186
6	No	Show	6	H	2	1	3	1.104546	140.7239	0	-2.01866	0.665681	0
7	No	Show	7	H	3	2	1	1.096506	111.6832	118.4033	-0.00618	1.702583	-0.89626
8	No	Show	8	H	3	2	1	1.096506	111.6832	-118.403	-0.00618	1.702583	0.896262
9	No	Show	9	H	4	2	1	1.099775	110.4537	-153.475	-1.98796	-1.46249	1.28294
10	No	Show	10	H	4	2	1	1.100588	111.3042	86.30465	-1.11484	-0.18563	2.168596
11	No	Show	11	H	4	2	1	1.100976	110.6879	-34.0322	-0.20871	-1.44998	1.297035
12	No	Show	12	H	5	2	1	1.099775	110.4537	153.4746	-1.98796	-1.46249	-1.28294
13	No	Show	13	H	5	2	1	1.100588	111.3042	-86.3047	-1.11484	-0.18563	-2.1686
14	No	Show	14	H	5	2	1	1.100976	110.6879	34.03224	-0.20871	-1.44998	-1.29704

1-BROMOPENTANE (no. 92)

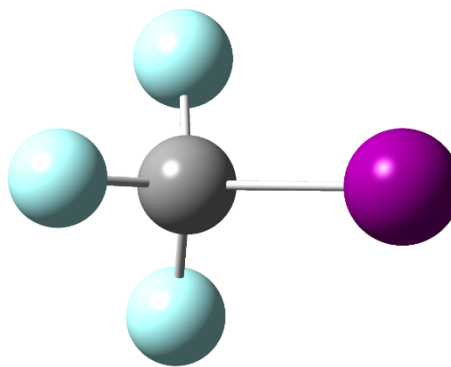
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-2.31999	-0.10827	-4E-06
2	No	Show	2	C	1			4.282117			1.93058	0.410574	0.000004
3	No	Show	3	C	2	1		1.52728	19.82941		0.567216	-0.27777	0.000002
4	No	Show	4	C	2	1	3	1.525678	132.3058	-0.00044	3.086643	-0.58502	0.000016
5	No	Show	5	C	3	2	1	1.513812	110.6648	-0.00054	-0.54805	0.745848	0.000012
6	No	Show	6	C	4	2	1	1.523486	112.4624	179.9987	4.446452	0.101948	-1.7E-05
7	No	Show	7	H	2	1	5	1.103737	98.30458	54.10218	2.011233	1.065535	0.884739
8	No	Show	8	H	2	1	5	1.103738	98.30475	-54.1052	2.011241	1.065525	-0.88474
9	No	Show	9	H	3	2	1	1.101462	109.8279	121.1074	0.474977	-0.92404	-0.88716
10	No	Show	10	H	3	2	1	1.101463	109.8279	-121.108	0.474981	-0.92405	0.887156
11	No	Show	11	H	4	2	1	1.102839	109.0802	57.93243	2.998722	-1.23958	-0.88321
12	No	Show	12	H	4	2	1	1.102839	109.0802	-57.9349	2.998741	-1.23953	0.883272
13	No	Show	13	H	5	3	2	1.096241	112.2742	61.90317	-0.53112	1.378806	-0.89487
14	No	Show	14	H	5	3	2	1.096241	112.2741	-61.9042	-0.53113	1.37878	0.894917
15	No	Show	15	H	6	4	2	1.099639	111.5625	179.9981	5.268317	-0.62863	0.000026
16	No	Show	16	H	6	4	2	1.10118	110.893	59.7529	4.5633	0.741599	0.888684
17	No	Show	17	H	6	4	2	1.101179	110.8931	-59.7566	4.563307	0.741503	-0.88879

2-BROMO-2-METHYLPROPANE (no. 93)

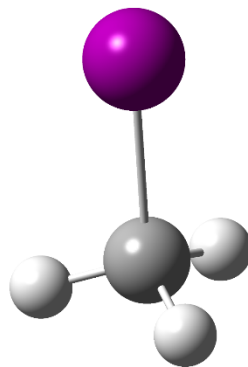
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.17164	-4.4E-05	0.000173
2	No	Show	2	C	1			2.017868			0.846224	0.000025	-0.00016
3	No	Show	3	C	2	1		1.518321	106.9073		1.287623	1.248839	-0.7424
4	No	Show	4	C	2	1	3	1.518334	106.9348	119.9928	1.288728	0.018561	1.452144
5	No	Show	5	C	2	1	3	1.518366	106.9152	-120.014	1.287928	-1.26726	-0.71032
6	No	Show	6	H	3	2	1	1.098405	111.3033	-60.9513	0.928093	1.244214	-1.78029
7	No	Show	7	H	3	2	1	1.098414	111.2909	60.96909	0.928474	2.158211	-0.24184
8	No	Show	8	H	3	2	1	1.102256	108.1651	-179.998	2.389611	1.269657	-0.75498
9	No	Show	9	H	4	2	1	1.098431	111.3075	-60.9649	0.929906	0.919924	1.967258
10	No	Show	10	H	4	2	1	1.09846	111.313	60.98583	0.930321	-0.86957	1.990085
11	No	Show	11	H	4	2	1	1.102257	108.1455	-179.984	2.390743	0.019193	1.475246
12	No	Show	12	H	5	2	1	1.098396	111.3099	60.91986	0.928061	-1.28953	-1.74786
13	No	Show	13	H	5	2	1	1.098391	111.2902	-61.0006	0.929389	-2.16362	-0.18646
14	No	Show	14	H	5	2	1	1.102265	108.1674	179.9707	2.389928	-1.28797	-0.72275

2-BROMOBUTANE (no. 94)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.38549	-0.19575	-0.00717
2	No	Show	2	C	1			1.991986			0.508481	0.296521	0.365079
3	No	Show	3	C	2	1		1.521524	108.3871		1.409865	-0.7621	-0.25288
4	No	Show	4	C	2	1	3	1.514062	108.6756	125.174	0.75138	1.703906	-0.13756
5	No	Show	5	C	3	2	1	1.527213	111.8297	-175.666	2.880967	-0.51822	0.076915
6	No	Show	6	H	2	1	4	1.097544	103.0622	117.7145	0.564408	0.256789	1.460477
7	No	Show	7	H	3	2	1	1.10174	108.9094	62.22518	1.259199	-0.76647	-1.34426
8	No	Show	8	H	3	2	1	1.099473	108.8201	-54.4138	1.106019	-1.74978	0.122608
9	No	Show	9	H	4	2	1	1.097494	111.3504	55.20654	0.035104	2.412679	0.297272
10	No	Show	10	H	4	2	1	1.100799	109.1033	174.3457	1.764262	2.02097	0.154494
11	No	Show	11	H	4	2	1	1.100125	110.7727	-66.2465	0.674767	1.7452	-1.23424
12	No	Show	12	H	5	3	2	1.09907	110.1055	173.6186	3.493153	-1.35642	-0.28448
13	No	Show	13	H	5	3	2	1.101049	110.9907	54.21673	3.032508	-0.43266	1.164124
14	No	Show	14	H	5	3	2	1.099192	111.8154	-66.6267	3.258453	0.400205	-0.39448

TRIFLUOROIODOMETHANE (no. 95)

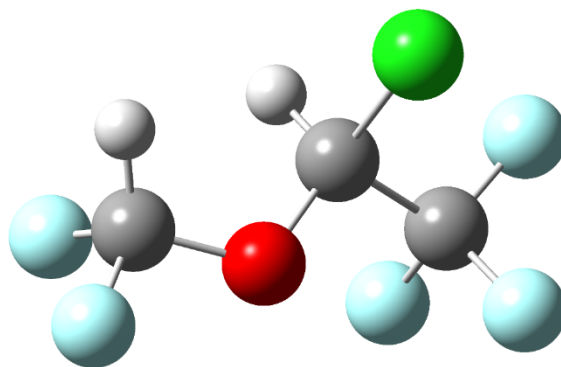
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							0.971744	0.000195	0.000185
2	No	Show	2	F	1			2.900241			-1.64929	0.164869	1.230816
3	No	Show	3	F	2	1		2.151685	68.19605		-1.64787	0.983265	-0.75915
4	No	Show	4	F	2	1	3	2.151712	68.14347	65.18282	-1.64541	-1.14938	-0.47288
5	No	Show	5	C	4	2	1	1.330917	36.06514	-39.1109	-1.16989	0.000149	0.000193

IODOMETHANE (no. 96)

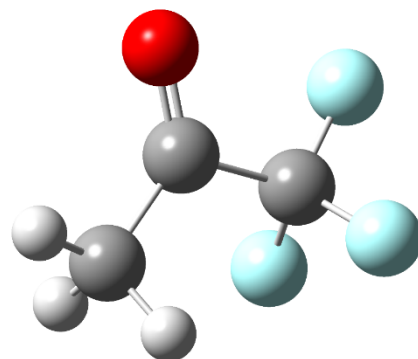
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							-1.3E-05	0.326637	0
2	No	Show	2	C	1			2.141952			-1.3E-05	-1.81532	0
3	No	Show	3	H	2	1		1.093804	107.3014		-1.04433	-2.14061	0
4	No	Show	4	H	2	1	3	1.093818	107.2471	-	0.522535	-2.13963	0.904547
5	No	Show	5	H	2	1	4	1.093818	107.2471	-	0.522535	-2.13963	-0.90455

HALOOXYGEN

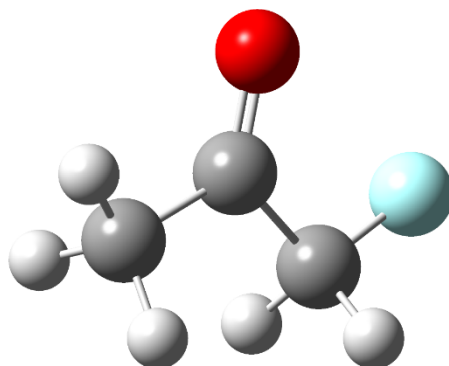
ISOFLURANE (no. 97)



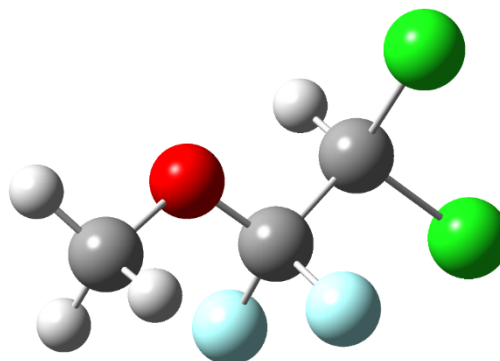
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0.633569	1.966919	-0.14733
2	No	Show	2	F	1			2.971524			2.518741	-0.27692	-0.63852
3	No	Show	3	F	2	1		2.155006	97.70118		1.171252	-1.89319	-0.17378
4	No	Show	4	F	3	2	1	2.154031	60.04679	-62.3565	1.694687	-0.45876	1.345512
5	No	Show	5	F	1	2	3	4.212097	103.1198	-1.40111	-2.94141	0.000518	0.898869
6	No	Show	6	F	5	1	2	2.161694	76.16696	-53.2771	-2.39076	-0.89774	-0.98868
7	No	Show	7	O	5	1	2	2.170847	31.91347	5.249254	-0.83052	-0.14775	0.414389
8	No	Show	8	C	7	5	1	1.389162	148.9515	-43.2213	0.237348	0.240942	-0.38457
9	No	Show	9	C	8	7	5	1.525401	106.3669	-174.994	1.429661	-0.60552	0.049865
10	No	Show	10	C	7	5	1	1.381516	36.28395	-72.9847	-2.082	0.088774	-0.12081
11	No	Show	11	H	8	7	5	1.088901	113.3851	-55.4062	0.062059	0.0823	-1.4475
12	No	Show	12	H	10	7	5	1.088586	113.7988	122.0896	-2.17119	1.051735	-0.62058

1,1,1-TRIFLUOROACETONE (no. 98)

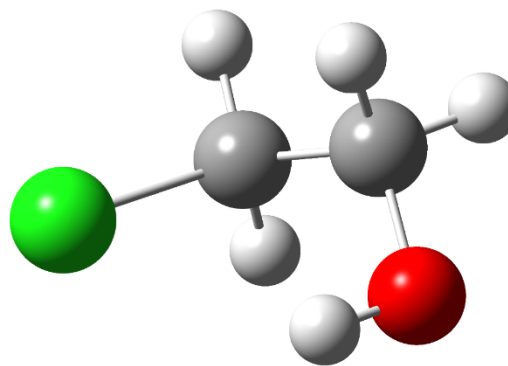
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							0.889523	-0.97264	-0.92139
2	No	Show	2	F	1			2.157005			0.954804	-0.53323	1.189379
3	No	Show	3	F	2	1		2.15512	59.99526		1.347794	1.023535	-0.24818
4	No	Show	4	O	3	2	1	2.61999	82.98205	92.14889	-1.22574	1.451934	-0.0079
5	No	Show	5	C	4	3	2	2.362016	30.31725	-32.3648	0.601104	-0.04531	-0.00489
6	No	Show	6	C	4	3	2	1.201131	65.43001	-39.1546	-0.9102	0.292991	-0.00779
7	No	Show	7	C	6	4	3	1.484271	126.669	-174.561	-1.82604	-0.87502	-0.0004
8	No	Show	8	H	7	6	4	1.085258	109.887	-10.185	-2.84319	-0.54543	0.185499
9	No	Show	9	H	7	6	4	1.092315	108.4032	110.0984	-1.76429	-1.36781	-0.97328
10	No	Show	10	H	7	6	4	1.090547	110.0458	-132.766	-1.50485	-1.59713	0.751059

FLUOROACETONE (no 99)

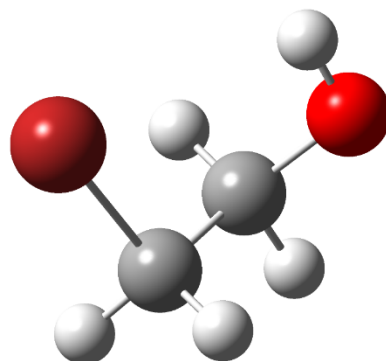
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							1.893387	0.009017	-0.03815
2	No	Show	2	O	1			2.637858			-0.35527	1.38715	0.012817
3	No	Show	3	C	2	1		1.212514	64.25603		-0.47674	0.180742	0.016827
4	No	Show	4	C	3	2	1	1.505396	121.1428	2.148211	0.727098	-0.72289	0.038016
5	No	Show	5	C	3	2	1	1.493107	123.6974	-176.958	-1.79516	-0.5192	-0.01776
6	No	Show	6	H	4	3	2	1.091353	109.6464	-124.52	0.682791	-1.413	-0.80628
7	No	Show	7	H	4	3	2	1.091392	109.1033	116.0898	0.72748	-1.29564	0.967044
8	No	Show	8	H	5	3	2	1.092425	107.8755	101.6677	-1.96266	-0.86853	-1.03919
9	No	Show	9	H	5	3	2	1.086241	110.3875	-17.8115	-2.5926	0.161621	0.265957
10	No	Show	10	H	5	3	2	1.089574	110.7491	-140.916	-1.78453	-1.3947	0.630747

METHOXYFLURANE (no. 100)

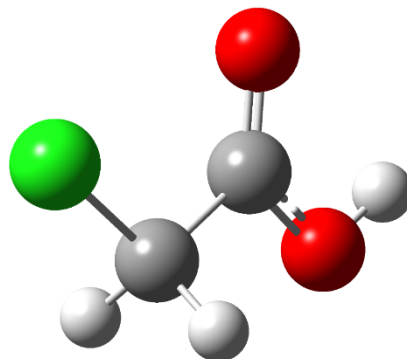
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.138091	1.741247	0.035472
2	No	Show	2	Cl	1			2.929057			1.950633	-1.07269	0.004914
3	No	Show	3	F	2	1		3.017806	61.49788		-0.65339	-0.34015	1.342688
4	No	Show	4	F	3	2	1	2.159474	66.3839	114.5436	-0.89958	-1.57372	-0.4126
5	No	Show	5	O	4	3	2	2.233659	61.22459	-110.476	-1.56808	0.556054	-0.49275
6	No	Show	6	C	5	4	3	1.34551	34.51605	36.08745	-0.64728	-0.2996	-0.01275
7	No	Show	7	C	6	5	4	1.531828	109.1142	119.6756	0.734845	0.107021	-0.53321
8	No	Show	8	C	5	4	3	1.440738	95.28353	-90.6474	-2.91453	0.289038	-0.05516
9	No	Show	9	H	7	6	5	1.094359	109.1886	-57.5739	0.719223	0.114607	-1.62743
10	No	Show	10	H	8	5	4	1.097475	110.2571	-27.6555	-3.21016	-0.73	-0.33555
11	No	Show	11	H	8	5	4	1.093465	105.4712	-146.501	-3.54059	1.018847	-0.57583
12	No	Show	12	H	8	5	4	1.09714	110.1379	94.64542	-2.99366	0.428648	1.030185

2-CHLOROETHANOL (no. 101)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.40283	-0.29169	0.06313
2	No	Show	2	O	1			3.130273			1.678722	-0.76627	-0.21511
3	No	Show	3	C	2	1		1.413949	60.62841		1.211299	0.446555	0.341494
4	No	Show	4	C	3	2	1	1.511001	112.4416	-34.1357	-0.08502	0.906449	-0.28394
5	No	Show	5	H	3	2	1	1.100102	107.0019	-151.956	1.971679	1.212454	0.128317
6	No	Show	6	H	3	2	1	1.103125	111.7013	89.90667	1.094359	0.374701	1.436047
7	No	Show	7	H	4	3	2	1.095623	111.7653	-177.642	-0.41544	1.867295	0.125926
8	No	Show	8	H	4	3	2	1.096036	111.4391	-53.4375	-0.0057	0.961509	-1.37572
9	No	Show	9	H	2	1	4	0.970287	54.18549	178.861	1.015754	-1.44506	-0.01218

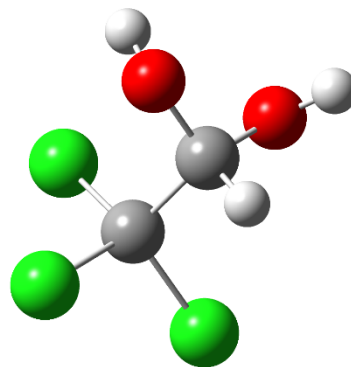
2-BROMOETHANOL (no. 102)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Br							-1.05937	-0.12881	0.027039
2	No	Show	2	O	1			3.268143			2.119957	-0.84201	-0.22594
3	No	Show	3	C	2	1		1.41708	61.2718		1.743341	0.393481	0.357007
4	No	Show	4	C	3	2	1	1.506752	112.9752	-35.5192	0.519405	0.996561	-0.28219
5	No	Show	5	H	3	2	1	1.090758	106.5617	-153.158	2.571706	1.08257	0.187533
6	No	Show	6	H	3	2	1	1.091682	110.945	89.23928	1.600674	0.289288	1.4343
7	No	Show	7	H	4	3	2	1.085051	111.2815	-176.851	0.287996	1.965841	0.147088
8	No	Show	8	H	4	3	2	1.085198	111.8643	-52.6459	0.621866	1.071949	-1.35991
9	No	Show	9	H	2	1	4	0.963858	57.66514	174.7201	1.459428	-1.50547	0.003281

CHLOROACETIC ACID (no. 103)

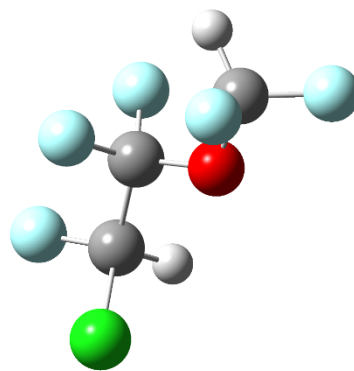
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.78782	0.072688	0.000041
2	No	Show	2	O	1			3.910827			2.064706	-0.60007	0.000072
3	No	Show	3	O	2	1		2.239203	49.1685		0.913911	1.320793	-0.00005
4	No	Show	4	C	2	1	3	2.322667	14.99618	-179.982	-0.2488	-0.80616	-9.9E-05
5	No	Show	5	C	3	2	1	1.203254	29.65833	-0.00113	0.940531	0.117834	0.000017
6	No	Show	6	H	4	2	1	1.086794	90.75053	125.5082	-0.20693	-1.43589	-0.88486
7	No	Show	7	H	4	2	1	1.086791	90.74446	-125.499	-0.20692	-1.43618	0.884453
8	No	Show	8	H	2	1	4	0.970857	131.8784	179.9819	2.827491	0.000535	0.000033

CHLORAL HYDRATE (no. 104)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.15614	1.457373	-0.46983
2	No	Show	2	Cl	1			2.90059			-0.0463	-0.0466	1.748212
3	No	Show	3	Cl	1	2		2.885945	60.05807		-1.15436	-1.42764	-0.54325
4	No	Show	4	O	3	1	2	3.008992	84.83826	-62.288	1.841195	-1.1572	-0.45626
5	No	Show	5	O	4	3	1	2.313762	94.34239	3.037878	1.803715	1.149242	-0.27618
6	No	Show	6	C	5	4	3	1.391869	33.89264	-25.7377	1.130908	0.013783	-0.71818
7	No	Show	7	C	6	5	4	1.54997	107.0075	122.388	-0.25057	0.003076	-0.01545
8	No	Show	8	H	6	5	4	1.09047	112.2945	-120.52	0.941796	0.036689	-1.79188
9	No	Show	9	H	4	3	1	0.967611	111.3725	88.75378	2.166399	-1.12892	0.454623
10	No	Show	10	H	5	4	3	0.965224	97.83827	-137.097	2.515996	1.341464	-0.89857

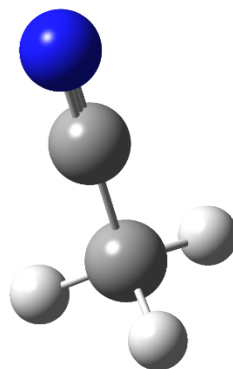
ENFLURANE (no. 105)



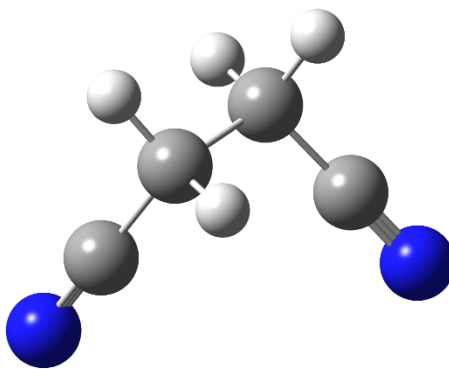
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.89063	-1.49805	-0.12883
2	No	Show	2	F	1			3.89571			-0.01106	1.913587	-0.196
3	No	Show	3	F	2	1		2.152238	50.25429		-0.20193	0.478747	1.396772
4	No	Show	4	F	1	3	2	2.555999	57.78638	-50.9167	-2.48181	0.9853	0.000021
5	No	Show	5	F	2	1	4	3.694995	83.70278	-172.618	2.924081	-0.18209	-0.99979
6	No	Show	6	F	5	2	1	2.157428	77.0008	-60.3071	2.309825	-0.92678	0.929624
7	No	Show	7	O	5	2	1	2.178875	33.58426	-2.55968	0.803038	-0.14303	-0.50265
8	No	Show	8	C	7	5	2	1.36348	144.5039	-20.4831	-0.19246	0.601987	0.056829
9	No	Show	9	C	8	7	5	1.528055	109.2743	153.8897	-1.53446	0.179836	-0.53965
10	No	Show	10	C	7	5	2	1.391886	36.13716	-73.0174	2.082612	0.032858	0.016105
11	No	Show	11	H	9	8	7	1.086297	110.3957	-57.3929	-1.52026	0.291045	-1.62014
12	No	Show	12	H	10	7	5	1.087438	113.9989	122.1323	2.250618	1.013024	0.45607

CYANIDE

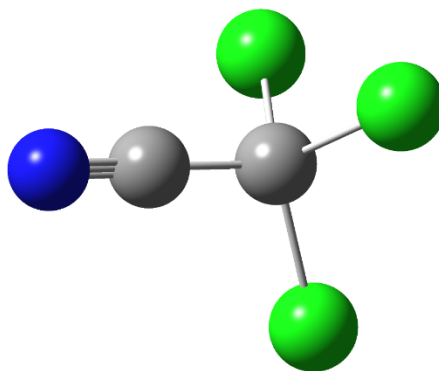
ACETONITRILE (no. 106)



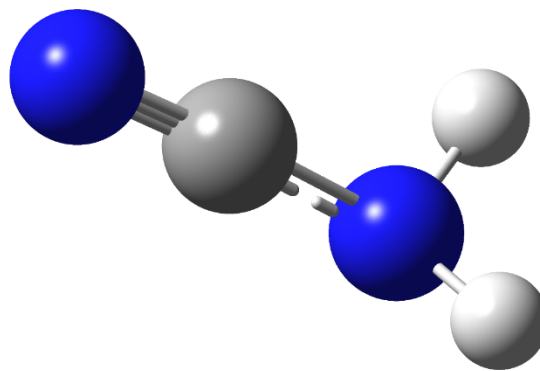
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-1.43591	0.000124	0.000054
2	No	Show	2	C	1			2.615708			1.179797	0.000057	0.000037
3	No	Show	3	C	1	2		1.158971	0.020509		-0.27694	-0.00028	-0.00013
4	No	Show	4	H	2	1	3	1.096944	109.4356	76.74333	1.5448	0.202886	-1.01432
5	No	Show	5	H	2	1	3	1.096952	109.4446	-43.2656	1.544944	-0.97973	0.331686
6	No	Show	6	H	2	1	3	1.096954	109.417	-163.269	1.544493	0.77733	0.68279

SUCCINONITRILE (no. 107)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							2.113753	-1.11185	0.199701
2	No	Show	2	C	1			1.158568			1.480571	-0.17773	-0.06254
3	No	Show	3	C	2	1		1.463248	179.1587		0.663726	0.992766	-0.38473
4	No	Show	4	C	3	2	1	1.534464	111.8765	14.5675	-0.66391	0.9928	0.384666
5	No	Show	5	C	4	3	2	1.463201	111.872	-60.902	-1.48052	-0.17786	0.062724
6	No	Show	6	N	5	4	3	1.15856	179.1544	13.02411	-2.11358	-1.11199	-0.19976
7	No	Show	7	H	3	2	1	1.097461	108.3288	134.9539	1.232693	1.893638	-0.12181
8	No	Show	8	H	3	2	1	1.098094	108.171	-107.839	0.487821	0.999747	-1.46862
9	No	Show	9	H	4	3	2	1.098093	110.8745	59.94581	-0.488	1.00006	1.468553
10	No	Show	10	H	4	3	2	1.097467	109.1724	179.2006	-1.23293	1.893588	0.12156

TRICHLOROACETONITRILE (no. 108)

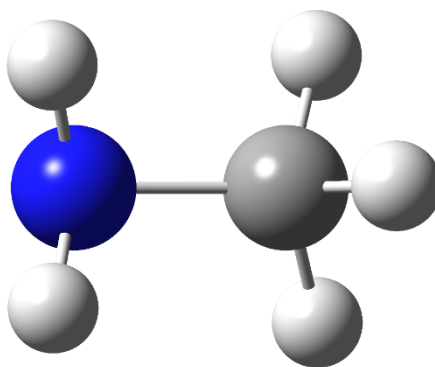
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0.529556	-1.64864	-0.36754
2	No	Show	2	Cl	1			2.918636			0.550446	0.501746	1.605739
3	No	Show	3	Cl	2	1		2.918099	60.01502		0.546749	1.136091	-1.24258
4	No	Show	4	N	1	2	3	3.607853	66.16419	-	-2.6486	0.017384	0.007036
5	No	Show	5	C	4	1	2	2.621829	27.84953	75.2193	-0.02683	0.000217	0.000027
6	No	Show	6	C	4	1	5	1.156356	27.86683	-	-1.49227	0.010123	0.004157

CYANAMIDE (no. 109)

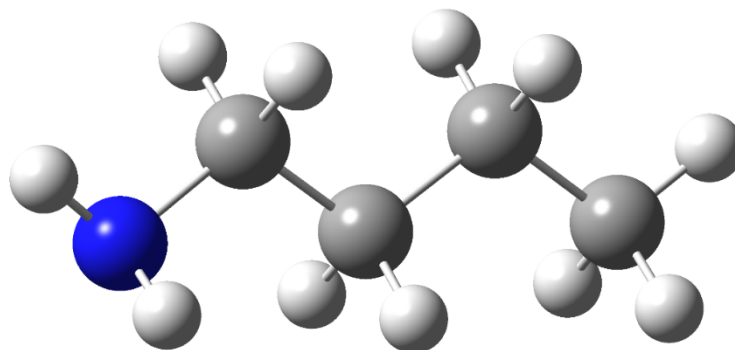
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.122306	-6.4E-05	-0.10108
2	No	Show	2	N	1			2.503548			-1.37858	-0.00012	0.014299
3	No	Show	3	C	2	1		1.164605	1.95153		-0.21406	0.000324	0.000274
4	No	Show	4	H	1	3	2	1.022573	112.1134	-116.674	1.538737	-0.84215	0.302809
5	No	Show	5	H	1	3	2	1.022571	112.1331	117.9088	1.539565	0.841524	0.302996

AMINE

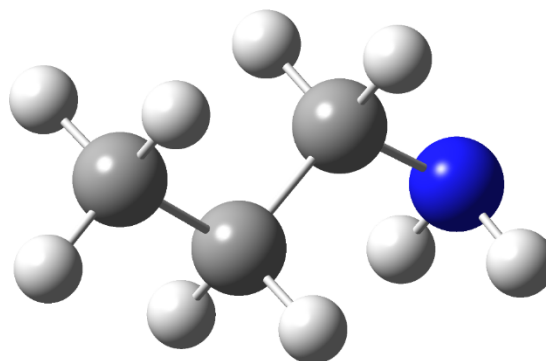
METHYLAMINE (no. 110)



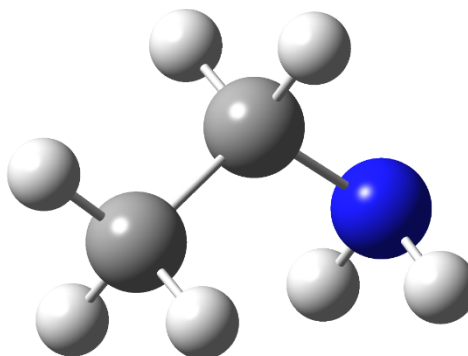
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.75445	0	-0.13787
2	No	Show	2	C	1			1.463356			0.700679	0	0.017045
3	No	Show	3	H	2	1		1.099179	109.7584		1.127064	0.883928	-0.47799
4	No	Show	4	H	2	1	3	1.099179	109.7583	-	1.127064	-0.88393	-0.47799
5	No	Show	5	H	2	1	4	1.10434	115.061	-	1.059925	-1E-06	1.061319
6	No	Show	6	H	1	2	3	1.022301	107.4924	-	-1.11848	-0.80354	0.378755
7	No	Show	7	H	1	2	3	1.022301	107.4924	-	-1.11848	0.803543	0.378755

BUTYLAMINE (no. 111)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-2.47225	-0.37788	-0.10284
2	No	Show	2	C	1			2.457424			-0.01607	-0.32897	-0.04192
3	No	Show	3	C	2	1		1.524611	146.9587		1.243579	0.526062	0.039643
4	No	Show	4	C	1	2	3	1.466335	35.30958	-2.08296	-1.29508	0.489327	0.008386
5	No	Show	5	C	3	2	1	1.523863	112.598	-178.798	2.519785	-0.30518	-0.01023
6	No	Show	6	H	2	1	4	1.103506	88.68902	-128.049	-0.00644	-0.92205	-0.97245
7	No	Show	7	H	2	1	4	1.105286	90.08311	125.42	-0.02074	-1.05352	0.792738
8	No	Show	8	H	3	2	1	1.103077	109.2347	59.10029	1.221727	1.117428	0.97055
9	No	Show	9	H	3	2	1	1.103201	109.1239	-56.7617	1.241137	1.253253	-0.78996
10	No	Show	10	H	4	1	2	1.106924	113.3588	-122.595	-1.28839	1.104301	0.928735
11	No	Show	11	H	4	1	2	1.101741	108.2246	119.5801	-1.30555	1.194692	-0.83789
12	No	Show	12	H	5	3	2	1.099623	111.6438	179.976	3.417867	0.326548	0.049219
13	No	Show	13	H	5	3	2	1.101241	110.8853	-59.7511	2.554974	-1.02103	0.825866
14	No	Show	14	H	5	3	2	1.10121	110.8865	59.69774	2.575384	-0.88342	-0.94576
15	No	Show	15	H	1	4	2	1.022157	107.943	176.8344	-3.30479	0.207994	-0.01095
16	No	Show	16	H	1	4	2	1.023728	107.1005	65.53468	-2.49274	-0.96647	0.734515

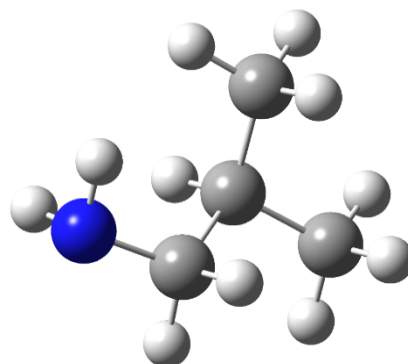
PROPYLAMINE (no. 112)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.95179	-0.02345	0.000004
2	No	Show	2	C	1			2.524899			-0.52342	-0.52189	0.000002
3	No	Show	3	C	1	2		1.464152	33.05617		0.591121	0.517219	0.000013
4	No	Show	4	C	2	1	3	1.523586	144.0956	0.00123	-1.90962	0.110387	-7E-06
5	No	Show	5	H	2	1	3	1.1037	90.52676	126.6864	-0.40321	-1.17027	-0.88505
6	No	Show	6	H	2	1	3	1.103699	90.52729	-126.685	-0.40322	-1.17028	0.885043
7	No	Show	7	H	3	1	2	1.102237	108.3283	122.6327	0.477363	1.169552	0.881175
8	No	Show	8	H	3	1	2	1.102236	108.3276	-122.632	0.47737	1.169564	-0.88114
9	No	Show	9	H	4	2	1	1.101343	110.9191	-59.7369	-2.05224	0.745291	0.888539
10	No	Show	10	H	4	2	1	1.101342	110.9195	59.74634	-2.0523	0.745144	-0.88865
11	No	Show	11	H	4	2	1	1.099355	111.6723	-179.995	-2.70297	-0.65065	0.000086
12	No	Show	12	H	1	3	2	1.023976	107.0435	55.14745	2.024106	-0.65419	-0.8034
13	No	Show	13	H	1	3	2	1.023977	107.0434	-55.1386	2.024062	-0.65433	0.803308

ETHYLAMINE (no. 113)

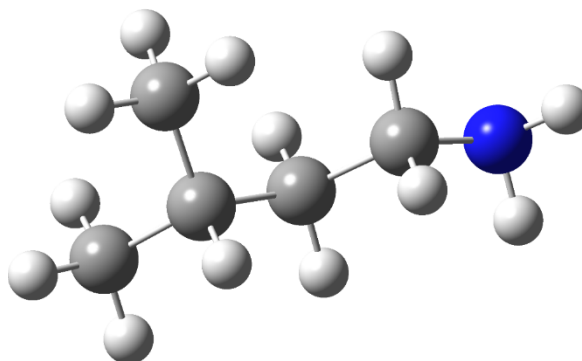
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.3057	-0.08271	0
2	No	Show	2	C	1			1.465429			0	0.582596	0
3	No	Show	3	C	2	1		1.521456	114.8103		-1.19583	-0.35806	0
4	No	Show	4	H	2	1	3	1.100794	108.1149	122.7097	-0.04828	1.241725	0.880321
5	No	Show	5	H	2	1	3	1.100794	108.1149	-122.71	-0.04828	1.241725	-0.88032
6	No	Show	6	H	3	2	1	1.101757	110.5655	-59.7233	-1.17847	-1.00611	-0.89084
7	No	Show	7	H	3	2	1	1.101757	110.5655	59.72334	-1.17847	-1.00611	0.890842
8	No	Show	8	H	3	2	1	1.100861	111.5467	180	-2.14665	0.196763	0
9	No	Show	9	H	1	2	3	1.024248	106.9783	55.07939	1.317603	-0.71814	-0.80322
10	No	Show	10	H	1	2	3	1.024248	106.9783	-55.0794	1.317603	-0.71814	0.803224

ISOBUTYLAMINE (no. 114)

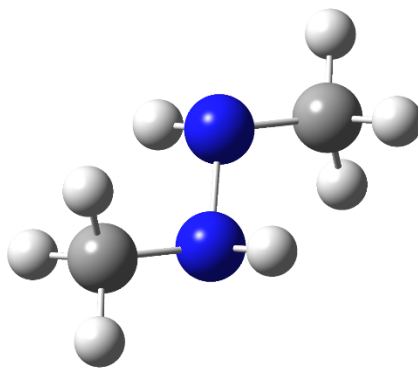


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-2.07018	-0.13307	-0.04796
2	No	Show	2	C	1			2.546179			0.455053	0.0023	-0.3444
3	No	Show	3	C	1	2		1.463331	32.55642		-0.75909	-0.70131	0.26742
4	No	Show	4	C	2	1	3	1.526203	94.45053	-125.966	0.550051	1.455772	0.111328
5	No	Show	5	C	2	1	3	1.525742	140.8642	5.301148	1.730164	-0.75915	0.005146
6	No	Show	6	H	2	1	3	1.105594	89.91879	125.5262	0.325386	-0.01252	-1.44227
7	No	Show	7	H	3	1	2	1.101859	108.1673	-122.587	-0.75451	-1.75475	-0.05559
8	No	Show	8	H	3	1	2	1.103632	108.1992	122.6154	-0.64332	-0.71273	1.364904
9	No	Show	9	H	4	2	1	1.103263	110.3069	87.56562	0.661807	1.50674	1.207732
10	No	Show	10	H	4	2	1	1.100468	111.1008	-152.885	1.419856	1.956465	-0.34009
11	No	Show	11	H	4	2	1	1.100374	111.8045	-32.6115	-0.34643	2.030473	-0.16593
12	No	Show	12	H	5	2	1	1.102808	110.384	-65.4423	1.88575	-0.76711	1.096895
13	No	Show	13	H	5	2	1	1.100295	111.3349	174.9691	2.61387	-0.29298	-0.45572
14	No	Show	14	H	5	2	1	1.100913	111.3926	54.29525	1.67958	-1.80483	-0.33543
15	No	Show	15	H	1	3	2	1.024155	107.3966	51.42658	-2.12454	-0.03493	-1.06595
16	No	Show	16	H	1	3	2	1.022597	107.8564	-59.8265	-2.08325	0.831922	0.290171

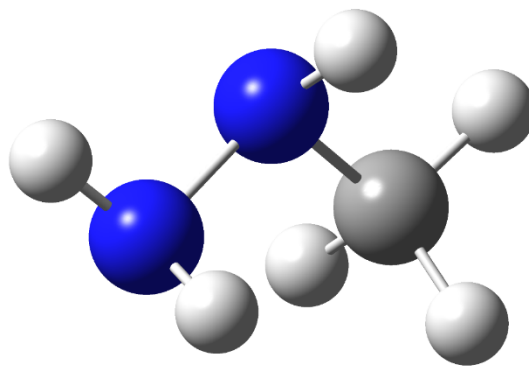
ISOAMYLAMINE (no. 115)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							2.746194	-0.2518	-0.22589
2	No	Show	2	C	1			3.839664			-1.04339	-0.02117	0.347593
3	No	Show	3	C	2	1		1.530228	19.48358		0.310349	-0.51555	-0.16678
4	No	Show	4	C	1	3	2	1.466262	35.59498	-8.55621	1.490316	0.365847	0.211382
5	No	Show	5	C	2	1	4	1.5279	102.5015	46.12651	-1.37	1.38222	-0.16063
6	No	Show	6	C	2	1	4	1.526583	129.5248	176.3165	-2.14697	-0.99951	-0.04666
7	No	Show	7	H	2	1	4	1.1048	96.0784	-64.0209	-0.99277	0.01543	1.450626
8	No	Show	8	H	3	2	1	1.104837	108.7158	116.0681	0.492194	-1.52976	0.23192
9	No	Show	9	H	3	2	1	1.10498	109.3385	-127.992	0.270615	-0.61244	-1.26679
10	No	Show	10	H	4	1	3	1.100297	107.8415	-119.977	1.403127	1.342405	-0.288
11	No	Show	11	H	4	1	3	1.107773	113.4288	122.2796	1.452818	0.564085	1.300628
12	No	Show	12	H	5	2	1	1.09987	112.1026	-45.6314	-0.6546	2.132401	0.206982
13	No	Show	13	H	5	2	1	1.103314	110.3618	74.73344	-1.35028	1.405363	-1.26352
14	No	Show	14	H	5	2	1	1.10074	110.8244	-165.937	-2.375	1.692047	0.16434
15	No	Show	15	H	6	2	1	1.100507	111.283	173.8918	-3.12088	-0.68831	0.36049
16	No	Show	16	H	6	2	1	1.102681	110.3671	-66.4825	-2.24119	-1.04978	-1.14416
17	No	Show	17	H	6	2	1	1.100728	111.3563	53.21771	-1.93207	-2.01501	0.319653
18	No	Show	18	H	1	4	3	1.023563	107.2102	-65.9405	2.866718	-1.11061	0.317806
19	No	Show	19	H	1	4	3	1.022021	108.0087	-177.471	3.516113	0.345739	0.081841

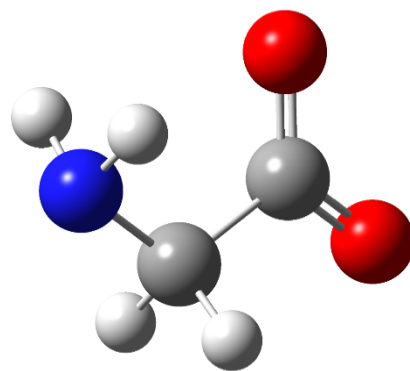
1,2-DIMETHYLHYDRAZINE (no. 116)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.00482	0.080242	-0.7255
2	No	Show	2	N	1			1.459888			0.004823	-0.08024	0.725504
3	No	Show	3	C	1	2		1.458115	107.6694		1.375562	0.00184	-1.18863
4	No	Show	4	C	2	1	3	1.458115	107.6694	-180	-1.37556	-0.00184	1.188633
5	No	Show	5	H	1	3	2	1.025218	105.9347	-109.836	-0.46048	-0.77811	-1.05214
6	No	Show	6	H	2	1	3	1.025218	103.1537	68.26326	0.460478	0.778105	1.052141
7	No	Show	7	H	3	1	2	1.10456	113.2574	50.0792	1.917195	-0.87819	-0.79846
8	No	Show	8	H	3	1	2	1.100719	109.4824	-70.5706	1.92034	0.904909	-0.87357
9	No	Show	9	H	3	1	2	1.09788	108.9366	171.6933	1.381933	-0.02965	-2.28604
10	No	Show	10	H	4	2	1	1.100719	109.4824	70.57062	-1.92034	-0.90491	0.873569
11	No	Show	11	H	4	2	1	1.10456	113.2574	-50.0792	-1.9172	0.878187	0.798455
12	No	Show	12	H	4	2	1	1.09788	108.9366	-171.693	-1.38193	0.029651	2.286043

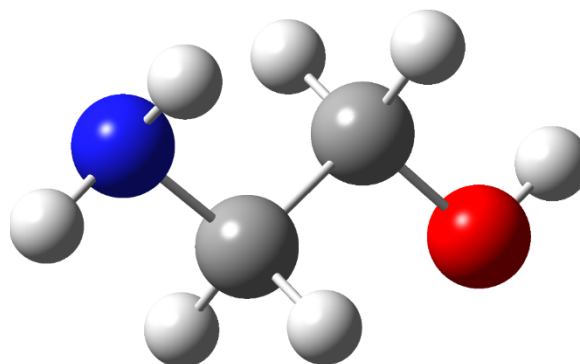
METHYLHYDRAZINE (no. 117)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.0324	0.576945	-0.10254
2	No	Show	2	N	1			1.434189			-1.15197	-0.31915	-0.08036
3	No	Show	3	C	1	2		1.454301	108.1034		1.183043	-0.21602	-0.00827
4	No	Show	4	H	3	1	2	1.098561	109.2067	-176.425	2.05036	0.456424	0.040887
5	No	Show	5	H	3	1	2	1.099048	109.3901	64.81183	1.277837	-0.84635	-0.9036
6	No	Show	6	H	3	1	2	1.107273	113.3937	-55.6517	1.207916	-0.87879	0.87839
7	No	Show	7	H	1	2	3	1.024433	109.0167	-115.724	-0.06362	1.170833	0.731601
8	No	Show	8	H	2	1	3	1.027835	109.22	76.02389	-1.30159	-0.64996	0.881209
9	No	Show	9	H	2	1	3	1.021189	106.6684	-171.039	-1.97856	0.239384	-0.29857

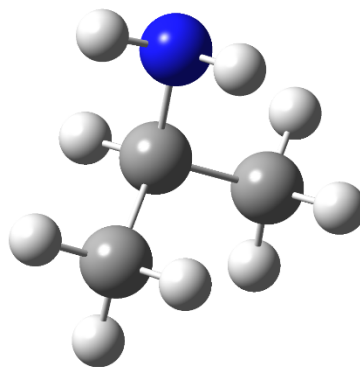
GLYCINATE (no. 118)



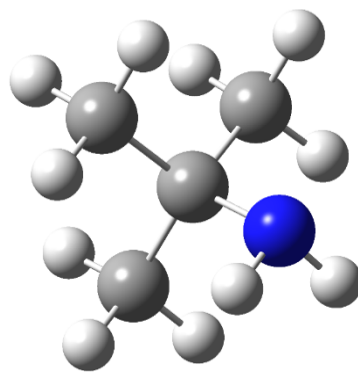
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.54974	1.313404	0.000212
2	No	Show	2	O	1			2.245493			1.722542	-0.60148	-0.00031
3	No	Show	3	N	1	2		2.772094	93.35483		-1.89489	0.006381	-0.00049
4	No	Show	4	C	3	1	2	1.459284	59.71678	0.043414	-0.65178	-0.75795	0.00034
5	No	Show	5	C	1	2	4	1.258446	27.01443	-0.00246	0.647856	0.058789	0.000033
6	No	Show	6	H	4	3	1	1.101269	109.7598	122.0979	-0.62348	-1.4218	0.878571
7	No	Show	7	H	4	3	1	1.101209	109.7792	-122.21	-0.62323	-1.42393	-0.8762
8	No	Show	8	H	3	1	5	1.024258	68.91878	-123.922	-1.8213	0.650549	-0.79342
9	No	Show	9	H	3	1	5	1.024309	68.97279	123.9202	-1.82249	0.650058	0.793015

ETHANOLAMINE (no. 119)

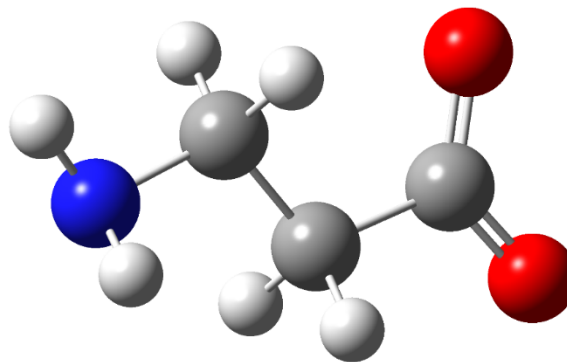
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.803236	-0.25124	0.040005
2	No	Show	2	N	1			3.662462			-1.82738	0.2109	-0.09666
3	No	Show	3	C	2	1		1.462425	22.01848		-0.55455	-0.49998	0.018376
4	No	Show	4	C	1	3	2	1.419682	37.41219	1.35119	0.592612	0.484039	-0.05614
5	No	Show	5	H	3	2	1	1.10051	108.9134	-117.791	-0.46269	-1.20524	-0.82144
6	No	Show	6	H	3	2	1	1.105814	114.2793	122.665	-0.44502	-1.08886	0.947917
7	No	Show	7	H	4	1	3	1.10597	111.0019	119.9292	0.506069	1.214831	0.769463
8	No	Show	8	H	4	1	3	1.104061	111.4839	-120.078	0.533866	1.043835	-1.00595
9	No	Show	9	H	2	1	4	1.023354	98.91981	-63.0122	-1.94937	0.762375	0.756719
10	No	Show	10	H	2	1	4	1.021398	129.8803	-179.781	-2.5777	-0.48076	-0.05338
11	No	Show	11	H	1	4	3	0.967655	107.4199	179.8799	2.532222	0.383119	-0.01019

ISOPROPYLAMINE (no. 120)

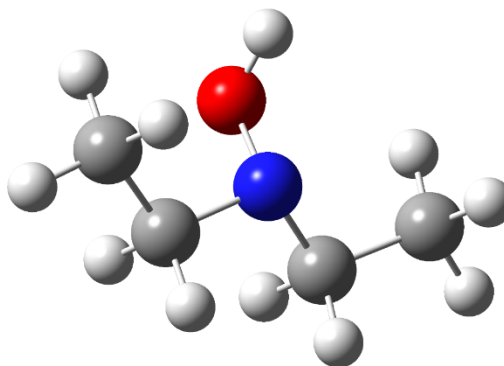
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.29702	1.403059	0.04862
2	No	Show	2	C	1			1.470197			0.001605	0.028808	-0.38002
3	No	Show	3	C	2	1		1.525157	113.1433		-1.0245	-0.98802	0.109126
4	No	Show	4	C	2	1	3	1.520914	108.9179	-123.939	1.400721	-0.3407	0.08808
5	No	Show	5	H	2	1	4	1.102423	106.9211	-116.877	-0.00714	0.027487	-1.48241
6	No	Show	6	H	3	2	1	1.101126	111.6177	177.8026	-0.7984	-2.00124	-0.25796
7	No	Show	7	H	3	2	1	1.102996	110.0045	-62.1845	-1.03162	-1.01638	1.211734
8	No	Show	8	H	3	2	1	1.100996	110.7922	57.23824	-2.03583	-0.71779	-0.23201
9	No	Show	9	H	4	2	1	1.099521	110.8786	-55.5444	2.140692	0.386177	-0.27668
10	No	Show	10	H	4	2	1	1.099658	111.1942	-176.518	1.687129	-1.34152	-0.26627
11	No	Show	11	H	4	2	1	1.103151	110.0273	63.9587	1.441088	-0.34632	1.190478
12	No	Show	12	H	1	2	4	1.025772	106.4453	-64.7262	-0.31396	1.390168	1.074171
13	No	Show	13	H	1	2	4	1.023756	107.3629	-175.078	-1.26976	1.59747	-0.20449

TERT-BUTYLAMINE (no. 121)

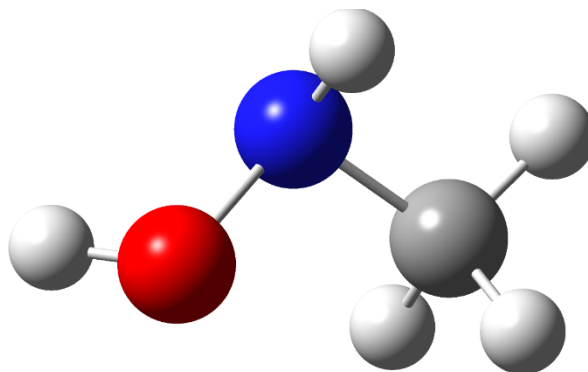
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.00013	-0.3609	1.448239
2	No	Show	2	C	1			1.47418			-1E-06	0.008319	0.021044
3	No	Show	3	C	2	1		1.526216	107.8041		1.250412	0.841932	-0.24521
4	No	Show	4	C	2	1	3	1.531005	111.8152	120.6235	0.000213	-1.22525	-0.88575
5	No	Show	5	C	2	1	3	1.526213	107.8042	-118.752	-1.2505	0.841713	-0.24549
6	No	Show	6	H	3	2	1	1.101988	110.4485	61.54611	2.157758	0.252831	-0.03531
7	No	Show	7	H	3	2	1	1.100147	110.9107	-178.672	1.28975	1.166284	-1.29572
8	No	Show	8	H	3	2	1	1.10041	110.5219	-58.1259	1.263704	1.734012	0.398929
9	No	Show	9	H	4	2	1	1.101811	110.3358	59.70487	-0.8918	-1.84253	-0.69272
10	No	Show	10	H	4	2	1	1.101812	110.3357	-59.7083	0.892331	-1.84234	-0.69257
11	No	Show	11	H	4	2	1	1.101464	111.6057	179.9985	0.000279	-0.94549	-1.9511
12	No	Show	12	H	5	2	1	1.10041	110.5215	58.11793	-1.26415	1.733715	0.398751
13	No	Show	13	H	5	2	1	1.100146	110.9104	178.6638	-1.28958	1.166184	-1.29597
14	No	Show	14	H	5	2	1	1.101987	110.4488	-61.5544	-2.15779	0.252411	-0.03593
15	No	Show	15	H	1	2	5	1.02452	106.9627	176.0095	0.806402	-0.97461	1.598287
16	No	Show	16	H	1	2	5	1.024521	106.9624	65.21805	-0.80678	-0.97447	1.598173

BETA-ALANINATE (no. 122)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.194765	-0.82244	0.016983
2	No	Show	2	O	1			2.242354			1.358491	1.258129	0.012326
3	No	Show	3	N	2	1		4.232918	91.04312		-2.59565	-0.24842	-0.10017
4	No	Show	4	C	1	2	3	2.377832	62.48292	0.311522	-0.17059	-0.58932	-0.05273
5	No	Show	5	C	3	2	1	1.467073	7.162735	153.7194	-1.29634	0.422284	0.019221
6	No	Show	6	C	2	1	4	1.260358	27.18915	0.211722	1.242477	0.0032	-0.00163
7	No	Show	7	H	4	1	6	1.103729	89.505	-130.618	-0.25698	-1.31606	0.773465
8	No	Show	8	H	4	1	6	1.103021	92.76882	123.7122	-0.25511	-1.18076	-0.97994
9	No	Show	9	H	5	3	2	1.105436	113.567	-143.749	-1.18719	1.012341	0.94761
10	No	Show	10	H	5	3	2	1.100191	108.5506	98.34673	-1.19279	1.135295	-0.81223
11	No	Show	11	H	3	2	1	1.022092	114.8443	170.5797	-3.3264	0.452579	0.038718
12	No	Show	12	H	3	2	1	1.023723	106.3376	56.28871	-2.69131	-0.86694	0.709952

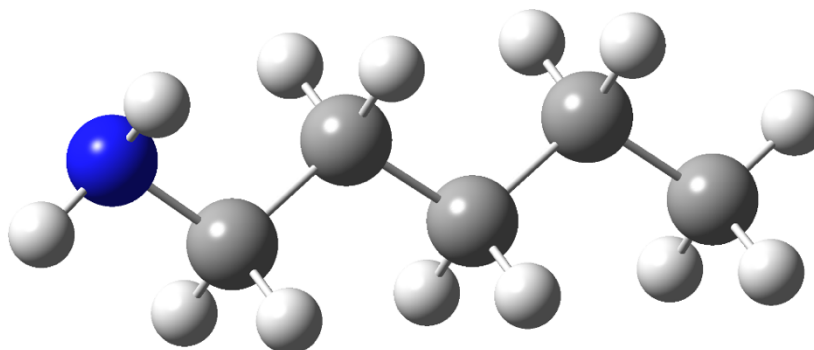
N,N-DIETHYLHYDROXYLAMINE (no. 123)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0	1.292149	-0.3686
2	No	Show	2	N	1			1.436569			0	0.004475	0.268285
3	No	Show	3	C	2	1		1.464763	105.3098		1.200126	-0.67267	-0.22841
4	No	Show	4	C	2	1	3	1.464763	105.3098	-116.31	-1.20013	-0.67267	-0.22841
5	No	Show	5	C	3	2	1	1.516034	111.9383	68.11996	2.470268	-0.02235	0.283625
6	No	Show	6	C	4	2	1	1.516034	111.9383	-68.1199	-2.47027	-0.02235	0.283625
7	No	Show	7	H	3	2	1	1.099265	106.4838	-171.177	1.136749	-1.71393	0.118183
8	No	Show	8	H	3	2	1	1.107661	109.8251	-54.9755	1.191827	-0.6876	-1.33594
9	No	Show	9	H	4	2	1	1.107661	109.8251	54.97567	-1.19183	-0.6876	-1.33594
10	No	Show	10	H	4	2	1	1.099265	106.4837	171.177	-1.13675	-1.71393	0.118187
11	No	Show	11	H	5	3	2	1.09874	110.6982	-61.265	2.536277	1.020778	-0.05514
12	No	Show	12	H	5	3	2	1.100029	110.7246	59.02778	2.497242	-0.03336	1.383268
13	No	Show	13	H	5	3	2	1.098995	110.309	178.9823	3.352134	-0.56142	-0.08988
14	No	Show	14	H	6	4	2	1.100028	110.7246	-59.0277	-2.49724	-0.03336	1.383267
15	No	Show	15	H	6	4	2	1.098739	110.6982	61.26514	-2.53628	1.020776	-0.05515
16	No	Show	16	H	6	4	2	1.098995	110.3089	-178.982	-3.35213	-0.56142	-0.08987
17	No	Show	17	H	1	2	3	0.969076	104.2759	-121.846	-8E-06	1.922709	0.367265

N-METHYL-N-TRITIOHYDROXYLAMINE (no. 124)

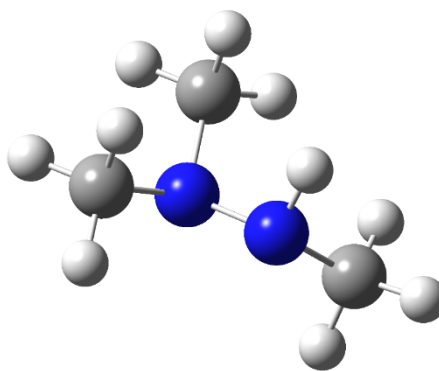
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.1563	-0.28794	0.131695
2	No	Show	2	N	1			1.433382			-0.04807	0.573205	-0.1596
3	No	Show	3	C	2	1		1.45624	106.4348		1.153885	-0.23254	0.00389
4	No	Show	4	H	3	2	1	1.098309	109.3488	70.1944	1.210945	-0.96985	-0.80814
5	No	Show	5	H	3	2	1	1.102949	112.969	51.1062	1.187477	-0.76438	0.969557
6	No	Show	6	H	3	2	1	1.098405	108.0913	171.764	2.02381	0.434329	-0.06694
7	No	Show	7	H	2	1	3	1.023823	102.7689	111.971	-0.06596	1.2366	0.620017
8	No	Show	8	H	1	2	3	0.968845	103.6394	122.812	-1.69275	-0.25045	-0.67421

AMYLAMINE (no. 125)

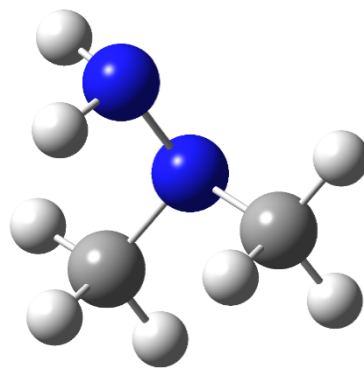


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-3.13241	0.256849	-0.08335
2	No	Show	2	C	1			3.826038			0.641199	-0.36685	0.013715
3	No	Show	3	C	2	1		1.524126	20.48871		-0.67949	0.391717	-0.04386
4	No	Show	4	C	2	1	3	1.525428	133.6959	-1.33652	1.861806	0.547041	-0.02937
5	No	Show	5	C	1	3	2	1.466253	35.33007	1.955406	-1.89282	-0.52156	0.002549
6	No	Show	6	C	4	2	1	1.523752	112.6664	-179.439	3.174891	-0.22392	0.027577
7	No	Show	7	H	2	1	5	1.104483	98.15567	-51.8506	0.675836	-0.97508	0.934985
8	No	Show	8	H	2	1	5	1.104617	97.47029	55.85788	0.69079	-1.07899	-0.82924
9	No	Show	9	H	3	2	1	1.103293	109.8806	-120.706	-0.72385	0.998466	-0.96426
10	No	Show	10	H	3	2	1	1.105089	109.3485	122.6844	-0.73212	1.099978	0.802794
11	No	Show	11	H	4	2	1	1.103146	109.098	-57.3061	1.82586	1.154112	-0.94975
12	No	Show	12	H	4	2	1	1.10319	109.0994	58.44453	1.810527	1.25776	0.812814
13	No	Show	13	H	5	1	3	1.106892	113.3583	122.5847	-1.83127	-1.14988	0.911742
14	No	Show	14	H	5	1	3	1.101728	108.2271	-119.583	-1.85872	-1.21112	-0.85603
15	No	Show	15	H	6	4	2	1.099695	111.6744	-179.989	4.043287	0.450022	-0.00429
16	No	Show	16	H	6	4	2	1.101298	110.8936	-59.7126	3.242329	-0.81696	0.953113
17	No	Show	17	H	6	4	2	1.101282	110.8949	59.7299	3.258084	-0.92119	-0.82078
18	No	Show	18	H	1	5	3	1.023713	107.1166	-65.5704	-3.18928	0.827424	0.764702
19	No	Show	19	H	1	5	3	1.022125	107.9594	-176.89	-3.91811	-0.39106	0.004014

TRIMETHYLHYDRAZINE (no. 126)



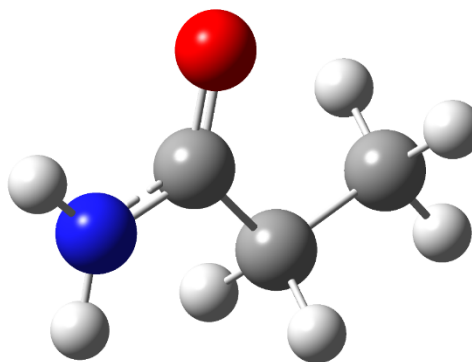
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.40861	-0.02262	-0.35461
2	No	Show	2	N	1			1.43164			0.7024	-0.5613	0.37001
3	No	Show	3	C	1	2		1.455701	107.2896		-1.56291	-0.85989	-0.06199
4	No	Show	4	C	1	2	3	1.459609	110.8745	119.118	-0.69027	1.346044	0.06717
5	No	Show	5	C	2	1	3	1.456254	111.1798	161.2112	1.966482	-0.08961	-0.17797
6	No	Show	6	H	2	1	3	1.030328	107.558	-80.6089	0.630491	-0.22787	1.342237
7	No	Show	7	H	3	1	2	1.097048	109.6661	-59.729	-1.3596	-1.89148	-0.37503
8	No	Show	8	H	3	1	2	1.09852	109.4993	-179.357	-2.43706	-0.48415	-0.61102
9	No	Show	9	H	3	1	2	1.109635	111.9168	60.71478	-1.80899	-0.8626	1.020011
10	No	Show	10	H	4	1	2	1.110169	111.4696	-59.8522	-0.93366	1.395845	1.149184
11	No	Show	11	H	4	1	2	1.098585	109.6735	-179.976	-1.54496	1.739365	-0.50001
12	No	Show	12	H	4	1	2	1.09782	110.4638	61.07622	0.174249	1.993665	-0.12879
13	No	Show	13	H	5	2	1	1.098515	108.338	176.1101	2.780714	-0.47255	0.452206
14	No	Show	14	H	5	2	1	1.104864	114.5888	55.6108	2.064264	1.009786	-0.22781
15	No	Show	15	H	5	2	1	1.098867	109.4364	-66.0777	2.098213	-0.49184	-1.19206

1,1-DIMETHYLHYDRAZINE (no. 127)

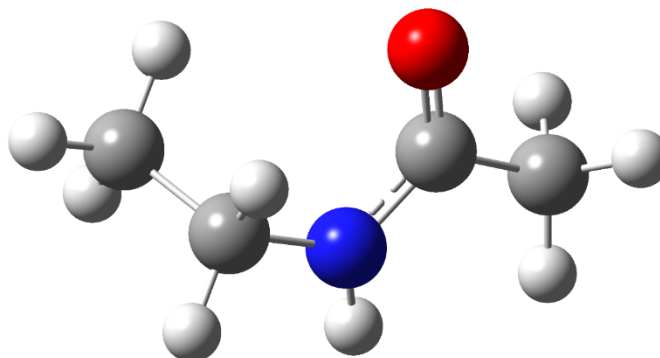
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							0.007313	0.020305	-0.43436
2	No	Show	2	N	1			1.432493			-0.47292	1.282771	0.042707
3	No	Show	3	C	1	2		1.45736	110.4487		-0.81949	-1.06528	0.077304
4	No	Show	4	C	1	2	3	1.453897	106.7653	-118.908	1.364557	-0.1281	0.065319
5	No	Show	5	H	3	1	2	1.110417	111.5437	-58.5809	-0.83293	-1.07915	1.187553
6	No	Show	6	H	3	1	2	1.098985	109.9773	-179.148	-0.4354	-2.03067	-0.28085
7	No	Show	7	H	3	1	2	1.098788	109.6184	61.60577	-1.85073	-0.94463	-0.28231
8	No	Show	8	H	4	1	2	1.098041	109.6716	-179.457	1.78429	-1.08132	-0.28237
9	No	Show	9	H	4	1	2	1.1106	111.7897	60.497	1.398633	-0.11777	1.175348
10	No	Show	10	H	4	1	2	1.097231	109.6118	-59.742	1.986586	0.694978	-0.30824
11	No	Show	11	H	2	1	4	1.022882	106.1953	175.4096	-1.39664	1.413606	-0.37671
12	No	Show	12	H	2	1	4	1.033573	107.6674	-73.4479	-0.66501	1.183688	1.053427

AMIDE

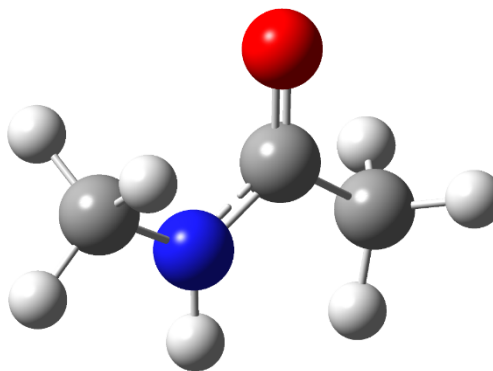
PROPIONAMIDE (no. 128)



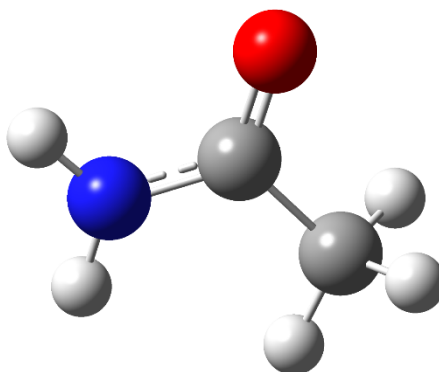
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.49334	1.358053	0.000081
2	No	Show	2	N	1			2.258208			-1.73944	-0.52522	-0.00015
3	No	Show	3	C	1	2		2.414096	62.27222		0.668953	-0.75783	0.000185
4	No	Show	4	C	3	1	2	1.518601	87.12568	179.9794	1.96162	0.039144	-0.00015
5	No	Show	5	C	1	2	3	1.234153	30.31028	-0.00072	-0.56182	0.125802	0.000043
6	No	Show	6	H	3	1	5	1.10136	119.8208	-67.1064	0.60673	-1.41685	0.880417
7	No	Show	7	H	3	1	5	1.101355	119.8429	67.05959	0.606582	-1.41744	-0.87959
8	No	Show	8	H	4	3	1	1.09821	110.501	179.9864	2.82886	-0.63462	0.000039
9	No	Show	9	H	4	3	1	1.09903	110.9054	-59.8576	2.024722	0.683672	-0.88811
10	No	Show	10	H	4	3	1	1.099029	110.9044	59.83043	2.02479	0.684279	0.887359
11	No	Show	11	H	2	1	5	1.012857	148.7359	0.015328	-1.77881	-1.53731	-0.00004
12	No	Show	12	H	2	1	5	1.014364	91.80056	179.9912	-2.60256	0.007661	-0.00012

N-ETHYLACETAMIDE (no. 129)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.744471	1.354503	0.257411
2	No	Show	2	N	1			2.260417			-0.07815	-0.75091	0.250778
3	No	Show	3	C	2	1		1.455385	93.98963		-1.4343	-0.33076	0.570889
4	No	Show	4	C	3	2	1	1.521964	112.9348	80.07401	-2.19687	0.185478	-0.64087
5	No	Show	5	C	1	2	3	1.238455	30.33466	-176.305	0.914425	0.141072	0.077212
6	No	Show	6	C	5	1	2	1.506253	121.5071	-179.594	2.251322	-0.41307	-0.34044
7	No	Show	7	H	3	2	1	1.096947	107.4725	-157.512	-1.9492	-1.19102	1.015999
8	No	Show	8	H	3	2	1	1.098642	107.6762	-41.697	-1.3684	0.453269	1.337683
9	No	Show	9	H	2	1	5	1.013936	146.0735	-7.90454	0.096147	-1.72152	0.014992
10	No	Show	10	H	4	3	2	1.099572	110.3667	-60.2603	-1.68375	1.056524	-1.07335
11	No	Show	11	H	4	3	2	1.099771	110.8245	60.0903	-2.27738	-0.59342	-1.41309
12	No	Show	12	H	4	3	2	1.099532	110.2276	-179.913	-3.212	0.491209	-0.34928
13	No	Show	13	H	6	5	1	1.099181	108.3291	-64.6333	2.488131	-0.02659	-1.34182
14	No	Show	14	H	6	5	1	1.09807	108.5071	51.90644	3.016473	-0.03545	0.350722
15	No	Show	15	H	6	5	1	1.096343	112.9676	173.938	2.273759	-1.50905	-0.35734

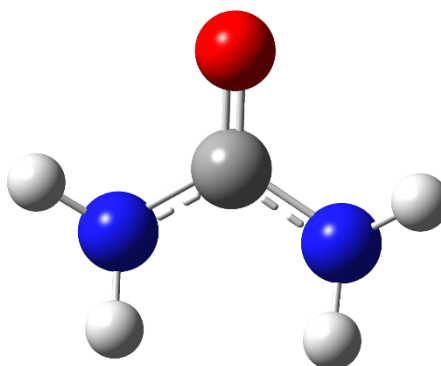
N-METHYLACETAMIDE (no. 130)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.360618	1.381427	-0.00023
2	No	Show	2	N	1			2.252508			-0.59967	-0.65613	-0.0034
3	No	Show	3	C	1	2		1.238302	30.57947		0.475975	0.148511	-0.00176
4	No	Show	4	C	2	1	3	1.44897	92.95819	179.7957	-1.9405	-0.10688	0.001721
5	No	Show	5	C	3	1	2	1.505417	121.9041	-179.876	1.822529	-0.52459	0.000886
6	No	Show	6	H	2	1	3	1.012987	147.1464	0.717449	-0.4654	-1.66016	0.002255
7	No	Show	7	H	4	2	1	1.094476	108.8441	179.1837	-2.66026	-0.93125	-0.01344
8	No	Show	8	H	4	2	1	1.099406	110.8457	59.29881	-2.10603	0.529327	-0.87949
9	No	Show	9	H	4	2	1	1.099597	110.9869	-60.8468	-2.11295	0.502685	0.9005
10	No	Show	10	H	5	3	1	1.098372	108.5427	-55.9068	2.398293	-0.15735	-0.85938
11	No	Show	11	H	5	3	1	1.098834	108.5037	60.74755	2.359663	-0.22641	0.911937
12	No	Show	12	H	5	3	1	1.096156	112.8116	-177.68	1.751372	-1.6176	-0.04185

ACETAMIDE (no. 131)

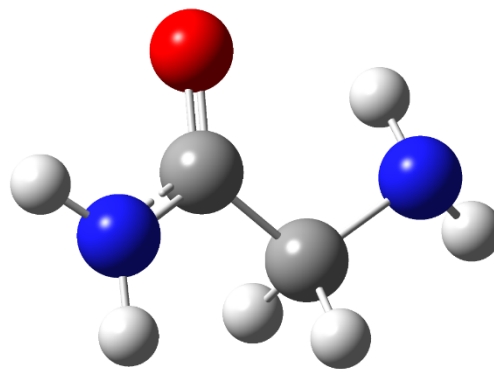
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.36333	1.334101	0
2	No	Show	2	N	1			2.258226			-1.29732	-0.19621	0
3	No	Show	3	C	1	2		2.396574	62.61574		0.99478	-0.97779	0
4	No	Show	4	C	1	2	3	1.235336	30.23462	0	0	0.153404	0
5	No	Show	5	H	3	1	4	1.098623	93.64901	-126.076	1.636017	-0.87513	0.886142
6	No	Show	6	H	3	1	4	1.098623	93.64901	126.0764	1.636017	-0.87513	-0.88614
7	No	Show	7	H	3	1	4	1.09616	139.0676	0	0.520183	-1.96588	0
8	No	Show	8	H	2	1	4	1.012368	148.9414	0	-1.58112	-1.16798	0
9	No	Show	9	H	2	1	4	1.014879	91.5653	180	-2.00519	0.531048	0

UREA (no. 132)

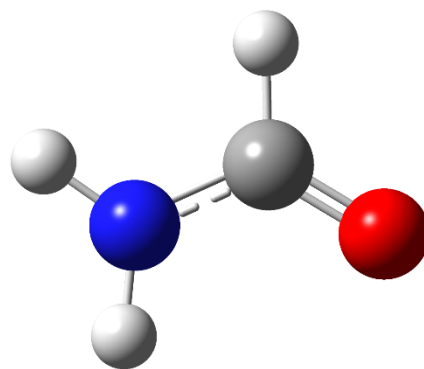


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.042032	1.363446	0
2	No	Show	2	N	1			2.278258			0.042032	-0.59982	1.155874
3	No	Show	3	N	1	2		2.278258	60.97495		0.042032	-0.59982	-1.15587
4	No	Show	4	C	1	3	2	1.236329	30.52085	-2.95648	0.009648	0.127541	0
5	No	Show	5	H	2	1	4	1.01524	143.272	-29.4783	-0.2836	-1.56099	1.127131
6	No	Show	6	H	2	1	4	1.014794	88.4057	-162.792	-0.2077	-0.07667	1.988796
7	No	Show	7	H	3	1	4	1.014794	88.4057	162.7917	-0.2077	-0.07667	-1.9888
8	No	Show	8	H	3	1	4	1.01524	143.272	29.47831	-0.2836	-1.56099	-1.12713

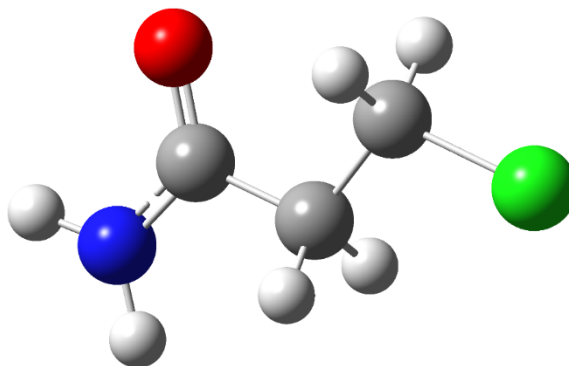
GLYCINAMIDE (no. 133)



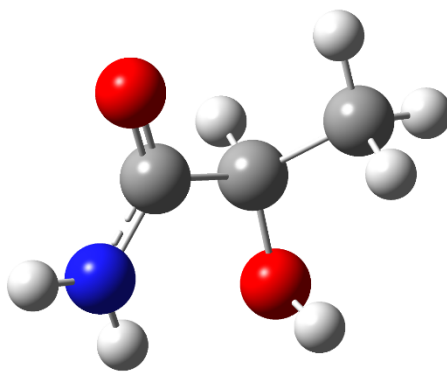
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.49131	1.357739	-0.05647
2	No	Show	2	N	1			2.727374			1.878313	0.044642	0.258534
3	No	Show	3	N	1	2		2.261815	92.63651		-1.69069	-0.55373	0.09713
4	No	Show	4	C	2	1	3	1.457066	61.47761	19.8125	0.710845	-0.71828	-0.16338
5	No	Show	5	C	1	3	4	1.233646	29.94849	-1.25521	-0.53895	0.125463	-0.02317
6	No	Show	6	H	4	2	1	1.106512	114.5092	107.9311	0.732511	-1.04329	-1.22086
7	No	Show	7	H	4	2	1	1.099252	110.634	-131.528	0.602692	-1.62831	0.443661
8	No	Show	8	H	2	1	5	1.022884	57.96314	149.7085	1.817655	0.948019	-0.21741
9	No	Show	9	H	2	1	5	1.020805	150.4959	89.14401	2.704228	-0.40539	-0.13818
10	No	Show	10	H	3	1	5	1.014789	92.09033	-176.531	-2.5692	-0.04581	0.103133
11	No	Show	11	H	3	1	5	1.013086	148.4155	-1.17152	-1.70209	-1.56665	0.111094

FORMAMIDE (no. 134)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.199945	-0.24171	0.000011
2	No	Show	2	N	1			2.275013			-1.0737	-0.16288	-6.5E-05
3	No	Show	3	C	1	2		1.229047	28.88446		0.145013	0.388906	0.000002
4	No	Show	4	H	2	1	3	1.016035	93.46871	- 179.986	-1.17028	-1.17432	0.000128
5	No	Show	5	H	2	1	3	1.013234	146.9795	- 0.03127	-1.90363	0.418371	0.000233
6	No	Show	6	H	3	1	2	1.107736	122.1542	- 179.997	0.120188	1.496364	-3E-06

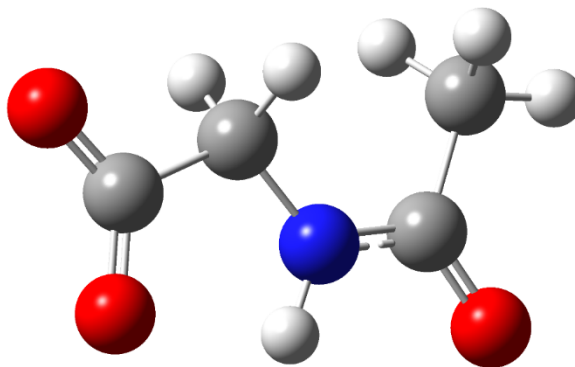
3-CHLOROPROPIONAMIDE (no. 135)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							2.505411	-0.17356	-0.00126
2	No	Show	2	O	1			4.518323			-1.7684	1.292627	-0.00947
3	No	Show	3	N	2	1		2.26184	92.68159		-2.60166	-0.81003	0.011861
4	No	Show	4	C	2	1	3	2.407566	30.42121	-1.07577	-0.2002	-0.53413	-0.01697
5	No	Show	5	C	4	2	1	1.513275	84.68154	0.833048	0.851468	0.553399	0.018772
6	No	Show	6	C	2	1	5	1.233734	62.74032	-171.006	-1.58979	0.071902	-0.00431
7	No	Show	7	H	4	2	1	1.100013	121.4952	112.0798	-0.09749	-1.20691	0.847233
8	No	Show	8	H	4	2	1	1.100295	119.3316	-109.984	-0.0936	-1.14926	-0.92301
9	No	Show	9	H	5	4	2	1.094734	111.8731	-60.4252	0.788361	1.210633	-0.85444
10	No	Show	10	H	5	4	2	1.094914	111.897	62.68904	0.785941	1.154962	0.931277
11	No	Show	11	H	3	2	1	1.01322	148.521	-0.70925	-2.42817	-1.80828	0.014656
12	No	Show	12	H	3	2	1	1.014668	91.94714	179.7944	-3.55711	-0.46846	0.013533

(S)-2-HYDROXYPROPANAMIDE (no. 136)

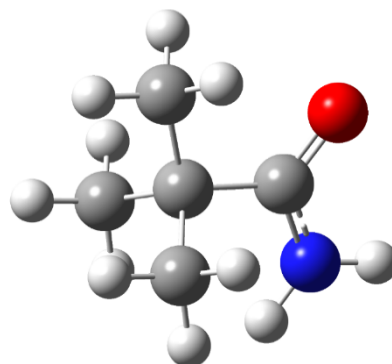
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.085594	-1.3652	-0.16123
2	No	Show	2	O	1			3.592609			-1.29322	1.326885	-0.13412
3	No	Show	3	N	2	1		2.268548	47.60786		-1.49959	-0.90035	0.244227
4	No	Show	4	C	1	3	2	1.416791	65.07966	-4.81926	0.674327	-0.03067	-0.40033
5	No	Show	5	C	4	1	3	1.519418	112.4404	128.6785	1.538332	0.982472	0.331571
6	No	Show	6	C	2	1	4	1.23512	18.26653	166.2851	-0.80228	0.194919	-0.07803
7	No	Show	7	H	4	1	5	1.101343	105.904	119.6792	0.764977	0.12295	-1.48713
8	No	Show	8	H	5	4	1	1.09788	109.8354	57.3077	2.588841	0.857256	0.038155
9	No	Show	9	H	5	4	1	1.096939	110.3556	177.7306	1.216181	2.00311	0.091171
10	No	Show	10	H	5	4	1	1.101652	109.991	-62.538	1.451766	0.834934	1.419861
11	No	Show	11	H	1	4	5	0.971171	107.3264	47.43692	1.21219	-1.4616	0.796821
12	No	Show	12	H	3	2	1	1.013051	146.6941	-6.19338	-1.04563	-1.80597	0.237219
13	No	Show	13	H	3	2	1	1.014558	92.58241	178.7618	-2.49243	-0.82204	0.437773

ACETURATE (no. 137)

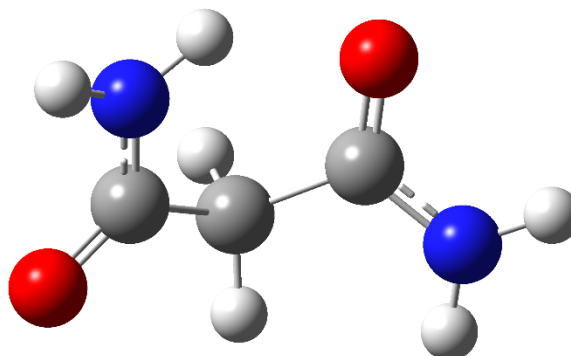


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.609855	-1.12917	0.000041
2	No	Show	2	O	1			5.843988			-2.91072	0.787983	-0.00001
3	No	Show	3	O	2	1		2.248664	47.82935		-2.03138	-1.28162	0.000315
4	No	Show	4	N	1	3	2	2.257688	20.6387	-0.025	0.472076	-0.40318	-0.00032
5	No	Show	5	C	4	1	3	1.444795	154.2564	179.9388	-0.55841	0.609504	-0.00024
6	No	Show	6	C	1	4	5	1.239483	30.3747	-0.03173	1.79884	-0.19185	-0.00018
7	No	Show	7	C	6	1	4	1.506602	121.9743	179.9739	2.243295	1.247704	0.000272
8	No	Show	8	C	2	1	6	1.254659	21.40194	179.9871	-1.95742	-0.02773	0.000055
9	No	Show	9	H	5	4	1	1.101205	111.6858	-59.8392	-0.48855	1.261057	0.884778
10	No	Show	10	H	5	4	1	1.101218	111.6784	59.9262	-0.48884	1.260733	-0.88553
11	No	Show	11	H	4	1	6	1.01856	90.74259	179.9893	0.132074	-1.36332	-0.00043
12	No	Show	12	H	7	6	1	1.099715	110.2971	120.7956	1.851684	1.768138	-0.88582
13	No	Show	13	H	7	6	1	1.094874	109.0989	0.024035	3.337541	1.284789	0.00036
14	No	Show	14	H	7	6	1	1.099721	110.2946	-120.744	1.851593	1.767563	0.886671

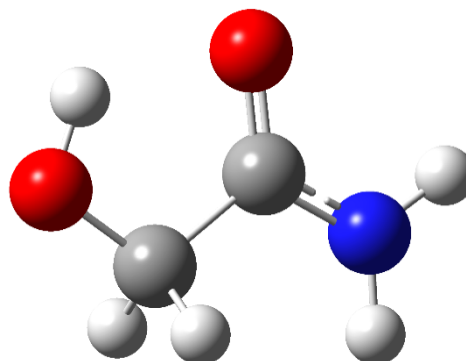
PIVALAMIDE (no. 138)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.44418	1.336827	-1.2E-05
2	No	Show	2	N	1			2.251332			-1.71918	-0.89765	0.000035
3	No	Show	3	C	1	2		2.428899	62.89603		0.566613	-0.02562	-0.00001
4	No	Show	4	C	3	1	2	1.534837	119.9842	70.99678	0.95879	-0.81428	-1.25697
5	No	Show	5	C	3	1	2	1.52651	83.44081	-179.996	1.27292	1.327659	0.00005
6	No	Show	6	C	3	1	2	1.534847	119.9876	-70.9922	0.958842	-0.81435	1.256897
7	No	Show	7	C	1	2	3	1.234779	30.69331	-0.00036	-0.94832	0.205987	0.000008
8	No	Show	8	H	4	3	1	1.100673	110.9424	32.20795	0.646808	-0.28217	-2.16856
9	No	Show	9	H	4	3	1	1.100568	109.3765	151.5253	2.052344	-0.9349	-1.28595
10	No	Show	10	H	4	3	1	1.099962	111.9459	-89.0163	0.508651	-1.81784	-1.26971
11	No	Show	11	H	5	3	1	1.099279	111.0459	-60.1107	1.002358	1.914212	-0.88943
12	No	Show	12	H	5	3	1	1.099282	111.0464	60.11946	1.002443	1.9141	0.889628
13	No	Show	13	H	5	3	1	1.099838	109.5335	-179.995	2.361981	1.174067	-1.5E-05
14	No	Show	14	H	6	3	1	1.099957	111.9464	89.02197	0.50881	-1.81795	1.269558
15	No	Show	15	H	6	3	1	1.100669	110.9417	-32.2043	0.646812	-0.28232	2.168518
16	No	Show	16	H	6	3	1	1.10057	109.3744	-151.521	2.05241	-0.93487	1.285851
17	No	Show	17	H	2	1	7	1.014472	91.01193	179.9976	-2.72809	-0.79153	0.000081
18	No	Show	18	H	2	1	7	1.012683	149.7617	-0.00478	-1.31989	-1.82829	0.000009

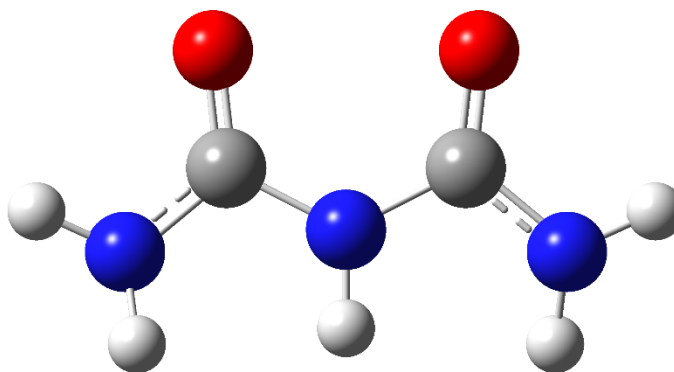
MALONAMIDE (no. 139)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.23946	-0.95091	0.234197
2	No	Show	2	O	1			4.228696			1.332552	1.284683	-0.11898
3	No	Show	3	N	1	2		2.264874	37.17082		-1.43645	1.164677	0.138677
4	No	Show	4	N	2	1	3	2.256689	80.98064	165.9321	2.2235	-0.73194	0.362765
5	No	Show	5	C	1	3	2	2.391573	62.9393	-16.1266	-0.00455	-0.67073	-0.56972
6	No	Show	6	C	1	3	5	1.232895	29.5932	1.735337	-1.32457	-0.1615	-0.01041
7	No	Show	7	C	2	1	6	1.237005	53.42019	-140.479	1.23491	0.052083	-0.08229
8	No	Show	8	H	5	1	6	1.095055	82.30883	162.5673	0.044249	-1.74689	-0.37315
9	No	Show	9	H	5	1	6	1.102435	108.4519	-90.7356	-0.04254	-0.52134	-1.66132
10	No	Show	10	H	3	1	6	1.014895	91.82069	-176.387	-2.29374	1.542232	0.529202
11	No	Show	11	H	3	1	6	1.016722	146.0735	-8.26979	-0.61792	1.750718	-0.00377
12	No	Show	12	H	4	2	1	1.012951	149.0072	21.62934	2.128674	-1.7402	0.385127
13	No	Show	13	H	4	2	1	1.015506	91.38863	-159.507	3.092393	-0.30303	0.666585

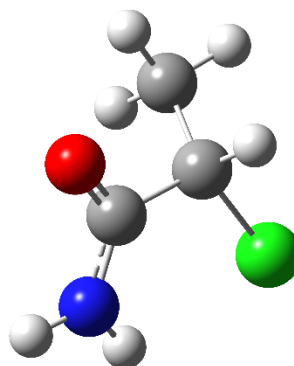
2-HYDROXYACETAMIDE (no. 140)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.88352	-0.00931	0.000397
2	No	Show	2	O	1			2.620959			0.359068	1.34725	-0.00013
3	No	Show	3	N	2	1		2.269297	95.16938		1.70378	-0.48072	0.000327
4	No	Show	4	C	1	2	3	1.408338	64.55879	-0.03902	-0.70762	-0.78434	-0.00031
5	No	Show	5	C	2	1	4	1.234629	65.91499	-0.02405	0.51135	0.122048	-7.5E-05
6	No	Show	6	H	4	1	5	1.102719	111.1538	120.0512	-0.65856	-1.43384	0.889483
7	No	Show	7	H	4	1	5	1.102742	111.1653	-120.047	-0.65873	-1.43286	-0.89085
8	No	Show	8	H	3	2	1	1.015002	92.71046	179.9967	2.548913	0.081405	0.000055
9	No	Show	9	H	3	2	1	1.01403	147.81	0.099629	1.777154	-1.49209	-0.00032
10	No	Show	10	H	1	4	5	0.976328	104.1645	0.080107	-1.56204	0.91258	-0.00048

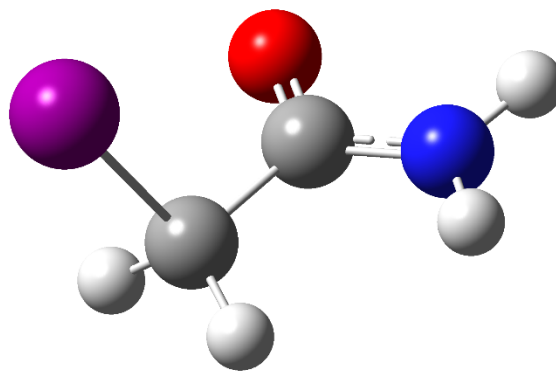
BIURET (no. 141)



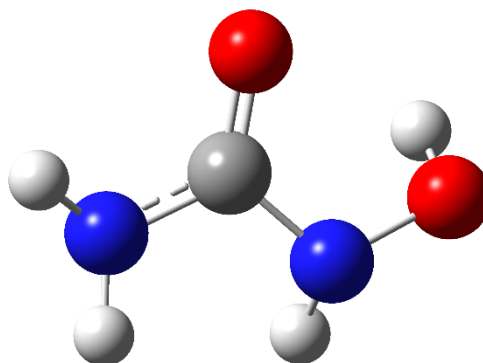
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.37903	1.276879	-0.08953
2	No	Show	2	O	1			2.763877			1.379043	1.276854	0.089517
3	No	Show	3	N	1	2		2.310707	53.26902		0.000005	-0.57506	-0.00023
4	No	Show	4	N	1	3	2	2.271297	60.1145	-175.836	-2.28368	-0.80477	-0.00521
5	No	Show	5	N	2	1	4	2.271298	113.2707	7.834972	2.283697	-0.80482	0.005592
6	No	Show	6	C	1	4	3	1.225182	30.05155	-1.57648	-1.23898	0.06177	-0.01904
7	No	Show	7	C	2	1	6	1.225184	83.23492	5.769943	1.238975	0.061742	0.019091
8	No	Show	8	H	3	1	6	1.017375	143.27	5.707203	-1E-06	-1.59243	-9E-06
9	No	Show	9	H	4	1	6	1.014936	145.0027	27.24786	-2.1489	-1.75742	0.317887
10	No	Show	10	H	4	1	6	1.014832	89.1036	167.3151	-3.19192	-0.38579	0.166375
11	No	Show	11	H	5	2	1	1.014946	144.9662	25.31177	2.148882	-1.75709	-0.31863
12	No	Show	12	H	5	2	1	1.014841	89.0916	165.2131	3.191717	-0.3857	-0.16687

2-CHLOROPROPIONAMIDE (no. 142)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							1.680517	-0.54735	0.126088
2	No	Show	2	O	1			3.93497			-2.122	0.428793	0.394453
3	No	Show	3	N	2	1		2.263688	48.253		-1.09234	-1.40744	-0.43762
4	No	Show	4	C	2	1	3	2.357201	16.85139	-164.861	0.233337	0.517814	0.364906
5	No	Show	5	C	4	2	1	1.518514	96.55801	133.5609	0.349195	1.754904	-0.50806
6	No	Show	6	C	2	1	4	1.232271	19.00979	158.9505	-1.09507	-0.18795	0.105427
7	No	Show	7	H	4	2	1	1.096425	90.31963	-115.31	0.242658	0.786005	1.427984
8	No	Show	8	H	5	4	2	1.098364	108.3576	30.62809	-0.52492	2.393208	-0.32126
9	No	Show	9	H	5	4	2	1.099064	110.43	-88.765	0.368253	1.474294	-1.57053
10	No	Show	10	H	5	4	2	1.096824	110.4161	150.0128	1.26011	2.313637	-0.26093
11	No	Show	11	H	3	2	1	1.015363	91.45669	175.8495	-1.98439	-1.85657	-0.62058
12	No	Show	12	H	3	2	1	1.012503	148.9728	-3.76608	-0.23294	-1.8925	-0.66414

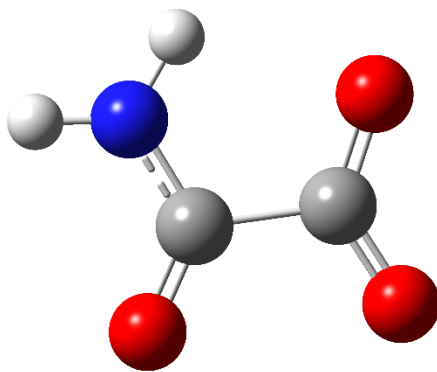
IDOACETAMIDE (no. 143)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	I							-1.09442	0.00987	-0.09154
2	No	Show	2	O	1			3.55821			2.221261	-1.27435	-0.22538
3	No	Show	3	N	2	1		2.256777	76.49476		2.516779	0.960313	-0.33489
4	No	Show	4	C	2	1	3	2.386998	35.81679	61.14569	0.728141	0.102985	1.028141
5	No	Show	5	C	2	1	4	1.232109	53.37115	-40.1804	1.887169	-0.13413	0.100779
6	No	Show	6	H	4	2	1	1.083365	137.3127	-133.436	0.749405	1.079375	1.497065
7	No	Show	7	H	4	2	1	1.083109	88.0923	106.1241	0.670584	-0.69065	1.762954
8	No	Show	8	H	3	2	1	1.008711	92.27454	-143.077	3.285466	0.867406	-0.98141
9	No	Show	9	H	3	2	1	1.007056	148.4589	35.04233	2.219299	1.880234	-0.05309

HYDROXYUREA (no. 144)

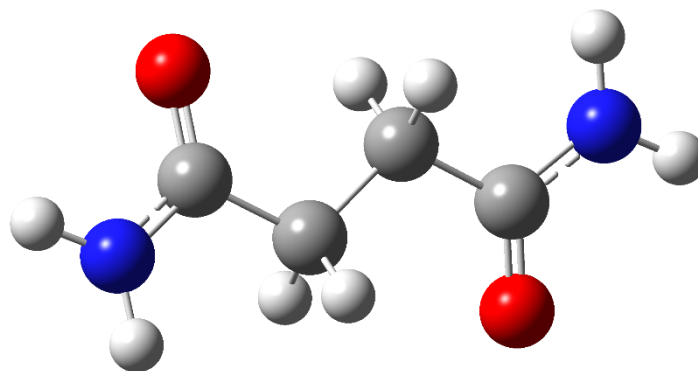
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.850118	-0.06567	0.019485
2	No	Show	2	O	1			2.635362			-0.36664	1.359426	0.034606
3	No	Show	3	N	1	2		1.388862	60.38595		0.62529	-0.70332	0.168285
4	No	Show	4	N	2	1	3	2.28715	91.60412	-10.6901	-1.65484	-0.52439	-0.11652
5	No	Show	5	C	2	1	3	1.226913	62.42922	-6.98425	-0.47711	0.137507	0.029573
6	No	Show	6	H	3	1	5	1.022906	111.3199	130.6666	0.574766	-1.54981	-0.40377
7	No	Show	7	H	4	2	1	1.016156	142.4416	34.41929	-1.69749	-1.49668	0.175725
8	No	Show	8	H	4	2	1	1.015645	89.81221	169.6862	-2.48368	0.031262	0.072723
9	No	Show	9	H	1	3	5	0.975495	106.8024	-51.1949	1.808053	0.434079	-0.81722

OXAMATE (no. 145)



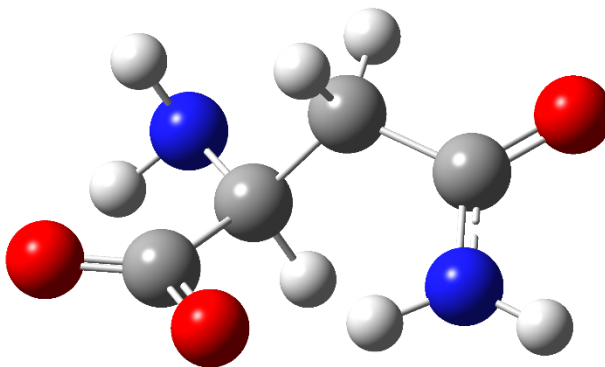
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.20369	-1.30501	-0.0003
2	No	Show	2	O	1			2.743864			1.523666	-1.00452	0.000356
3	No	Show	3	O	2	1		2.254408	88.80187		1.229974	1.23068	-0.00035
4	No	Show	4	N	1	2	3	2.271946	88.9569	-0.03239	-1.41135	0.957427	0.000292
5	No	Show	5	C	1	4	3	1.23248	29.16377	0.01214	-0.70398	-0.17838	-4.1E-05
6	No	Show	6	C	2	1	5	1.247745	63.01887	-0.01874	0.8392	0.038735	-2.5E-05
7	No	Show	7	H	4	1	5	1.013028	144.8492	0.000345	-0.90627	1.83556	0.000487
8	No	Show	8	H	4	1	5	1.014134	93.75621	179.9937	-2.42515	0.931092	0.000231

SUCCINAMIDE (no. 146)

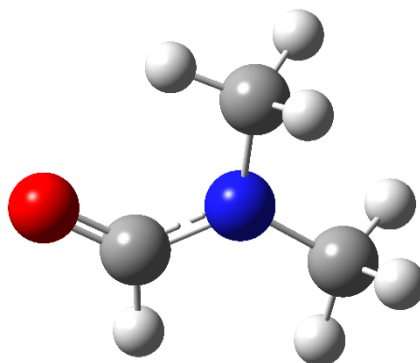


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.08769	1.330843	-0.2403
2	No	Show	2	O	1			4.951596			2.087686	-1.33084	-0.24032
3	No	Show	3	N	1	2		2.258381	80.81388		-2.96089	-0.70966	0.177024
4	No	Show	4	N	2	1	3	2.25838	80.81391	-158.421	2.960888	0.709646	0.177061
5	No	Show	5	C	1	3	2	2.413109	62.16724	-3.70788	-0.55729	-0.51375	0.039813
6	No	Show	6	C	5	1	3	1.515929	87.02904	-171.105	0.557289	0.513757	0.039728
7	No	Show	7	C	1	3	5	1.234298	30.2363	-0.3604	-1.92721	0.127296	-0.01846
8	No	Show	8	C	2	1	7	1.234298	50.67023	-153.129	1.927211	-0.12729	-0.01849
9	No	Show	9	H	5	1	7	1.100856	115.1548	78.2284	-0.46205	-1.17927	-0.83191
10	No	Show	10	H	5	1	7	1.099982	125.106	-56.7269	-0.50272	-1.16126	0.927346
11	No	Show	11	H	6	5	1	1.100858	110.2497	-50.9006	0.462038	1.179148	-0.83209
12	No	Show	12	H	6	5	1	1.099981	111.2579	66.63722	0.502738	1.1614	0.927163
13	No	Show	13	H	3	1	7	1.013009	148.7426	-1.30188	-2.81187	-1.69725	0.346275
14	No	Show	14	H	3	1	7	1.014368	91.71452	-178.366	-3.90764	-0.35103	0.113819
15	No	Show	15	H	4	2	1	1.01301	148.7426	2.764095	2.811864	1.697236	0.346313
16	No	Show	16	H	4	2	1	1.014368	91.71451	-174.299	3.907636	0.35101	0.113883

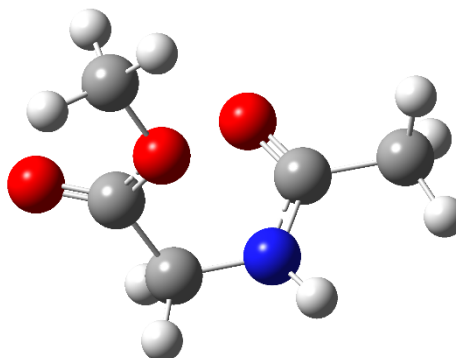
ASPARAGINATE (no. 147)



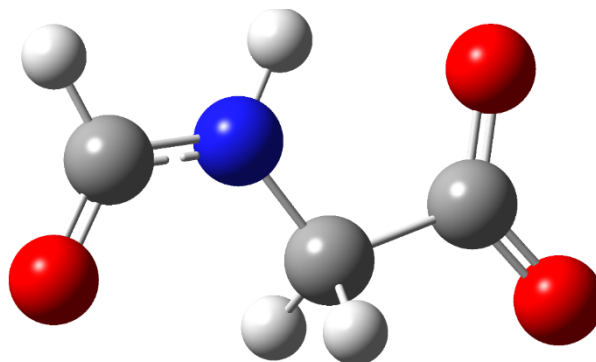
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.979217	0.62241	0.129015
2	No	Show	2	O	1			5.784648			-2.70731	-0.43098	0.255242
3	No	Show	3	O	2	1		2.234818	46.48351		-0.90225	-1.74142	0.117735
4	No	Show	4	N	2	1	3	2.724576	50.23166	-160.043	-1.37275	1.860682	-0.36972
5	No	Show	5	N	1	3	2	2.267869	26.97514	-154.731	1.721373	-1.19553	-0.3771
6	No	Show	6	C	4	2	1	1.463546	61.54771	16.77357	-0.62953	0.599898	-0.36594
7	No	Show	7	C	6	4	2	1.540314	108.8183	-127.134	0.613691	0.758685	0.529467
8	No	Show	8	C	1	5	7	1.239654	29.57641	-0.29342	1.878586	0.054873	0.071962
9	No	Show	9	C	2	1	8	1.251072	20.96855	-11.8754	-1.48901	-0.61819	0.041084
10	No	Show	10	H	6	4	2	1.102845	107.8252	115.6849	-0.28967	0.405267	-1.3969
11	No	Show	11	H	7	6	4	1.097018	108.4113	-23.7334	0.865982	1.824793	0.586141
12	No	Show	12	H	7	6	4	1.103229	110.3135	93.56564	0.393033	0.417571	1.555169
13	No	Show	13	H	4	2	1	1.025859	75.94814	-100.09	-1.67651	2.005718	0.599347
14	No	Show	14	H	4	2	1	1.023592	60.89686	147.558	-2.25963	1.657382	-0.8386
15	No	Show	15	H	5	1	8	1.034481	144.7158	-9.13364	0.780886	-1.61954	-0.3006
16	No	Show	16	H	5	1	8	1.014648	91.34111	-177.913	2.545854	-1.71902	-0.65223

N,N-DIMETHYLFORMAMIDE (no. 148)

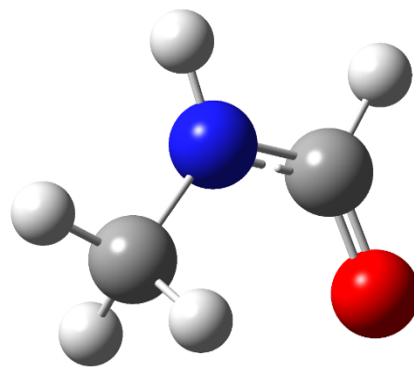
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.95298	-0.08765	0.000015
2	No	Show	2	N	1			2.289442			0.335518	-0.02193	-1.2E-05
3	No	Show	3	C	2	1		1.450143	95.44263		0.431563	1.425034	0
4	No	Show	4	C	2	1	3	1.448857	147.5056	179.9969	1.579389	-0.76487	0.000008
5	No	Show	5	C	1	2	4	1.232518	28.52485	-0.00548	-0.85363	-0.6449	-2.8E-05
6	No	Show	6	H	3	2	1	1.100222	110.1695	-120.188	0.974844	1.769169	-0.8927
7	No	Show	7	H	3	2	1	1.100221	110.1693	120.1865	0.974843	1.769152	0.892702
8	No	Show	8	H	3	2	1	1.094313	108.9853	-0.00067	-0.57737	1.848795	0.000004
9	No	Show	9	H	4	2	1	1.100248	110.3893	120.1017	2.173702	-0.51741	-0.89224
10	No	Show	10	H	4	2	1	1.09674	109.6227	0.003503	1.365864	-1.84063	-5E-06
11	No	Show	11	H	4	2	1	1.100248	110.3892	-120.095	2.173663	-0.51743	0.892283
12	No	Show	12	H	5	1	2	1.108129	122.0236	179.9934	-0.75428	-1.74856	0.000022

METHYL 2-ACETAMIDOACETATE (no. 149)

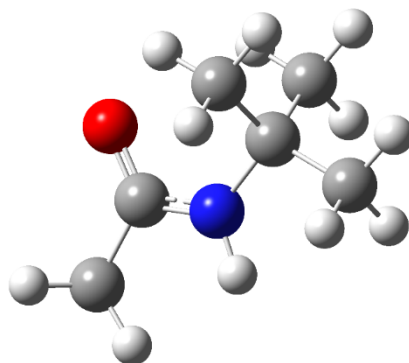
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.16899	0.653609	0.578115
2	No	Show	2	O	1			2.242797			-2.13474	-0.90258	-0.71639
3	No	Show	3	O	1	2		3.038676	81.39349		1.13314	0.169523	-1.34527
4	No	Show	4	N	3	1	2	2.247268	59.48285	-100.92	1.137957	-0.76486	0.698534
5	No	Show	5	C	4	3	1	1.440194	91.19776	59.73981	-0.09012	-1.46204	0.415796
6	No	Show	6	C	2	1	5	1.212123	29.68997	-1.4864	-1.23243	-0.55164	0.01293
7	No	Show	7	C	3	1	6	1.235579	76.6529	-105.028	1.661773	0.058649	-0.234
8	No	Show	8	C	7	3	1	1.502562	122.5259	-127.808	2.896793	0.821997	0.152931
9	No	Show	9	C	1	6	2	1.434118	115.128	-2.91825	-2.22372	1.553937	0.212537
10	No	Show	10	H	5	4	3	1.097956	111.7328	63.72615	0.031588	-2.18466	-0.40183
11	No	Show	11	H	5	4	3	1.097251	108.9181	-176.751	-0.40348	-2.00913	1.313824
12	No	Show	12	H	4	3	1	1.01339	147.8557	-107.61	1.526887	-0.77993	1.634197
13	No	Show	13	H	8	7	3	1.097678	108.6349	-50.976	3.656088	0.679175	-0.62679
14	No	Show	14	H	8	7	3	1.09921	108.188	65.71789	2.644044	1.891349	0.182384
15	No	Show	15	H	8	7	3	1.096071	112.6937	-173.122	3.29652	0.514384	1.126052
16	No	Show	16	H	9	1	6	1.093844	105.7231	-179.634	-2.01948	2.483965	0.750894
17	No	Show	17	H	9	1	6	1.097494	110.3262	60.83032	-3.19659	1.142374	0.51026
18	No	Show	18	H	9	1	6	1.097825	109.9658	-60.3499	-2.21029	1.726595	-0.87154

2-FORMAMIDOACETATE (no. 150)

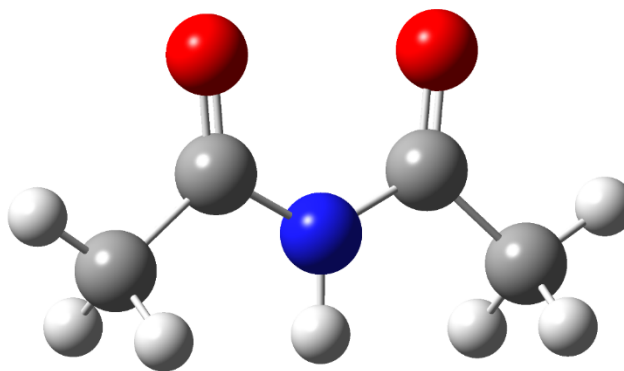
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.743492	1.201173	0.007443
2	No	Show	2	O	1			2.247927			2.437585	-0.93691	0.002112
3	No	Show	3	O	1	2		4.837034	84.98596		-2.70905	-0.68875	0.008851
4	No	Show	4	N	3	1	2	2.269032	10.59204	-177.095	-0.81875	0.566176	-0.01193
5	No	Show	5	C	4	3	1	1.444575	96.27567	2.517616	0.107033	-0.54275	-0.00839
6	No	Show	6	C	2	1	5	1.254258	26.48846	0.011389	1.558885	-0.04189	0.001167
7	No	Show	7	C	3	1	6	1.234667	39.70229	-179.115	-2.14278	0.408378	0.001148
8	No	Show	8	H	5	4	3	1.101265	110.9709	-58.4388	-0.04854	-1.18324	0.873859
9	No	Show	9	H	5	4	3	1.101217	111.0674	60.13891	-0.03712	-1.1816	-0.8937
10	No	Show	10	H	4	3	1	1.01707	148.1474	-176.241	-0.39578	1.491124	-0.01008
11	No	Show	11	H	7	3	1	1.107376	122.345	-179.279	-2.70239	1.363953	0.002618

N-METHYLFORMAMIDE (no. 151)

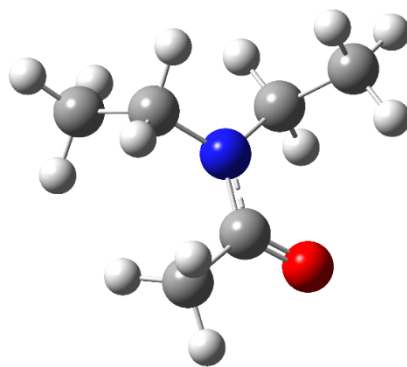
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.362675	-0.67796	0.000006
2	No	Show	2	N	1			2.26697			-0.46676	0.660814	0.000104
3	No	Show	3	C	2	1		1.450622	94.18412		-1.40656	-0.44421	-2.3E-05
4	No	Show	4	C	1	2	3	1.232462	29.36329	179.9868	0.852753	0.444065	-3.2E-05
5	No	Show	5	H	3	2	1	1.094173	108.8976	179.9685	-2.42472	-0.04349	0.000566
6	No	Show	6	H	3	2	1	1.099264	110.796	60.05409	-1.26866	-1.07394	0.890371
7	No	Show	7	H	3	2	1	1.099292	110.8047	-60.1139	-1.26946	-1.07328	-0.89104
8	No	Show	8	H	2	1	4	1.013572	145.6113	0.030043	-0.80368	1.616751	-0.00024
9	No	Show	9	H	4	1	2	1.10708	122.5852	179.9949	1.455301	1.372807	-0.0001

N-TERT-BUTYLACETAMIDE (no. 152)

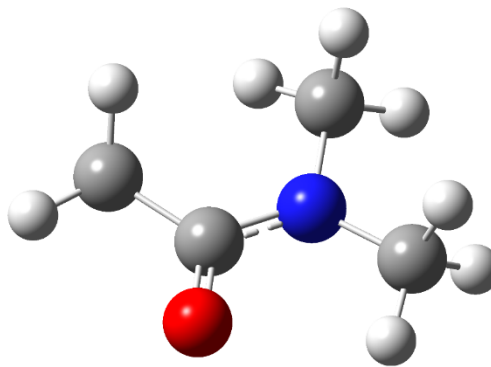
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.49808	-1.3043	0.000019
2	No	Show	2	N	1			2.276961			-0.30412	0.634522	-0.00006
3	No	Show	3	C	2	1		1.475446	99.04267		1.058194	0.067925	-1.4E-05
4	No	Show	4	C	3	2	1	1.526689	106.1925	-179.969	2.014309	1.258144	0.000731
5	No	Show	5	C	3	2	1	1.530377	110.317	-61.2383	1.283618	-0.77368	1.258138
6	No	Show	6	C	3	2	1	1.530378	110.3115	61.29869	1.284025	-0.77255	-1.25885
7	No	Show	7	C	1	2	3	1.238509	29.52481	179.9946	-1.45268	-0.06662	0.000016
8	No	Show	8	C	7	1	2	1.509381	120.6958	179.9961	-2.72147	0.750945	0.000012
9	No	Show	9	H	4	3	2	1.100644	110.7271	60.32751	1.860778	1.880574	0.895397
10	No	Show	10	H	4	3	2	1.098804	109.7916	-179.971	3.053351	0.900705	0.000285
11	No	Show	11	H	4	3	2	1.100647	110.7258	-60.2742	1.860505	1.881884	-0.89298
12	No	Show	12	H	5	3	2	1.097512	111.0483	62.43914	0.595228	-1.62788	1.289549
13	No	Show	13	H	5	3	2	1.100173	110.3553	-58.2418	1.130307	-0.16245	2.159955
14	No	Show	14	H	5	3	2	1.100054	109.59	-177.572	2.315739	-1.15415	1.267346
15	No	Show	15	H	6	3	2	1.100171	110.3562	58.30563	1.132178	-0.16022	-2.16017
16	No	Show	16	H	6	3	2	1.100054	109.595	177.6402	2.315747	-1.15411	-1.26751
17	No	Show	17	H	6	3	2	1.097523	111.0424	-62.3734	0.59477	-1.62601	-1.29176
18	No	Show	18	H	2	1	7	1.014738	143.9533	0.00075	-0.38235	1.64624	-4.7E-05
19	No	Show	19	H	8	7	1	1.098656	108.3027	-58.2111	-3.30912	0.475929	-0.8866
20	No	Show	20	H	8	7	1	1.098656	108.3023	58.15542	-3.30958	0.475204	0.886088
21	No	Show	21	H	8	7	1	1.096124	113.2687	179.9723	-2.54003	1.831948	0.000497

DIACETAMIDE (no. 153)

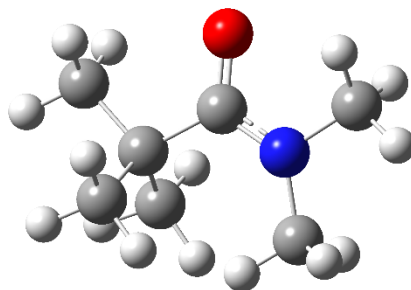
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.377199	1.309625	-0.04435
2	No	Show	2	O	1			2.755851			-1.37723	1.309626	0.044213
3	No	Show	3	N	2	1		2.291058	53.02724		0.000007	-0.52075	0.000685
4	No	Show	4	C	1	3	2	1.217104	30.66365	177.3176	1.243922	0.100314	-0.0105
5	No	Show	5	C	2	1	4	1.217104	83.66562	-2.78232	-1.24395	0.100305	0.010725
6	No	Show	6	C	4	1	3	1.502307	123.5884	179.9886	2.396843	-0.86228	0.022826
7	No	Show	7	C	5	2	1	1.502296	123.5911	-177.809	-2.39681	-0.86232	-0.02333
8	No	Show	8	H	3	2	1	1.017946	143.0251	-179.944	-3.7E-05	-1.5387	0.000504
9	No	Show	9	H	6	4	1	1.094244	109.1682	-0.99602	3.335198	-0.30014	-0.00644
10	No	Show	10	H	6	4	1	1.099384	109.6012	119.6656	2.34669	-1.46619	0.940119
11	No	Show	11	H	6	4	1	1.099155	109.8989	-121.96	2.337659	-1.54674	-0.83517
12	No	Show	12	H	7	5	2	1.099138	109.9052	-122.099	-2.33704	-1.54823	0.833439
13	No	Show	13	H	7	5	2	1.099394	109.5862	119.5264	-2.34707	-1.46457	-0.94174
14	No	Show	14	H	7	5	2	1.094247	109.1699	-1.12119	-3.33521	-0.30032	0.007318

N,N-DIETHYLACETAMIDE (no. 154)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.790045	-1.89315	-0.5746
2	No	Show	2	N	1			2.259551			0.042219	0.163259	-0.01113
3	No	Show	3	C	2	1		1.461834	90.87629		1.274182	0.772352	-0.50936
4	No	Show	4	C	2	1	3	1.461117	151.9069	-177.374	-0.95412	1.056433	0.575734
5	No	Show	5	C	1	2	4	1.240649	30.73916	3.229021	-0.1033	-1.17744	-0.09617
6	No	Show	6	C	3	2	1	1.521819	112.355	-83.7675	2.393954	0.739186	0.520662
7	No	Show	7	C	4	2	1	1.521762	112.757	-97.9761	-1.87254	1.679145	-0.46566
8	No	Show	8	C	5	1	2	1.510024	120.7994	-179.757	-1.38847	-1.78319	0.41528
9	No	Show	9	H	3	2	1	1.097502	108.3595	38.36942	1.578588	0.241214	-1.42026
10	No	Show	10	H	3	2	1	1.098844	107.3094	154.4071	1.036664	1.807862	-0.79001
11	No	Show	11	H	4	2	1	1.096368	109.3365	25.59275	-1.53559	0.5084	1.326454
12	No	Show	12	H	4	2	1	1.100166	107.0927	140.5772	-0.40563	1.841144	1.117717
13	No	Show	13	H	6	3	2	1.100331	110.8736	-58.6749	2.096363	1.264854	1.440358
14	No	Show	14	H	6	3	2	1.099547	110.2437	61.64727	2.645266	-0.30033	0.776093
15	No	Show	15	H	6	3	2	1.099482	110.3396	-178.621	3.295059	1.226453	0.12136
16	No	Show	16	H	7	4	2	1.100274	110.8413	-57.618	-1.29227	2.236506	-1.21615
17	No	Show	17	H	7	4	2	1.100128	110.7552	62.65374	-2.45541	0.903921	-0.98486
18	No	Show	18	H	7	4	2	1.099414	110.1937	-177.335	-2.57251	2.377676	0.014775
19	No	Show	19	H	8	5	1	1.094964	107.9839	-9.52098	-1.40649	-2.83733	0.119641
20	No	Show	20	H	8	5	1	1.099901	110.1194	109.3782	-1.4268	-1.71851	1.512609
21	No	Show	21	H	8	5	1	1.09797	111.8731	-130.512	-2.2714	-1.26841	0.014047

N,N-DIMETHYLACETAMIDE (no. 155)

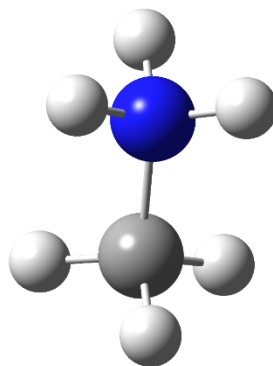
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.0369	-1.49389	0.032406
2	No	Show	2	N	1			2.26831			0.586363	0.083245	-0.11891
3	No	Show	3	C	1	2		1.237832	30.53423		-0.71112	-0.30089	-0.02087
4	No	Show	4	C	2	1	3	1.4538	149.7487	17.40866	1.014037	1.464087	0.035703
5	No	Show	5	C	2	1	3	1.453667	92.10176	172.9434	1.638846	-0.91054	0.014614
6	No	Show	6	C	3	1	2	1.509381	120.6753	179.1858	-1.7589	0.7853	0.003312
7	No	Show	7	H	4	2	1	1.094239	111.2779	-44.5906	0.270573	2.157701	-0.36867
8	No	Show	8	H	4	2	1	1.097953	108.6232	-163.412	1.949695	1.605782	-0.52105
9	No	Show	9	H	4	2	1	1.102688	111.4955	77.43005	1.201275	1.713063	1.093471
10	No	Show	10	H	5	2	1	1.098353	109.4152	139.0444	2.455039	-0.67368	-0.68116
11	No	Show	11	H	5	2	1	1.093255	109.4987	19.02039	1.237378	-1.90064	-0.21716
12	No	Show	12	H	5	2	1	1.102591	110.9055	-101.439	2.046111	-0.91705	1.039211
13	No	Show	13	H	6	3	1	1.094729	107.9978	-0.22079	-2.74124	0.30632	0.066721
14	No	Show	14	H	6	3	1	1.099236	110.7947	119.7555	-1.61558	1.446558	0.869637
15	No	Show	15	H	6	3	1	1.098842	111.0997	-120.317	-1.70981	1.402554	-0.90446

(CH₃)₃CCON(CH₃)₂ (no. 156)

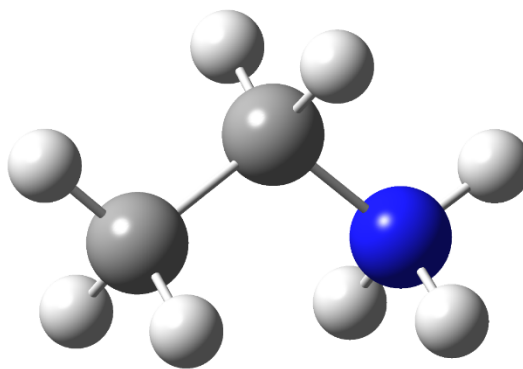
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							-1.14742	0.093592	-0.01066
2	No	Show	2	C	1			1.533011			-2.20939	-1.01164	0.017707
3	No	Show	3	H	2	1		1.09855	111.2431		-2.12653	-1.61996	0.928687
4	No	Show	4	H	2	1	3	1.099793	108.949	119.6719	-3.20692	-0.5491	-0.00541
5	No	Show	5	H	2	1	4	1.098643	111.2621	119.7102	-2.11251	-1.67958	-0.84917
6	No	Show	6	C	1	2	3	1.538174	107.2268	-58.1029	-1.34634	0.949001	1.252147
7	No	Show	7	H	6	1	2	1.10094	110.2599	64.48955	-1.14842	0.349273	2.153935
8	No	Show	8	H	6	1	2	1.096194	114.077	-173.585	-0.71346	1.84321	1.29084
9	No	Show	9	H	6	1	2	1.100712	108.7455	-53.5079	-2.39483	1.281564	1.292573
10	No	Show	10	C	1	2	6	1.536527	107.3864	-120.895	-1.35897	0.900601	-1.30097
11	No	Show	11	H	10	1	2	1.09664	114.163	178.7615	-0.66501	1.74081	-1.4238
12	No	Show	12	H	10	1	2	1.100708	110.0962	-59.7271	-1.25452	0.244681	-2.1787
13	No	Show	13	H	10	1	2	1.100762	108.9434	58.38228	-2.38136	1.308522	-1.30374
14	No	Show	14	C	1	2	6	1.542516	107.4784	119.3486	0.234592	-0.59147	-0.00074
15	No	Show	15	O	14	1	2	1.239539	119.5486	-2.89348	0.304154	-1.82637	0.080682
16	No	Show	16	N	14	1	2	1.359648	121.6813	175.5019	1.386341	0.122554	-0.11158
17	No	Show	17	C	16	14	1	1.458912	116.1461	177.5982	2.62659	-0.64173	-0.03366
18	No	Show	18	H	17	16	14	1.095838	108.4806	169.6507	3.456977	0.01353	-0.31993
19	No	Show	19	H	17	16	14	1.102001	111.4696	-70.3767	2.803976	-1.01983	0.986132
20	No	Show	20	H	17	16	14	1.095995	110.4343	49.9391	2.591144	-1.49917	-0.71539
21	No	Show	21	C	16	14	1	1.455972	127.4348	15.9359	1.559049	1.557078	0.067772
22	No	Show	22	H	21	16	14	1.102278	110.6497	97.5639	1.924404	1.780641	1.083426
23	No	Show	23	H	21	16	14	1.098646	108.8797	-143.643	2.30576	1.918079	-0.65273
24	No	Show	24	H	21	16	14	1.088815	112.2512	-24.1093	0.63503	2.107845	-0.10064

AMMONIUM

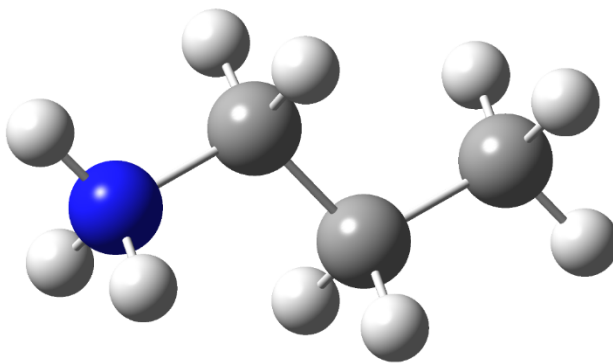
METHYL AMMONIUM HYDRIDE (no. 157)



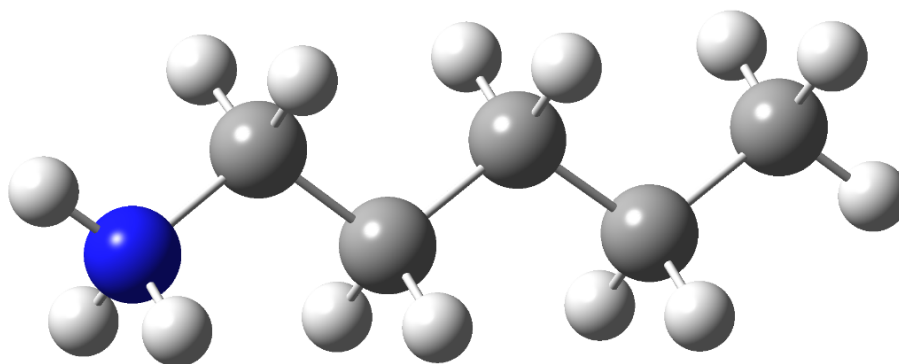
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							0.000085	0.697665	0
2	No	Show	2	C	1			1.483424			0.000085	-0.78576	0
3	No	Show	3	H	1	2		1.027284	111.4207		-0.95624	1.072842	0
4	No	Show	4	H	1	2	3	1.027286	111.4849	119.9794	0.477739	1.073914	0.82801
5	No	Show	5	H	1	2	3	1.027286	111.4849	-119.979	0.477739	1.073914	-0.82801
6	No	Show	6	H	2	1	3	1.09299	108.3725	180	1.037362	-1.13026	0
7	No	Show	7	H	2	1	3	1.0932	108.3408	59.99339	-0.51885	-1.12976	-0.89859
8	No	Show	8	H	2	1	3	1.0932	108.3408	-59.9934	-0.51885	-1.12976	0.898586

ETHYLAMMONIUM (no. 158)

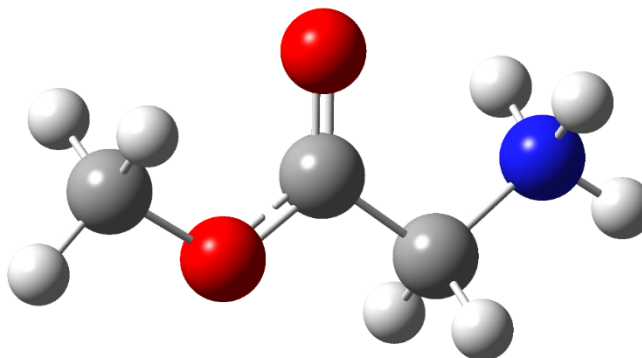
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.181693	-0.24556	0
2	No	Show	2	C	1			1.492366			-0.04482	0.604629	0
3	No	Show	3	C	2	1		1.510403	110.2233		-1.28135	-0.26273	0
4	No	Show	4	H	2	1	3	1.095111	106.5309	121.9031	0.015177	1.238131	0.89126
5	No	Show	5	H	2	1	3	1.095112	106.531	-121.903	0.015177	1.238132	-0.89126
6	No	Show	6	H	1	2	3	1.027251	111.7116	180	2.037714	0.322303	0
7	No	Show	7	H	1	2	3	1.028396	110.9718	59.64029	1.207695	-0.85414	-0.82859
8	No	Show	8	H	1	2	3	1.028396	110.9718	-59.6403	1.207695	-0.85414	0.828589
9	No	Show	9	H	3	2	1	1.097791	109.2345	180	-2.17265	0.378148	0
10	No	Show	10	H	3	2	1	1.099349	110.8894	-60.6142	-1.31284	-0.90043	-0.89494
11	No	Show	11	H	3	2	1	1.099348	110.8895	60.61428	-1.31284	-0.90043	0.894939

TRIDEUTERIO(PROPYL)AZANIUM (no. 159)

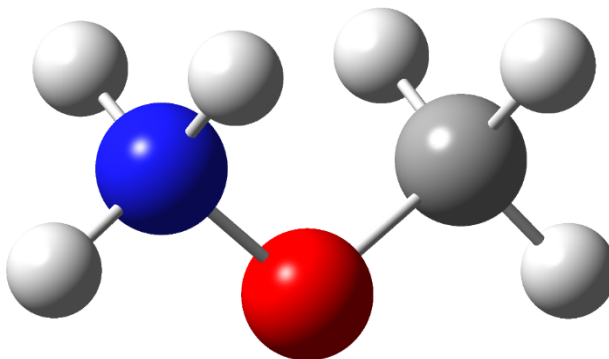
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-1.84359	-0.11155	0
2	No	Show	2	C	1			1.490702			-0.49637	0.526566	0
3	No	Show	3	C	2	1		1.515437	110.6567		0.593765	-0.52612	0
4	No	Show	4	C	3	2	1	1.522953	110.7359	180	1.971034	0.123891	0
5	No	Show	5	H	2	1	3	1.09646	106.7802	-121.82	-0.44722	1.16229	0.892
6	No	Show	6	H	2	1	3	1.09646	106.7802	121.8201	-0.44722	1.16229	-0.892
7	No	Show	7	H	3	2	1	1.10154	109.065	-58.4989	0.474709	-1.16739	0.887689
8	No	Show	8	H	3	2	1	1.10154	109.065	58.49886	0.474709	-1.16739	-0.88769
9	No	Show	9	H	1	2	3	1.028375	111.0393	59.64816	-1.96964	-0.70791	0.828264
10	No	Show	10	H	1	2	3	1.028375	111.0392	-59.6482	-1.96964	-0.70791	-0.82827
11	No	Show	11	H	1	2	3	1.026897	111.7562	180	-2.59585	0.587475	0
12	No	Show	12	H	4	3	2	1.100189	110.9156	-60.0047	2.106938	0.756151	-0.89005
13	No	Show	13	H	4	3	2	1.100188	110.9156	60.00472	2.106938	0.756151	0.890051
14	No	Show	14	H	4	3	2	1.09809	110.7305	180	2.760878	-0.63896	0

PENTYLAZANIUM (no. 160)

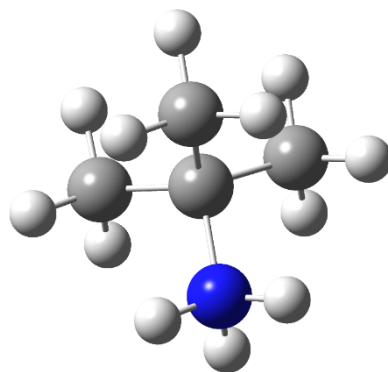
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-1.46543	-2.71308	0
2	No	Show	2	C	1			2.470933			0	-0.7236	0
3	No	Show	3	C	2	1		1.524719	145.7051		0.055342	0.80011	0
4	No	Show	4	C	1	2	3	1.490814	35.01911	0	-1.43015	-1.22269	0
5	No	Show	5	C	3	2	1	1.524943	112.5589	180	1.483911	1.333627	0
6	No	Show	6	C	5	3	2	1.523368	112.4271	180	1.535703	2.856114	0
7	No	Show	7	H	2	1	4	1.102562	89.65138	126.3322	0.521962	-1.11641	0.888202
8	No	Show	8	H	2	1	4	1.102562	89.65138	-126.332	0.521962	-1.11641	-0.8882
9	No	Show	9	H	3	2	1	1.103545	109.3285	58.16507	-0.48032	1.185061	0.884697
10	No	Show	10	H	3	2	1	1.103545	109.3285	-58.1651	-0.48032	1.185061	-0.8847
11	No	Show	11	H	4	1	2	1.096312	106.735	-121.811	-1.97595	-0.894	0.892175
12	No	Show	12	H	4	1	2	1.096312	106.735	121.8114	-1.97595	-0.894	-0.89218
13	No	Show	13	H	5	3	2	1.102815	109.0789	57.93682	2.015175	0.941434	-0.88326
14	No	Show	14	H	5	3	2	1.102815	109.0789	-57.9368	2.015175	0.941434	0.883257
15	No	Show	15	H	1	4	2	1.028365	111.0752	-59.6335	-0.98922	-3.09425	-0.82793
16	No	Show	16	H	1	4	2	1.02713	111.7498	180	-2.42818	-3.07101	0
17	No	Show	17	H	1	4	2	1.028365	111.0752	59.63352	-0.98922	-3.09425	0.827932
18	No	Show	18	H	6	5	3	1.101141	110.9012	-59.7617	1.031316	3.26634	-0.88872
19	No	Show	19	H	6	5	3	1.099439	111.5459	180	2.571453	3.224878	0
20	No	Show	20	H	6	5	3	1.101141	110.9012	59.76167	1.031316	3.26634	0.888718

2-METHOXY-2-OXOETHANAMINIUM (no. 161)

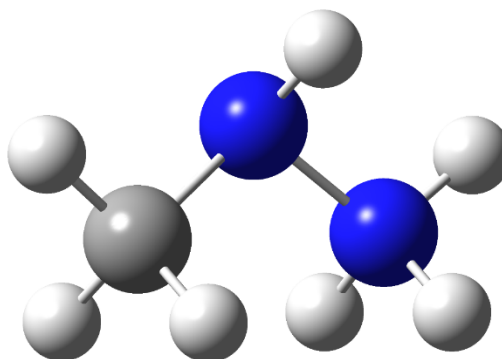
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.17856	-0.69748	0.000063
2	No	Show	2	O	1			2.252017			-0.08357	1.27041	0.000033
3	No	Show	3	N	2	1		2.668302	93.61756		2.325296	0.12272	-3.2E-05
4	No	Show	4	C	3	2	1	1.475363	63.12015	0	1.157088	-0.77838	-4E-06
5	No	Show	5	C	2	1	4	1.210162	28.60649	-0.00114	-0.09384	0.060292	0.000044
6	No	Show	6	C	1	5	2	1.438918	115.3262	0.005798	-2.428	0.016233	-6.1E-05
7	No	Show	7	H	4	3	2	1.09526	109.2826	120.2624	1.18889	-1.41182	-0.89294
8	No	Show	8	H	4	3	2	1.095262	109.2833	-120.264	1.188937	-1.41185	0.892916
9	No	Show	9	H	3	2	1	1.027919	174.374	0.115574	3.205458	-0.40825	-0.00026
10	No	Show	10	H	3	2	1	1.029402	74.67625	-123.602	2.316053	0.735755	0.826873
11	No	Show	11	H	3	2	1	1.029403	74.65777	123.6159	2.315782	0.736025	-0.82674
12	No	Show	12	H	6	1	5	1.097089	109.9015	60.57435	-2.50086	0.641453	-0.89861
13	No	Show	13	H	6	1	5	1.097093	109.9006	-60.6342	-2.50139	0.6408	0.898907
14	No	Show	14	H	6	1	5	1.093252	105.513	179.9711	-3.2044	-0.75345	-0.00056

METHOXYAZANIUM (no. 162)

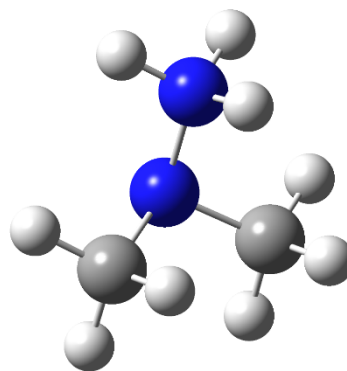
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.027702	-0.61492	0
2	No	Show	2	N	1			1.38611			-1.10062	0.190182	0
3	No	Show	3	C	1	2		1.433569	109.2725		1.198876	0.211799	0
4	No	Show	4	H	2	1	3	1.035368	111.2069	-60.9832	-1.13354	0.788857	0.844092
5	No	Show	5	H	2	1	3	1.030535	107.1693	180	-1.92015	-0.43461	-1E-06
6	No	Show	6	H	2	1	3	1.035368	111.2069	60.98303	-1.13354	0.788859	-0.84409
7	No	Show	7	H	3	1	2	1.099944	110.0953	-61.3016	1.221566	0.834986	-0.90609
8	No	Show	8	H	3	1	2	1.094201	104.4936	180	2.033531	-0.49575	0
9	No	Show	9	H	3	1	2	1.099944	110.0953	61.30163	1.221566	0.834986	0.90609

TERT-BUTYLAMMONIUM (no. 163)

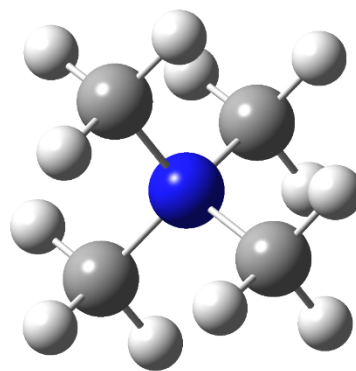
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.01373	-0.05074	1.436607
2	No	Show	2	C	1			1.509678			0.000666	0.002709	-0.07206
3	No	Show	3	C	2	1		1.521135	106.9765		-1.31048	-0.6022	-0.55044
4	No	Show	4	C	2	1	3	1.521147	107.0655	120.0019	0.124424	1.466817	-0.4657
5	No	Show	5	C	2	1	3	1.521279	106.9839	-120.005	1.200904	-0.80986	-0.53406
6	No	Show	6	H	1	2	3	1.02889	110.9473	59.97968	-0.09651	-1.02076	1.769534
7	No	Show	7	H	1	2	3	1.029083	111.0601	-59.9473	-0.80715	0.482232	1.817965
8	No	Show	8	H	1	2	3	1.028835	111.063	-179.973	0.850599	0.346145	1.828925
9	No	Show	9	H	3	2	1	1.099869	110.8443	60.65785	-2.16811	-0.02785	-0.17056
10	No	Show	10	H	3	2	1	1.098162	108.9879	-179.977	-1.33468	-0.58016	-1.64812
11	No	Show	11	H	3	2	1	1.099924	110.8473	-60.6378	-1.40286	-1.64734	-0.22034
12	No	Show	12	H	4	2	1	1.099833	110.8678	60.51459	1.055403	1.900851	-0.07261
13	No	Show	13	H	4	2	1	1.099853	110.9036	-60.8153	-0.73009	2.04798	-0.08923
14	No	Show	14	H	4	2	1	1.098164	108.9489	179.8416	0.140719	1.541389	-1.56121
15	No	Show	15	H	5	2	1	1.099934	110.8613	60.52945	1.117259	-1.85528	-0.20245
16	No	Show	16	H	5	2	1	1.098121	108.9977	179.9207	1.242274	-0.79416	-1.63129
17	No	Show	17	H	5	2	1	1.099954	110.8234	-60.7351	2.136156	-0.38265	-0.1433

2-METHYLHYDRAZINIUM (no. 164)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.03756	0.601956	-0.16596
2	No	Show	2	N	1			1.43409			1.127372	-0.21385	0.01842
3	No	Show	3	C	1	2		1.463064	108.3778		-1.22203	-0.23601	0.022219
4	No	Show	4	H	2	1	3	1.030315	109.2935	66.22838	1.175732	-0.91376	-0.73613
5	No	Show	5	H	2	1	3	1.029155	110.0242	-176.272	1.976343	0.364195	-0.04693
6	No	Show	6	H	2	1	3	1.035063	113.9461	-54.2932	1.146256	-0.72157	0.920207
7	No	Show	7	H	1	2	3	1.024527	104.2932	115.4396	0.005251	1.280873	0.600129
8	No	Show	8	H	3	1	2	1.102389	112.9045	54.4248	-1.223	-0.76677	0.988427
9	No	Show	9	H	3	1	2	1.097917	109.1637	-67.5727	-1.28108	-0.96558	-0.79611
10	No	Show	10	H	3	1	2	1.095168	107.2064	174.8471	-2.09598	0.421922	-0.03013

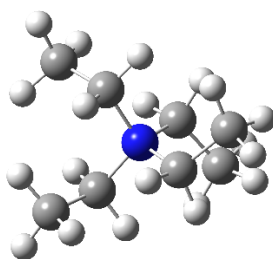
1,1-DIMETHYLHYDRAZINIUM (no. 165)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							0	-0.05108	-0.44075
2	No	Show	2	N	1			1.436206			-1E-06	1.293633	0.063664
3	No	Show	3	C	1	2		1.463207	106.8882		-1.20514	-0.69938	0.077254
4	No	Show	4	C	1	2	3	1.463207	106.8882	-118.802	1.205142	-0.69938	0.077254
5	No	Show	5	H	2	1	4	1.030011	109.7636	179.6939	-0.83171	1.794589	-0.28017
6	No	Show	6	H	2	1	4	1.037707	113.179	-59.4011	-2E-06	1.341026	1.100288
7	No	Show	7	H	2	1	4	1.030011	109.7636	61.50376	0.831712	1.79459	-0.28016
8	No	Show	8	H	3	1	2	1.097315	109.5199	61.40698	-2.09315	-0.16955	-0.28994
9	No	Show	9	H	3	1	2	1.105216	111.7918	-60.3995	-1.21562	-0.72309	1.182166
10	No	Show	10	H	3	1	2	1.095106	107.5938	179.6558	-1.21995	-1.72514	-0.30595
11	No	Show	11	H	4	1	2	1.097316	109.52	-61.407	2.093149	-0.16955	-0.28994
12	No	Show	12	H	4	1	2	1.095105	107.5938	-179.656	1.219947	-1.72514	-0.30595
13	No	Show	13	H	4	1	2	1.105216	111.7918	60.39943	1.215623	-0.72309	1.182166

TETRAMETHYLAMMONIUM (no. 166)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-0.00016	0.000065	-0.00018
2	No	Show	2	C	1			1.48968			0.872838	0.648626	-1.01821
3	No	Show	3	C	1	2		1.489944	109.4291		0.847518	-0.62626	1.052952
4	No	Show	4	C	1	2	3	1.489665	109.5034	-119.992	-0.83379	-1.04696	-0.65432
5	No	Show	5	C	1	4	3	1.489692	109.4563	-120.007	-0.88649	1.024554	0.619521
6	No	Show	6	H	2	1	4	1.095679	108.312	-179.975	1.476535	1.413407	-0.51704
7	No	Show	7	H	2	1	4	1.095492	108.3216	-59.9859	1.515295	-0.1203	-1.46106
8	No	Show	8	H	2	1	4	1.095597	108.3161	60.02616	0.232131	1.102699	-1.78218
9	No	Show	9	H	3	1	4	1.095592	108.3385	-59.942	0.18871	-1.09777	1.790496
10	No	Show	10	H	3	1	4	1.095536	108.2844	60.06091	1.490804	-1.37423	0.576593
11	No	Show	11	H	3	1	4	1.09559	108.3379	-179.933	1.450844	0.158848	1.521913
12	No	Show	12	H	4	1	2	1.09551	108.2886	179.9462	-1.46599	-1.51073	0.110783
13	No	Show	13	H	4	1	2	1.095486	108.3553	-60.0664	-1.44901	-0.5674	-1.42349
14	No	Show	14	H	4	1	2	1.095581	108.3058	59.96393	-0.1644	-1.78911	-1.10312
15	No	Show	15	H	5	1	4	1.095507	108.3384	60.231	-1.5157	0.529197	1.367084
16	No	Show	16	H	5	1	4	1.095529	108.2964	-179.776	-0.25513	1.785859	1.090677
17	No	Show	17	H	5	1	4	1.095521	108.3498	-59.7603	-1.5034	1.469309	-0.16901

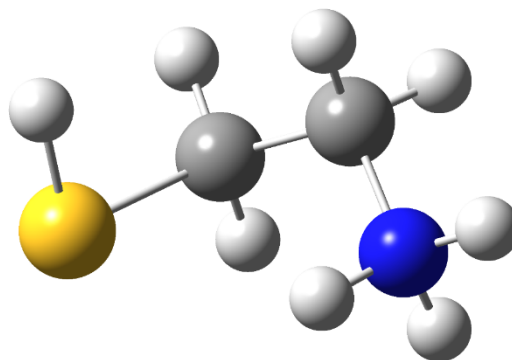
TETRAETHYLAMMONIUM (no. 167)



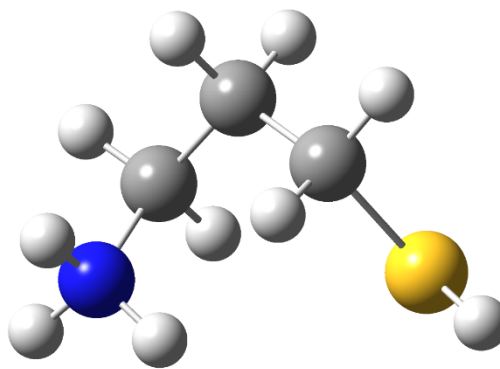
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							0.000177	0.000004	-8E-06
2	No	Show	2	C	1			1.513101			0.855706	0.837649	0.925139
3	No	Show	3	C	1	2		1.513101	111.138		0.855704	-0.83765	-0.92515
4	No	Show	4	C	1	3	2	1.513099	108.6464	119.4845	-0.85537	0.925169	-0.83761
5	No	Show	5	C	1	4	2	1.513099	111.136	119.4852	-0.85537	-0.92516	0.83759
6	No	Show	6	C	2	1	4	1.516567	115.1996	-66.0724	1.895409	1.701518	0.237591
7	No	Show	7	C	3	1	4	1.516566	115.1994	172.8992	1.895386	-1.70153	-0.2376
8	No	Show	8	C	4	1	5	1.51656	115.1994	-53.3684	-1.89578	0.237707	-1.70068
9	No	Show	9	C	5	1	4	1.516559	115.1997	-53.372	-1.89574	-0.2377	1.700721
10	No	Show	10	H	2	1	4	1.095678	105.8354	55.89898	0.158147	1.464761	1.4914
11	No	Show	11	H	2	1	4	1.096762	106.1194	170.6084	1.326458	0.135331	1.62373
12	No	Show	12	H	3	1	4	1.095678	105.8352	-65.1297	0.158141	-1.46475	-1.49142
13	No	Show	13	H	3	1	4	1.096762	106.1196	49.57981	1.326471	-0.13533	-1.62374
14	No	Show	14	H	4	1	5	1.096761	106.1187	69.94692	-1.32553	1.624196	-0.13533
15	No	Show	15	H	4	1	5	1.095678	105.8364	-175.344	-0.15789	1.49094	-1.46525
16	No	Show	16	H	5	1	4	1.09676	106.1186	69.94352	-1.32557	-1.62415	0.1353
17	No	Show	17	H	5	1	4	1.09568	105.8363	-175.347	-0.15789	-1.49098	1.46519
18	No	Show	18	H	6	2	1	1.098563	106.9506	178.8215	2.418259	2.261277	1.025079
19	No	Show	19	H	6	2	1	1.097753	112.7555	-63.0454	2.645403	1.111992	-0.30558
20	No	Show	20	H	6	2	1	1.097428	112.5379	61.01575	1.448085	2.434209	-0.44609
21	No	Show	21	H	7	3	1	1.098563	106.9506	178.8214	2.418237	-2.2613	-1.02508
22	No	Show	22	H	7	3	1	1.097753	112.7556	-63.0455	2.645383	-1.11202	0.305581
23	No	Show	23	H	7	3	1	1.097428	112.5378	61.01563	1.448041	-2.43422	0.446071
24	No	Show	24	H	8	4	1	1.098562	106.9508	-178.823	-2.4186	1.025186	-2.26048
25	No	Show	25	H	8	4	1	1.097429	112.5382	-61.0169	-1.44911	-0.44645	-2.43333
26	No	Show	26	H	8	4	1	1.097756	112.7539	63.04442	-2.64569	-0.30491	-1.11053
27	No	Show	27	H	9	5	1	1.098563	106.9507	-178.823	-2.41855	-1.02519	2.260516
28	No	Show	28	H	9	5	1	1.097428	112.5382	-61.0166	-1.44902	0.446413	2.433374
29	No	Show	29	H	9	5	1	1.097756	112.7539	63.04497	-2.64566	0.304947	1.110621

HYDROGEN SULFIDE

CYSTEAMINIUM (no. 168)



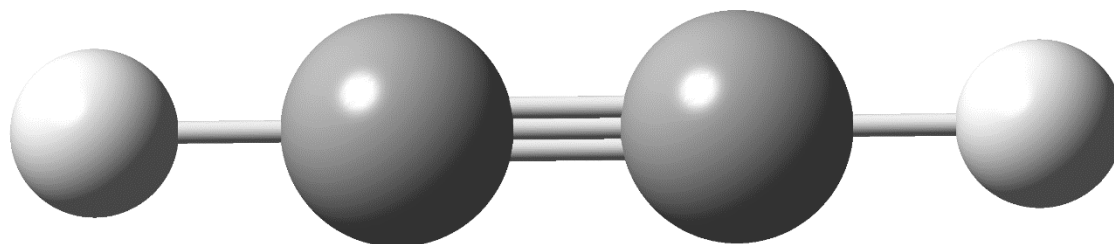
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.47779	-0.34586	-0.00729
2	No	Show	2	N	1			3.17667			1.675857	-0.70914	-0.12456
3	No	Show	3	C	2	1		1.486977	61.97062		1.139753	0.593237	0.352409
4	No	Show	4	C	3	2	1	1.514643	110.8635	-31.0018	-0.18269	0.909197	-0.31503
5	No	Show	5	H	3	2	1	1.096168	107.1434	91.15394	1.037777	0.52133	1.441452
6	No	Show	6	H	3	2	1	1.095845	107.2917	-151.73	1.884288	1.360127	0.1107
7	No	Show	7	H	4	3	2	1.096355	108.948	-177.614	-0.52756	1.892474	0.025891
8	No	Show	8	H	4	3	2	1.099432	110.6979	-59.0279	-0.0665	0.950463	-1.40752
9	No	Show	9	H	2	1	4	1.02748	148.011	117.0096	2.542744	-0.96224	0.365506
10	No	Show	10	H	2	1	4	1.029264	103.2688	-76.3357	1.87948	-0.68166	-1.13311
11	No	Show	11	H	2	1	4	1.030716	54.31611	-178.544	0.989409	-1.46169	0.033025
12	No	Show	12	H	1	4	3	1.355046	96.12336	64.90359	-1.56836	-0.13563	1.328283

3-SULFANYLPROPYLAZANIUM (no. 169)

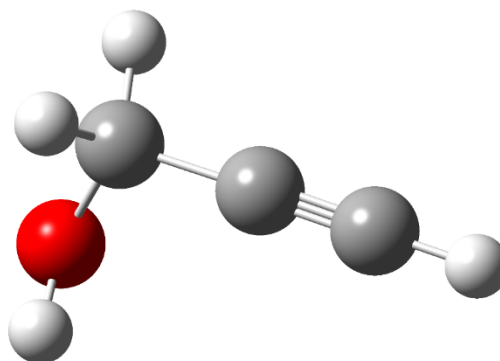
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							1.669217	-0.46987	-0.26338
2	No	Show	2	N	1			3.564966			-1.80687	-0.86246	0.423412
3	No	Show	3	C	2	1		2.486309	50.80817		-0.54354	1.19794	-0.16009
4	No	Show	4	C	2	1	3	1.491304	62.49253	39.52355	-1.42283	0.070496	-0.67481
5	No	Show	5	C	3	2	1	1.525247	91.79634	-37.8106	0.658403	0.75281	0.666695
6	No	Show	6	H	3	2	1	1.100806	95.74173	-145.851	-1.1463	1.876745	0.46255
7	No	Show	7	H	3	2	1	1.09974	140.6232	88.01183	-0.21155	1.771683	-1.0376
8	No	Show	8	H	4	2	1	1.096227	106.29	62.83924	-0.92162	-0.53953	-1.43532
9	No	Show	9	H	4	2	1	1.094723	106.9952	178.6659	-2.35177	0.463314	-1.10046
10	No	Show	10	H	5	3	2	1.099102	111.0181	-40.7246	0.338025	0.294295	1.612817
11	No	Show	11	H	5	3	2	1.096601	109.4474	-159.692	1.278438	1.62447	0.908147
12	No	Show	12	H	2	1	5	1.02754	130.8893	172.4565	-2.48214	-1.5643	0.095887
13	No	Show	13	H	2	1	5	1.029318	119.9413	-22.7989	-2.23455	-0.35941	1.213044
14	No	Show	14	H	2	1	5	1.029571	49.2948	-110.731	-0.98906	-1.3721	0.785989
15	No	Show	15	H	1	5	3	1.352547	96.1416	-173.124	2.508935	-0.76744	0.75432

ALKYNE

ACETYLENE (no. 170)



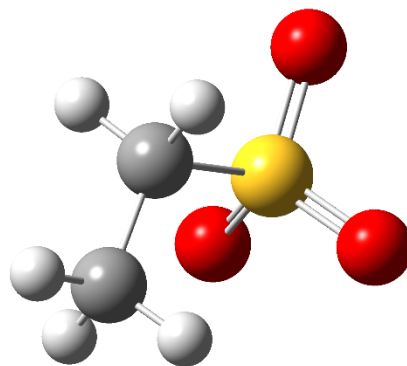
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0	0	0.604439
2	No	Show	2	C	1			1.208878			0	0	-0.60444
3	No	Show	3	H	1	2		1.076971	180		0	0	1.68141
4	No	Show	4	H	3	2		3.36282	0		0	0	-1.68141

PROPARGYL ALCOHOL (no. 171)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.53781	-0.49333	-0.11715
2	No	Show	2	C	1			1.415151			-0.63414	0.585195	0.033896
3	No	Show	3	C	2	1		1.473934	112.6837		0.77513	0.154479	0.00355
4	No	Show	4	C	3	2	1	1.211271	179.0604	-30.6158	1.927936	-0.21691	-0.01347
5	No	Show	5	H	2	1	3	1.098296	106.8999	119.6767	-0.81523	1.273046	-0.80296
6	No	Show	6	H	2	1	3	1.101802	111.8466	-122.918	-0.81433	1.143538	0.9665
7	No	Show	7	H	1	2	3	0.969444	107.089	65.20742	-1.43489	-1.06233	0.660972
8	No	Show	8	H	4	3	2	1.076554	179.7949	162.0685	2.953373	-0.54422	-0.03115

SULFATE

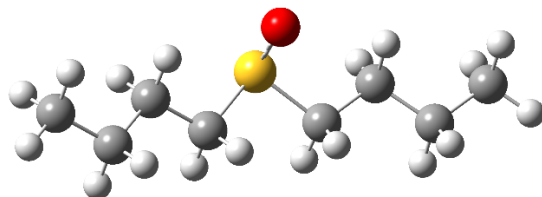
ETHANESULFONATE (no. 172)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0.467838	0.221589	0
2	No	Show	2	O	1			1.500481			0.87995	1.664366	0
3	No	Show	3	O	1	2		1.502323	112.8816		0.87995	-0.50363	1.249476
4	No	Show	4	O	1	2	3	1.502323	112.8816	-129.039	0.87995	-0.50363	-1.24948
5	No	Show	5	C	1	2	3	1.795159	105.8346	115.4805	-1.32732	0.224933	0
6	No	Show	6	C	5	1	2	1.517063	111.5041	180	-1.88605	-1.18549	0
7	No	Show	7	H	5	1	2	1.098932	105.6501	57.56995	-1.62271	0.79296	-0.89316
8	No	Show	8	H	5	1	2	1.098932	105.6501	-57.57	-1.62271	0.79296	0.893163
9	No	Show	9	H	6	5	1	1.09846	110.4007	180	-2.98427	-1.16229	0
10	No	Show	10	H	6	5	1	1.098912	110.3734	-59.9357	-1.54715	-1.73125	-0.89157
11	No	Show	11	H	6	5	1	1.098912	110.3734	59.93568	-1.54715	-1.73125	0.891573

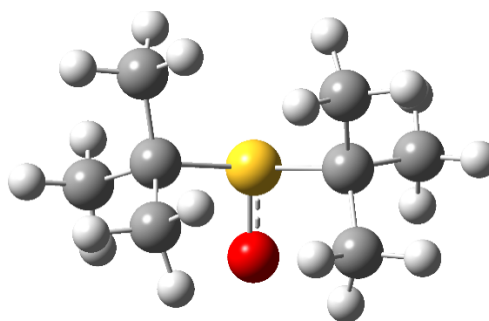
SULFOXIDE

DIBUTYL SULPHOXIDE (no. 173)

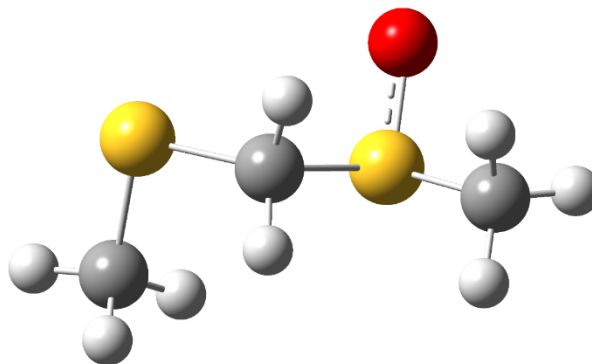


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0	0.500369	-0.53647
2	No	Show	2	O	1			1.552209			0	1.573288	0.585222
3	No	Show	3	C	1	2		1.818498	104.6885		-1.36977	-0.6159	-0.10682
4	No	Show	4	C	1	2	3	1.818498	104.6884	-102.282	1.36977	-0.6159	-0.10682
5	No	Show	5	C	3	1	2	1.520552	110.0049	65.11737	-2.69353	0.127021	-0.19522
6	No	Show	6	C	4	1	2	1.520551	110.005	-65.1176	2.693525	0.127019	-0.19523
7	No	Show	7	C	5	3	1	1.526045	111.8439	-174.49	-3.85964	-0.73129	0.286744
8	No	Show	8	C	6	4	1	1.526045	111.844	174.4895	3.85964	-0.73129	0.286747
9	No	Show	9	C	7	5	3	1.523331	112.0352	179.9944	-5.1882	0.008958	0.200156
10	No	Show	10	C	8	6	4	1.52333	112.0352	-179.994	5.188201	0.008958	0.200154
11	No	Show	11	H	3	1	2	1.101089	105.8856	-55.6122	-1.16656	-0.96153	0.91868
12	No	Show	12	H	3	1	2	1.100781	107.0199	-172.426	-1.31941	-1.46944	-0.80011
13	No	Show	13	H	4	1	2	1.100781	107.0199	172.4257	1.319406	-1.46945	-0.80011
14	No	Show	14	H	4	1	2	1.101089	105.8855	55.61201	1.166563	-0.96152	0.918682
15	No	Show	15	H	5	3	1	1.102808	109.6538	63.57554	-2.87137	0.445447	-1.23598
16	No	Show	16	H	5	3	1	1.102119	108.556	-53.2422	-2.62478	1.040305	0.417844
17	No	Show	17	H	6	4	1	1.102121	108.5559	53.24205	2.62478	1.040308	0.417837
18	No	Show	18	H	6	4	1	1.102808	109.6538	-63.5757	2.871368	0.44544	-1.23598
19	No	Show	19	H	7	5	3	1.102408	109.0025	58.09993	-3.6701	-1.04282	1.327094
20	No	Show	20	H	7	5	3	1.102435	109.1855	-57.9552	-3.90319	-1.65408	-0.31485
21	No	Show	21	H	8	6	4	1.102434	109.1855	57.95506	3.903184	-1.65409	-0.31484
22	No	Show	22	H	8	6	4	1.102408	109.0024	-58.1	3.670101	-1.04281	1.3271
23	No	Show	23	H	9	7	5	1.099362	111.4307	-179.422	-6.01952	-0.61446	0.559116
24	No	Show	24	H	9	7	5	1.100938	110.8063	-59.2006	-5.165	0.926474	0.808178
25	No	Show	25	H	9	7	5	1.10091	110.9016	60.33951	-5.40799	0.301281	-0.83823
26	No	Show	26	H	10	8	6	1.099363	111.4306	179.4222	6.019519	-0.61446	0.559119
27	No	Show	27	H	10	8	6	1.10091	110.9016	-60.3395	5.407994	0.301273	-0.83823
28	No	Show	28	H	10	8	6	1.100938	110.8063	59.20063	5.165003	0.926478	0.808169

DI-TERT-BUTYL SULFOXIDE (no. 174)



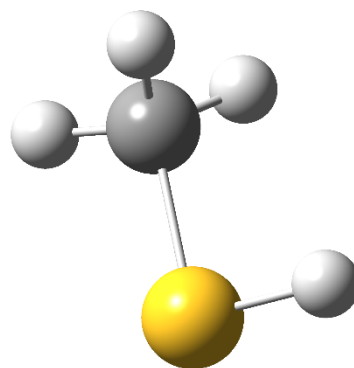
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.00372	-0.62036	-0.61635
2	No	Show	2	O	1			1.556624			0.014479	-1.9904	0.122386
3	No	Show	3	C	1	2		1.881582	103.4995		1.53872	0.24526	0.025482
4	No	Show	4	C	1	2	3	1.87336	104.384	-115.239	-1.53899	0.236628	0.030176
5	No	Show	5	C	3	1	2	1.521804	111.0091	-37.6999	1.757394	-0.053	1.501663
6	No	Show	6	C	3	1	2	1.532179	101.1546	78.71993	2.629278	-0.43582	-0.80782
7	No	Show	7	C	3	1	2	1.521584	111.0345	-164.075	1.493437	1.736128	-0.27532
8	No	Show	8	C	4	1	2	1.525556	109.1898	-172.037	-1.77458	1.514154	-0.76967
9	No	Show	9	C	4	1	2	1.531229	102.1885	-56.1136	-2.63734	-0.77987	-0.29389
10	No	Show	10	C	4	1	2	1.520158	112.1717	61.8239	-1.47356	0.476496	1.529864
11	No	Show	11	H	5	3	1	1.098629	110.3489	42.44798	1.568913	-1.11534	1.70878
12	No	Show	12	H	5	3	1	1.100992	108.2806	160.9307	2.80787	0.167607	1.746647
13	No	Show	13	H	5	3	1	1.096199	112.3726	-79.7644	1.120809	0.56024	2.150007
14	No	Show	14	H	6	3	1	1.099907	111.3535	63.94894	2.509117	-0.21827	-1.87928
15	No	Show	15	H	6	3	1	1.100028	110.6974	-57.2984	2.606513	-1.52584	-0.66156
16	No	Show	16	H	6	3	1	1.100139	108.8203	-176.437	3.610908	-0.06057	-0.4824
17	No	Show	17	H	7	3	1	1.098121	111.8114	76.41305	0.816784	2.269375	0.40561
18	No	Show	18	H	7	3	1	1.101428	108.0708	-165.003	2.506592	2.144216	-0.13346
19	No	Show	19	H	7	3	1	1.101106	111.907	-46.598	1.19478	1.936364	-1.31606
20	No	Show	20	H	8	4	1	1.100769	111.3413	47.73239	-1.69996	1.328579	-1.85211
21	No	Show	21	H	8	4	1	1.101174	108.0845	165.879	-2.79669	1.865648	-0.55916
22	No	Show	22	H	8	4	1	1.096025	112.7477	-75.1529	-1.0821	2.318725	-0.49688
23	No	Show	23	H	9	4	1	1.097315	111.0397	61.93482	-2.46828	-1.72523	0.236967
24	No	Show	24	H	9	4	1	1.101051	111.4011	-59.518	-2.68967	-0.98401	-1.37459
25	No	Show	25	H	9	4	1	1.100101	108.2371	-178.387	-3.60213	-0.35718	0.023511
26	No	Show	26	H	10	4	1	1.098121	111.7896	76.21049	-0.81231	1.316824	1.779796
27	No	Show	27	H	10	4	1	1.101373	108.7129	-164.565	-2.48482	0.717472	1.89361
28	No	Show	28	H	10	4	1	1.100228	110.4894	-46.0225	-1.12894	-0.42963	2.050133

METHYL (METHYLSULFINYL)METHYL SULFIDE (no. 175)

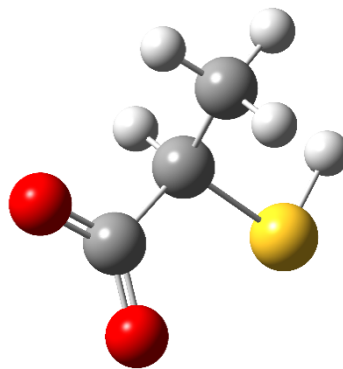
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							1.060414	0.00194	-0.48233
2	No	Show	2	S	1			3.006878			-1.75567	0.451651	0.470959
3	No	Show	3	O	1	2		1.542047	92.58446		1.434567	1.486338	-0.29664
4	No	Show	4	C	2	1	3	1.802145	34.49376	-113.382	-0.17657	-0.3414	0.824867
5	No	Show	5	C	1	3	4	1.806085	105.2718	-101.024	2.411962	-0.92748	0.273603
6	No	Show	6	C	2	1	3	1.816105	90.02733	140.7694	-2.36887	-0.69516	-0.79674
7	No	Show	7	H	4	2	1	1.099899	108.5453	116.2021	0.234691	0.094191	1.747309
8	No	Show	8	H	4	2	1	1.100472	111.5156	-121.836	-0.28672	-1.43137	0.929085
9	No	Show	9	H	5	1	3	1.098179	108.2066	52.5209	2.559146	-0.55003	1.29432
10	No	Show	10	H	5	1	3	1.097144	106.5019	-66.3888	3.301716	-0.73806	-0.33973
11	No	Show	11	H	5	1	3	1.097912	109.4185	174.3783	2.166505	-1.9976	0.268858
12	No	Show	12	H	6	2	1	1.097526	106.7884	-146.673	-3.35331	-0.32458	-1.10994
13	No	Show	13	H	6	2	1	1.098098	110.3226	94.47184	-2.47447	-1.70498	-0.37849
14	No	Show	14	H	6	2	1	1.098109	110.8883	-28.02	-1.69917	-0.71146	-1.66684

THIOL

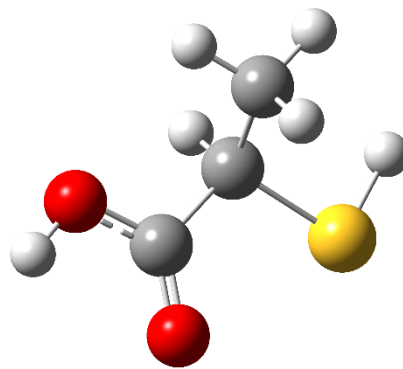
METHANETHIOL (no. 176)



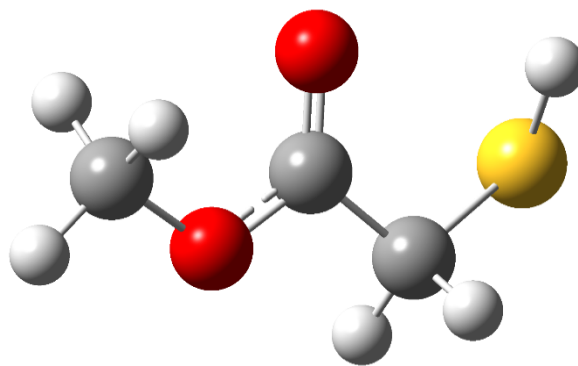
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.04861	-0.66675	0
2	No	Show	2	C	1			1.822794			-0.04861	1.156047	0
3	No	Show	3	H	2	1		1.097337	106.2648		-1.10203	1.463385	0
4	No	Show	4	H	2	1	3	1.096458	111.0105	118.4283	0.438661	1.549169	0.900132
5	No	Show	5	H	2	1	3	1.096458	111.0105	-118.428	0.438661	1.549169	-0.90013
6	No	Show	6	H	1	2	4	1.352725	96.93383	-61.5717	1.294217	-0.83005	0

THIOLACTATE (no. 177)

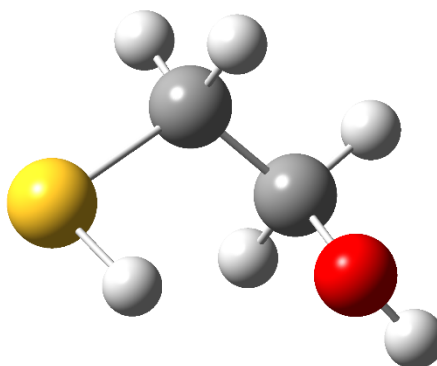
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							1.661148	-0.53588	-0.04607
2	No	Show	2	O	1			3.929564			-2.18638	0.223918	-0.29252
3	No	Show	3	O	2	1		2.244128	44.92147		-0.95131	-1.50839	0.421493
4	No	Show	4	C	1	3	2	1.835665	57.72018	2.303777	0.164906	0.474155	-0.37888
5	No	Show	5	C	4	1	3	1.52429	112.442	121.8882	0.16155	1.783753	0.40112
6	No	Show	6	C	3	2	1	1.253853	26.7858	1.364648	-1.09555	-0.3565	-0.05232
7	No	Show	7	H	4	1	6	1.099958	108.0519	-116.106	0.134783	0.694019	-1.45622
8	No	Show	8	H	5	4	1	1.0995	109.1975	-179.688	-0.75667	2.341499	0.167265
9	No	Show	9	H	5	4	1	1.099431	111.3943	60.37017	1.02755	2.408558	0.139565
10	No	Show	10	H	5	4	1	1.100673	110.4778	-60.2599	0.187702	1.587173	1.48378
11	No	Show	11	H	1	4	5	1.35532	95.34975	-58.4222	2.544303	0.410139	-0.44854

2-MERCAPTOPROPIONIC ACID (no. 178)

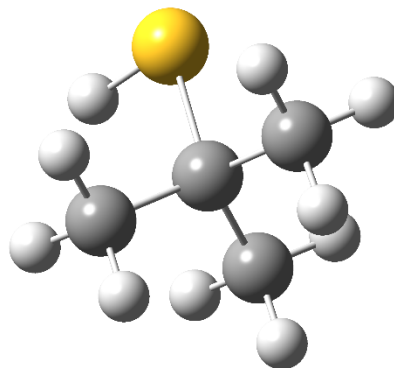
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							1.709281	-0.55296	-0.05459
2	No	Show	2	O	1			3.928743			-2.12102	0.277635	-0.32648
3	No	Show	3	O	2	1		2.241753	45.98331		-0.95849	-1.47655	0.446066
4	No	Show	4	C	1	3	2	1.832841	57.16072	3.800352	0.225548	0.47518	-0.37205
5	No	Show	5	C	4	1	3	1.527396	113.1318	120.6169	0.218894	1.780262	0.421457
6	No	Show	6	C	3	2	1	1.210648	29.97187	2.529655	-0.98527	-0.36554	-0.03415
7	No	Show	7	H	4	1	6	1.099388	108.9676	-115.153	0.166728	0.69522	-1.44759
8	No	Show	8	H	5	4	1	1.09891	109.9381	179.0309	-0.68172	2.361496	0.179263
9	No	Show	9	H	5	4	1	1.097965	109.8521	59.69243	1.101095	2.379658	0.160739
10	No	Show	10	H	5	4	1	1.099127	110.5304	-60.4091	0.236012	1.57503	1.501118
11	No	Show	11	H	1	4	6	1.353352	94.11069	177.0526	2.576079	0.390113	-0.49145
12	No	Show	12	H	2	1	4	0.976247	126.8895	-174.378	-2.86558	-0.30232	-0.07681

METHYL THIOGLYCOLATE (no. 179)

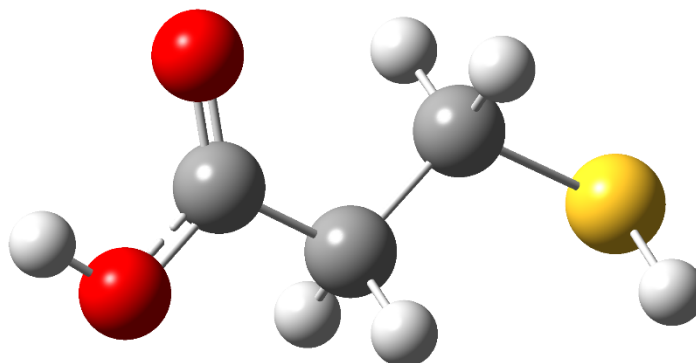
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							2.31798	0.049193	-0.15343
2	No	Show	2	O	1			3.952085			-1.56291	-0.68926	-0.04218
3	No	Show	3	O	2	1		2.243469	50.41036		-0.4757	1.268665	0.090667
4	No	Show	4	C	1	3	2	1.814746	52.44136	-14.8103	0.762414	-0.81276	0.207896
5	No	Show	5	C	3	2	1	1.210167	29.76956	-8.65616	-0.4617	0.058798	0.067622
6	No	Show	6	C	2	1	4	1.43531	138.4073	156.1114	-2.79683	0.041321	-0.10388
7	No	Show	7	H	4	1	5	1.097348	107.6998	121.2672	0.683567	-1.66221	-0.48232
8	No	Show	8	H	4	1	5	1.099918	111.183	-121.354	0.761212	-1.21889	1.230088
9	No	Show	9	H	6	2	1	1.097568	110.1742	51.64982	-2.80343	0.699649	-0.98207
10	No	Show	10	H	6	2	1	1.097661	110.1774	-69.5131	-2.929	0.638882	0.807335
11	No	Show	11	H	6	2	1	1.093863	105.6714	171.0559	-3.58376	-0.71413	-0.18499
12	No	Show	12	H	1	4	5	1.353355	95.55271	49.99976	2.069212	1.110222	0.649009

BETA-MERCAPTOETHANOL (no. 180)

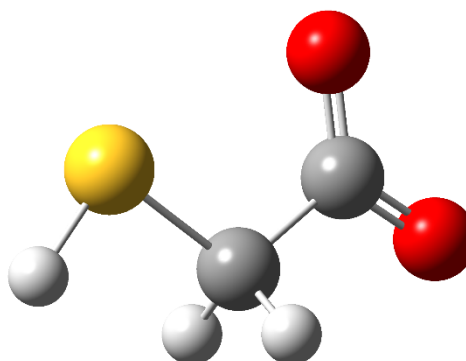
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.47353	-0.26031	-0.09325
2	No	Show	2	O	1			3.127195			1.595793	-0.76399	0.230632
3	No	Show	3	C	1	2		1.830315	49.09811		-0.10559	0.889518	0.302594
4	No	Show	4	C	2	1	3	1.419628	63.17303	-34.455	1.206446	0.481057	-0.32938
5	No	Show	5	H	3	1	4	1.098053	105.9194	120.5551	-0.41813	1.871389	-0.07684
6	No	Show	6	H	3	1	4	1.098923	109.3126	-122.905	0.005956	0.959756	1.393582
7	No	Show	7	H	4	2	1	1.104612	110.8003	151.7768	1.958449	1.260741	-0.11316
8	No	Show	8	H	4	2	1	1.102885	111.1836	-87.7033	1.088962	0.406628	-1.42346
9	No	Show	9	H	1	3	4	1.352619	95.01947	51.69961	-0.80469	-1.37405	0.283313
10	No	Show	10	H	2	1	3	0.968153	142.0423	-118.676	2.374478	-1.07109	-0.25584

2-METHYL-2-PROPANETHIOL (no. 181)

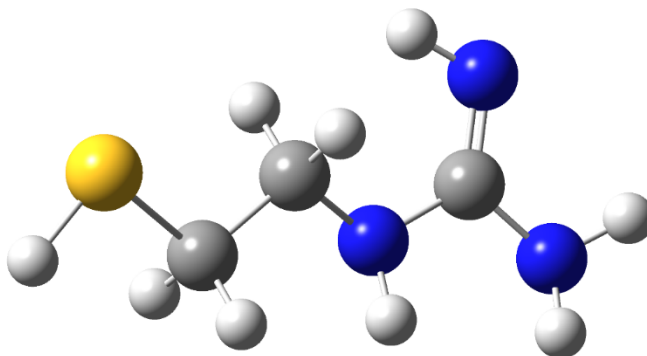
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.50427	-0.08711	0.000035
2	No	Show	2	C	1			1.857386			0.35087	0.004132	0.000002
3	No	Show	3	C	2	1		1.52739	105.7		0.835911	-1.4442	-0.0005
4	No	Show	4	C	2	1	3	1.525661	109.7667	119.1436	0.831822	0.728272	-1.25377
5	No	Show	5	C	2	1	3	1.525656	109.7672	-119.144	0.831918	0.72744	1.254213
6	No	Show	6	H	3	2	1	1.100156	111.255	60.69169	0.48661	-1.98146	-0.89475
7	No	Show	7	H	3	2	1	1.101023	109.0892	-179.999	1.936879	-1.45522	-0.00053
8	No	Show	8	H	3	2	1	1.100172	111.2574	-60.6908	0.486674	-1.98212	0.893396
9	No	Show	9	H	4	2	1	1.100434	111.0242	62.16859	0.462679	1.764679	-1.27719
10	No	Show	10	H	4	2	1	1.099252	111.073	-58.7505	0.489558	0.214023	-2.16303
11	No	Show	11	H	4	2	1	1.102366	109.4804	-178.552	1.933787	0.756868	-1.26188
12	No	Show	12	H	5	2	1	1.099254	111.0749	58.74593	0.489668	0.212662	2.163184
13	No	Show	13	H	5	2	1	1.10237	109.4816	178.5479	1.933889	0.755979	1.262311
14	No	Show	14	H	5	2	1	1.100436	111.0242	-62.1708	0.462813	1.763847	1.278322
15	No	Show	15	H	1	2	5	1.354514	96.23307	60.87905	-1.7173	1.250551	-5.6E-05

3-MERCAPTOPROPIONIC ACID (no. 182)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							2.54611	-0.11052	-0.0749
2	No	Show	2	O	1			5.153299			-2.54586	-0.90121	-0.01911
3	No	Show	3	O	2	1		2.240999	63.44594		-1.86284	1.232702	0.025472
4	No	Show	4	C	2	1	3	2.361465	0.478057	-63.8402	-0.21365	-0.53077	-0.02676
5	No	Show	5	C	4	2	1	1.51741	143.3967	119.1767	0.848172	0.551064	0.041908
6	No	Show	6	C	3	2	1	1.212811	30.22546	-0.61982	-1.60076	0.048872	-0.00223
7	No	Show	7	H	4	2	1	1.100532	90.14935	-8.9319	-0.11845	-1.13078	-0.94441
8	No	Show	8	H	4	2	1	1.101052	88.37689	-115.503	-0.13095	-1.23282	0.817401
9	No	Show	9	H	5	4	2	1.097282	110.9768	57.92133	0.748125	1.141895	0.961113
10	No	Show	10	H	5	4	2	1.098532	110.5222	-61.3447	0.751056	1.240486	-0.80782
11	No	Show	11	H	1	5	4	1.354169	96.42646	-62.2254	2.494958	-0.85916	1.052357
12	No	Show	12	H	2	1	5	0.975969	144.1818	6.041097	-3.41546	-0.45825	-0.00871

THIOGLYCOLATE (no. 183)

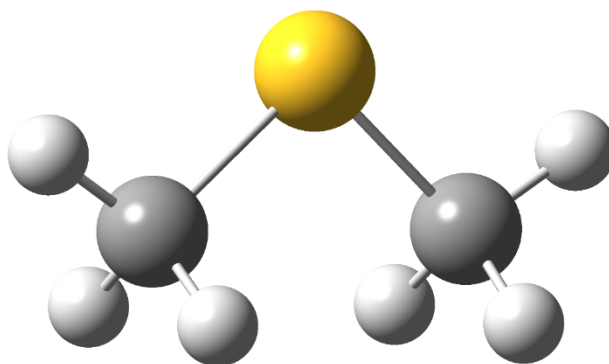
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.70509	0.147244	-1.2E-05
2	No	Show	2	O	1			3.941038			2.175168	-0.54224	-0.00016
3	No	Show	3	O	2	1		2.246718	45.4592		0.903742	1.310115	0.000014
4	No	Show	4	C	1	3	2	1.827253	56.66067	0.011985	-0.16634	-0.83819	0.000193
5	No	Show	5	C	3	2	1	1.253374	26.59157	0.015374	1.075437	0.068557	0.000064
6	No	Show	6	H	4	1	5	1.098864	110.3312	-120.532	-0.12711	-1.48507	-0.88723
7	No	Show	7	H	4	1	5	1.098877	110.3261	120.5235	-0.12716	-1.48462	0.887957
8	No	Show	8	H	1	4	5	1.354603	95.96457	179.9555	-2.55021	-0.9114	-0.0009

H2NC(=NH)NHCH2CH2SH (no. 184)

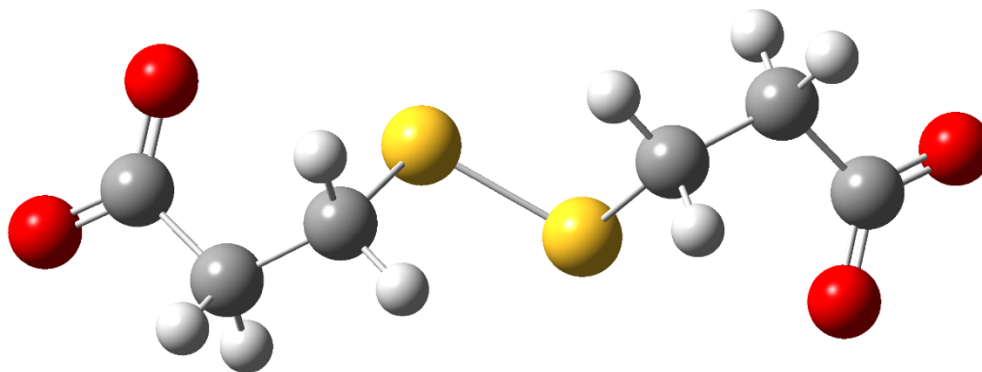
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							3.208763	-0.72853	0.066941
2	No	Show	2	H	1			1.017003			4.018268	-0.25601	0.461553
3	No	Show	3	H	1	2		1.018105	111.1835		3.010378	-1.59501	0.563314
4	No	Show	4	C	1	2	3	1.388446	111.1625	128.2621	2.122952	0.131635	-0.02746
5	No	Show	5	N	4	1	2	1.287243	120.0428	20.84944	2.30819	1.405478	-0.02965
6	No	Show	6	H	5	4	1	1.02254	109.6189	175.7819	1.41529	1.882012	-0.17536
7	No	Show	7	N	4	1	5	1.387457	113.476	175.2443	0.914354	-0.52271	-0.21761
8	No	Show	8	H	7	4	1	1.019139	113.1898	30.18181	0.888785	-1.44943	0.205691
9	No	Show	9	C	7	4	1	1.454336	118.1432	165.3696	-0.31299	0.229063	-0.00893
10	No	Show	10	H	9	7	4	1.100306	109.0916	65.5654	-0.38257	1.022435	-0.76813
11	No	Show	11	H	9	7	4	1.10541	111.6896	-53.0265	-0.32931	0.717521	0.982576
12	No	Show	12	C	9	7	4	1.518725	109.2392	-175.098	-1.50218	-0.70485	-0.15094
13	No	Show	13	H	12	9	7	1.098899	110.1579	60.50724	-1.44558	-1.50668	0.598364
14	No	Show	14	H	12	9	7	1.097515	110.0975	-59.8678	-1.51406	-1.15049	-1.15384
15	No	Show	15	S	12	9	7	1.831838	108.7449	-179.883	-3.03974	0.255882	0.110806
16	No	Show	16	H	15	12	9	1.352344	96.14468	178.4986	-3.89124	-0.77318	-0.10089

SULFIDE/DISULFIDE

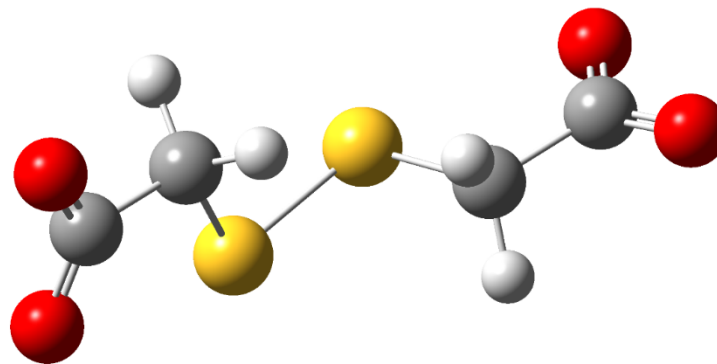
DIMETHYLSULFIDE (no. 185)



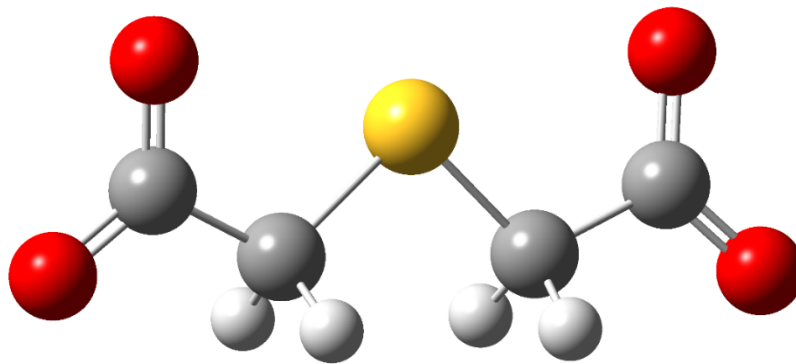
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0	0.667001	0
2	No	Show	2	C	1			1.813216			-1.37353	-0.51671	0
3	No	Show	3	C	1	2		1.813216	98.49003		1.373526	-0.51671	0
4	No	Show	4	H	2	1	3	1.09794	107.5574	179.9991	-2.30779	0.060021	0.000016
5	No	Show	5	H	2	1	3	1.098965	110.5947	60.91478	-1.33989	-1.14789	0.899007
6	No	Show	6	H	2	1	3	1.098964	110.5946	-60.9166	-1.33991	-1.14786	-0.89902
7	No	Show	7	H	3	1	2	1.09794	107.5574	-179.999	2.30779	0.060022	0.000012
8	No	Show	8	H	3	1	2	1.098965	110.5946	60.91637	1.339905	-1.14787	-0.89902
9	No	Show	9	H	3	1	2	1.098965	110.5947	-60.915	1.339892	-1.14788	0.899009

3,3'-DITHIODIPROPIONATE (no. 186)

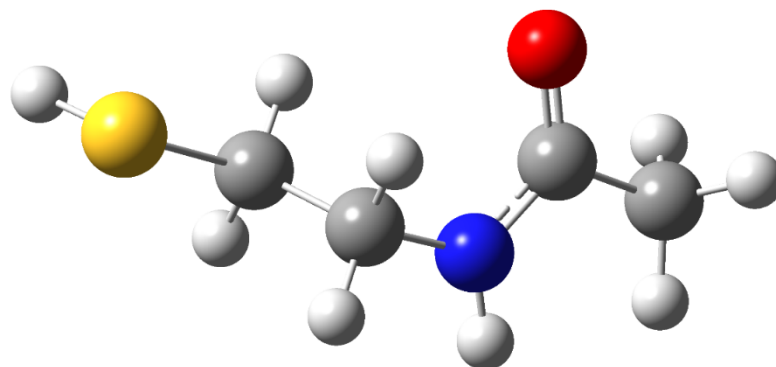
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0.898017	-0.52506	-0.32775
2	No	Show	2	S	1			2.080485			-0.89803	0.525007	-0.32732
3	No	Show	3	O	1	2		3.034038	163.5171		3.821507	-1.28907	-0.05411
4	No	Show	4	O	2	1	3	3.033581	163.5304	-142.894	-3.82095	1.2893	-0.05341
5	No	Show	5	O	3	1	2	2.243388	109.9556	-39.1192	5.122866	0.402125	-0.7463
6	No	Show	6	O	4	2	1	2.243391	109.972	-39.0947	-5.12312	-0.40097	-0.74633
7	No	Show	7	C	1	2	4	1.844276	102.8839	-114.237	1.869401	0.3211	0.992013
8	No	Show	8	C	2	1	7	1.844278	102.8854	-85.5739	-1.86946	-0.32222	0.991728
9	No	Show	9	C	7	1	2	1.51495	111.5992	-118.162	3.131746	0.9501	0.438916
10	No	Show	10	C	8	2	1	1.514947	111.5985	-118.177	-3.13198	-0.95043	0.438134
11	No	Show	11	C	5	3	1	1.259055	27.03188	37.05028	4.10388	-0.06774	-0.17523
12	No	Show	12	C	6	4	2	1.259054	27.03172	37.03988	-4.10383	0.068154	-0.17521
13	No	Show	13	H	7	1	2	1.097373	106.5736	4.613079	1.200823	1.063922	1.445275
14	No	Show	14	H	7	1	2	1.098035	106.8368	120.987	2.117168	-0.44098	1.742694
15	No	Show	15	H	8	2	1	1.097374	106.5741	4.597924	-1.201	-1.06562	1.444214
16	No	Show	16	H	8	2	1	1.098036	106.8372	120.9727	-2.11701	0.439187	1.743164
17	No	Show	17	H	9	7	1	1.10353	109.6525	178.0756	3.669286	1.475586	1.24681
18	No	Show	18	H	9	7	1	1.101213	110.9699	60.67623	2.892993	1.708377	-0.32311
19	No	Show	19	H	10	8	2	1.10353	109.6513	178.0882	-3.66966	-1.47639	1.24563
20	No	Show	20	H	10	8	2	1.101212	110.9707	60.68881	-2.89345	-1.70818	-0.32448

2,2'-DISULFANEDIYLDIACETATE (no. 187)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.94124	-1.02848	0.416439
2	No	Show	2	S	1			2.058598			0.941293	-1.02842	-0.41656
3	No	Show	3	O	1	2		3.936475	123.4604		-3.78658	1.474068	-0.64994
4	No	Show	4	O	2	1	3	3.936443	123.4609	80.69916	3.786296	1.474637	0.649399
5	No	Show	5	O	3	1	2	2.234841	45.85467	177.4851	-3.67402	-0.23422	0.786584
6	No	Show	6	O	4	2	1	2.234843	45.85317	177.4403	3.674238	-0.23469	-0.78593
7	No	Show	7	C	1	2	6	1.8198	101.1384	84.50118	-1.7314	0.33046	-0.50041
8	No	Show	8	C	2	1	7	1.819798	101.137	80.88398	1.731392	0.330437	0.500463
9	No	Show	9	C	5	3	1	1.252242	27.06357	-0.761	-3.18631	0.531362	-0.07605
10	No	Show	10	C	6	4	2	1.252244	27.0632	-0.78603	3.186277	0.531422	0.076092
11	No	Show	11	H	7	1	2	1.088608	109.2699	58.44959	-1.70189	0.109786	-1.566
12	No	Show	12	H	7	1	2	1.088953	109.5663	-60.1932	-1.1838	1.255299	-0.3254
13	No	Show	13	H	8	2	1	1.088615	109.2676	58.45686	1.701961	0.109535	1.566023
14	No	Show	14	H	8	2	1	1.088948	109.5689	-60.1857	1.183722	1.255273	0.325695

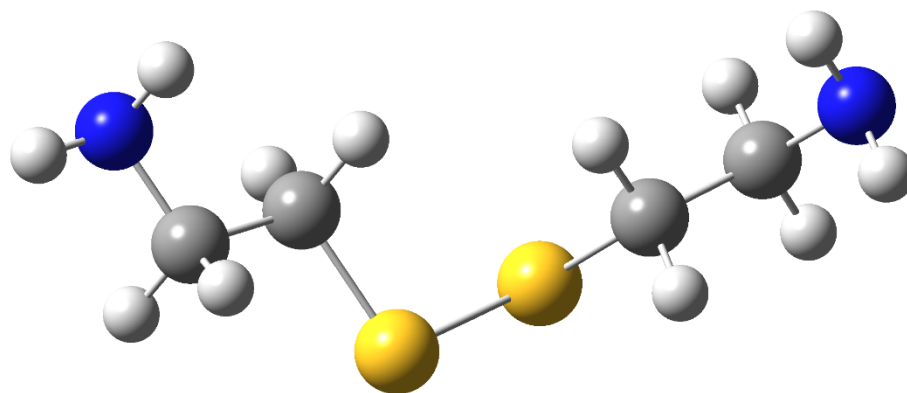
2,2'-SULFANEDIYLDIACETATE (no. 188)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.00022	0.527531	0.00025
2	No	Show	2	O	1			2.933241			-2.85188	1.193397	0.169198
3	No	Show	3	O	1	2		2.932687	153.7379		2.850604	1.194281	-0.1698
4	No	Show	4	O	2	1	3	2.232539	98.70359	170.4675	-3.69508	-0.84977	-0.14502
5	No	Show	5	O	3	1	2	2.23262	98.76342	170.9575	3.696504	-0.85015	0.129091
6	No	Show	6	C	1	3	5	1.811254	151.2392	-13.7967	-1.35084	-0.67927	0.00923
7	No	Show	7	C	1	6	4	1.811174	96.4651	-173.703	1.350961	-0.67855	0.005614
8	No	Show	8	C	2	1	7	1.252408	71.44651	-13.0598	-2.74035	-0.04362	0.008318
9	No	Show	9	C	3	1	7	1.252367	71.49021	-4.05078	2.740479	-0.04305	-0.01069
10	No	Show	10	H	6	1	7	1.089631	109.7103	-58.4107	-1.26802	-1.33	-0.86082
11	No	Show	11	H	6	1	7	1.091253	109.6486	59.42037	-1.27491	-1.30836	0.897666
12	No	Show	12	H	7	1	6	1.089739	109.7112	-58.8574	1.273025	-1.31389	0.88755
13	No	Show	13	H	7	1	6	1.091154	109.6493	58.96296	1.270686	-1.32338	-0.87096

N-ACETYLCYSTEAMINE (no. 189)

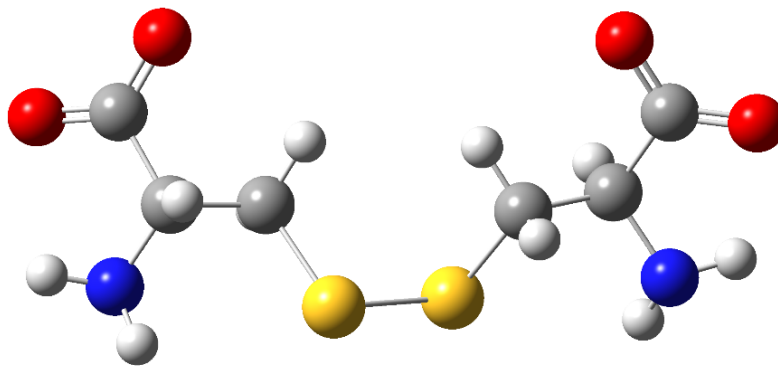
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-2.91336	0.171317	0.032491
2	No	Show	2	O	1			4.660359			1.583407	1.366026	0.298443
3	No	Show	3	N	2	1		2.254921	60.30028		1.009714	-0.81288	0.209379
4	No	Show	4	C	3	2	1	1.450476	94.77178	-18.5389	-0.36824	-0.59108	0.604245
5	No	Show	5	C	4	3	2	1.521731	111.5135	81.61559	-1.22328	-0.15287	-0.57582
6	No	Show	6	C	2	1	5	1.237081	88.99913	-32.0765	1.887326	0.189972	0.064134
7	No	Show	7	C	6	2	1	1.500314	121.223	162.9495	3.269532	-0.18122	-0.38605
8	No	Show	8	H	4	3	2	1.087751	107.9522	-157.037	-0.75033	-1.51911	1.023739
9	No	Show	9	H	4	3	2	1.089404	108.5422	-40.028	-0.38684	0.167692	1.385733
10	No	Show	10	H	5	4	3	1.087113	110.1274	-57.9002	-0.81666	0.75416	-1.01602
11	No	Show	11	H	5	4	3	1.087211	110.1364	63.01322	-1.25577	-0.93849	-1.32666
12	No	Show	12	H	3	2	1	1.007552	146.1786	155.6176	1.302025	-1.7462	-0.03275
13	No	Show	13	H	7	6	2	1.089209	108.4295	-58.2015	3.489581	0.360748	-1.30487
14	No	Show	14	H	7	6	2	1.089292	108.3979	58.69876	3.978088	0.14609	0.373801
15	No	Show	15	H	7	6	2	1.086837	112.7625	-179.765	3.384038	-1.24859	-0.55583
16	No	Show	16	H	1	5	4	1.340696	96.73895	-176.889	-3.45767	0.455676	-1.15928

CYSTAMINE (no. 190)

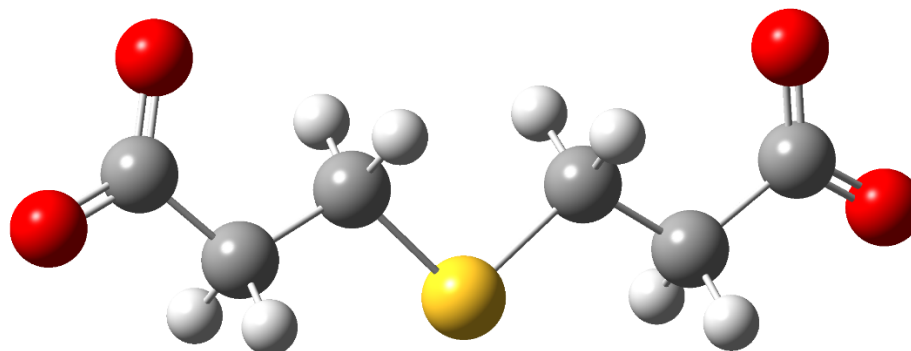


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.88736	-1.11994	0.513694
2	No	Show	2	S	1			2.049621			0.895649	-1.13028	-0.4971
3	No	Show	3	N	1	2		4.04779	123.1201		-3.92127	1.406495	-0.37915
4	No	Show	4	N	2	1	3	4.086034	124.5015	82.49223	3.996383	1.422759	0.253309
5	No	Show	5	C	1	2	4	1.823595	102.2253	82.95867	-1.81211	0.194553	-0.34796
6	No	Show	6	C	2	1	5	1.825552	102.4328	83.11434	1.815022	0.222407	0.313845
7	No	Show	7	C	3	1	5	1.464297	20.54325	178.6	-3.1764	0.343803	0.299105
8	No	Show	8	C	4	2	1	1.461291	18.21688	-177.913	3.180627	0.367409	-0.34347
9	No	Show	9	H	5	1	2	1.090003	108.483	-59.1293	-1.24857	1.123985	-0.26621
10	No	Show	10	H	5	1	2	1.088012	108.65	59.70649	-1.90876	-0.07825	-1.39677
11	No	Show	11	H	6	2	1	1.089629	108.6203	-58.64	1.243278	1.143936	0.208092
12	No	Show	12	H	6	2	1	1.089027	108.4635	60.22156	1.922104	-0.01839	1.370505
13	No	Show	13	H	7	3	1	1.089731	108.3833	-120.039	-3.73374	-0.58682	0.195035
14	No	Show	14	H	7	3	1	1.094125	112.8166	121.2116	-3.05029	0.530881	1.369715
15	No	Show	15	H	8	4	2	1.089898	108.5045	-121.088	3.724717	-0.57405	-0.26933
16	No	Show	16	H	8	4	2	1.089684	108.5297	122.7727	3.05575	0.584176	-1.40405
17	No	Show	17	H	3	1	5	1.014741	99.4822	-62.8597	-3.46005	2.292092	-0.19834
18	No	Show	18	H	3	1	5	1.013723	129.4424	177.1966	-4.84185	1.480542	0.038807
19	No	Show	19	H	4	2	1	1.014865	98.23172	55.02159	4.10596	1.231077	1.243865
20	No	Show	20	H	4	2	1	1.014885	98.70592	-52.5266	3.490237	2.300487	0.194983

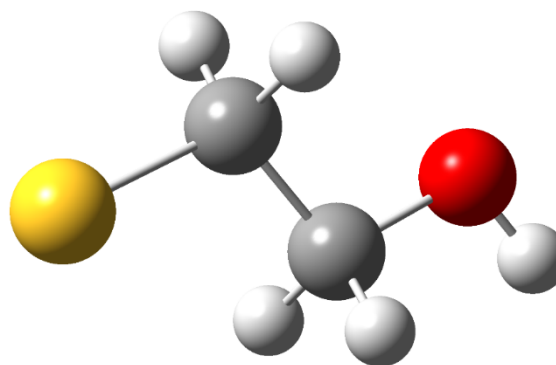
L-CYSTINE ANION (no. 191)



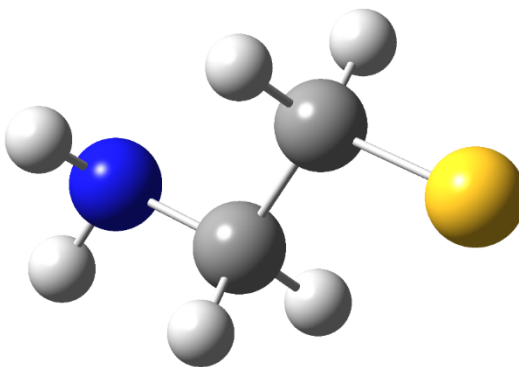
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0.864458	-1.48703	-0.464
2	No	Show	2	S	1			2.046755			-0.87983	-1.4517	0.606242
3	No	Show	3	O	1	2		4.539527	110.5835		3.264986	2.295032	0.27137
4	No	Show	4	O	2	1	3	4.537057	113.2792	51.86183	-3.29347	2.338114	-0.02347
5	No	Show	5	O	3	1	2	2.230551	90.32778	140.1724	5.151476	1.105482	0.309865
6	No	Show	6	O	4	2	1	2.23082	89.80158	123.7747	-5.04261	1.10897	-0.66086
7	No	Show	7	N	5	3	1	2.677437	94.27625	4.808374	3.948795	-1.19716	-0.33825
8	No	Show	8	N	6	4	2	2.680557	94.4212	11.33092	-3.96893	-1.21147	0.144231
9	No	Show	9	C	7	5	3	1.459453	62.99226	9.763808	3.148465	0.019276	-0.43701
10	No	Show	10	C	8	6	4	1.458803	63.07931	2.8304	-3.19818	-0.00093	0.406262
11	No	Show	11	C	9	7	5	1.521748	110.8458	-128.816	1.829613	-0.13845	0.305605
12	No	Show	12	C	10	8	6	1.523177	110.7202	-123.72	-1.80812	-0.10361	-0.20795
13	No	Show	13	C	5	3	1	1.253212	27.28889	9.238995	3.921673	1.237009	0.107812
14	No	Show	14	C	6	4	2	1.252603	27.28783	12.00736	-3.90707	1.249046	-0.15101
15	No	Show	15	H	9	7	5	1.097663	112.2602	110.4612	2.919847	0.283257	-1.47764
16	No	Show	16	H	10	8	6	1.096811	112.479	115.2312	-3.08277	0.198849	1.478531
17	No	Show	17	H	11	9	7	1.089206	110.5724	57.26961	2.006403	-0.39215	1.349995
18	No	Show	18	H	11	9	7	1.086049	110.4269	179.345	1.244764	0.774141	0.237487
19	No	Show	19	H	12	10	8	1.089134	110.3108	54.65853	-1.88019	-0.33253	-1.27032
20	No	Show	20	H	12	10	8	1.086278	110.4396	176.6383	-1.25929	0.822301	-0.06139
21	No	Show	21	H	7	5	3	1.012866	56.87269	148.4838	4.899005	-0.97374	-0.60859
22	No	Show	22	H	7	5	3	1.013381	153.7737	90.18147	3.606343	-1.89118	-0.99247
23	No	Show	23	H	8	6	4	1.01287	60.15341	137.3758	-4.94555	-1.01684	0.329269
24	No	Show	24	H	8	6	4	1.013259	158.3953	78.64257	-3.68298	-1.94688	0.779913

3,3'-THIODIPROPANOATE (no. 192)

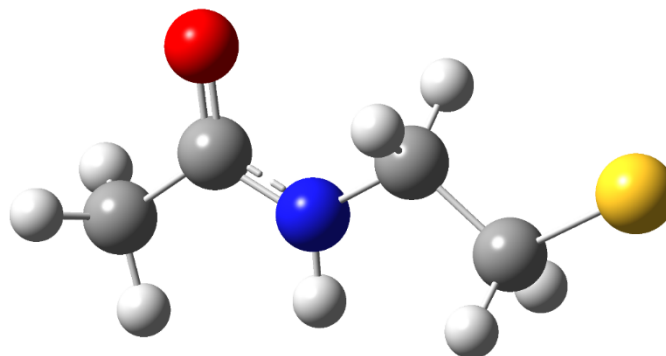
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0.000001	-1.07726	-1E-06
2	No	Show	2	O	1			4.561916			-3.7209	1.556324	-0.17393
3	No	Show	3	O	1	2		4.561911	109.4787		3.720893	1.556322	0.173942
4	No	Show	4	O	2	1	3	2.242764	91.40841	-171.137	-5.05949	-0.22074	0.109295
5	No	Show	5	O	3	1	2	2.242765	91.40844	-171.136	5.059486	-0.22073	-0.10935
6	No	Show	6	C	1	3	5	1.824364	103.9865	-173.239	-1.38285	0.112708	0.000387
7	No	Show	7	C	1	6	2	1.824362	98.57528	157.8923	1.382857	0.112703	-0.00039
8	No	Show	8	C	6	1	7	1.51749	110.7333	-178.391	-2.71539	-0.61222	0.04062
9	No	Show	9	C	7	1	6	1.517489	110.7333	-178.392	2.715389	-0.61222	-0.04058
10	No	Show	10	C	2	1	7	1.258742	64.3778	-173.293	-3.93181	0.326283	-0.00978
11	No	Show	11	C	3	1	7	1.258743	64.37788	-150.739	3.931812	0.326283	0.009775
12	No	Show	12	H	6	1	7	1.100368	108.6627	-56.7742	-1.27692	0.775369	0.872434
13	No	Show	13	H	6	1	7	1.099606	108.696	60.22257	-1.31288	0.734712	-0.90369
14	No	Show	14	H	7	1	6	1.100369	108.6627	-56.7764	1.276942	0.775339	-0.87246
15	No	Show	15	H	7	1	6	1.099606	108.6961	60.22019	1.312858	0.734736	0.903662
16	No	Show	16	H	8	6	1	1.101571	110.9059	60.33508	-2.80043	-1.22826	0.949859
17	No	Show	17	H	8	6	1	1.102799	110.5205	-57.0204	-2.80218	-1.3091	-0.80967
18	No	Show	18	H	9	7	1	1.10157	110.9058	60.3333	2.800437	-1.22831	-0.94979
19	No	Show	19	H	9	7	1	1.1028	110.5207	-57.0223	2.802181	-1.30906	0.809747

S⁻**2-HYDROXYETHANETHIOLATE (no. 193)**

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.77086	-0.11944	0.000001
2	No	Show	2	O	1			4.053243			2.272382	0.165131	-0.00012
3	No	Show	3	C	2	1		1.436812	21.93889		0.980597	-0.46393	-0.00006
4	No	Show	4	C	3	2	1	1.510935	109.1222	-0.00532	-0.08942	0.602837	0.000058
5	No	Show	5	H	3	2	1	1.092487	109.7351	-120.541	0.877736	-1.09521	0.885623
6	No	Show	6	H	3	2	1	1.092492	109.7363	120.5304	0.877593	-1.09514	-0.88578
7	No	Show	7	H	4	3	2	1.092049	108.4287	-57.9835	0.053968	1.235523	0.878534
8	No	Show	8	H	4	3	2	1.092051	108.4293	57.97408	0.053942	1.235708	-0.87829
9	No	Show	9	H	2	1	4	0.9628	130.2369	179.9101	2.944368	-0.52437	0.00088

2-LAMBDA1-SULFANYLETHANAMINE (no. 194)

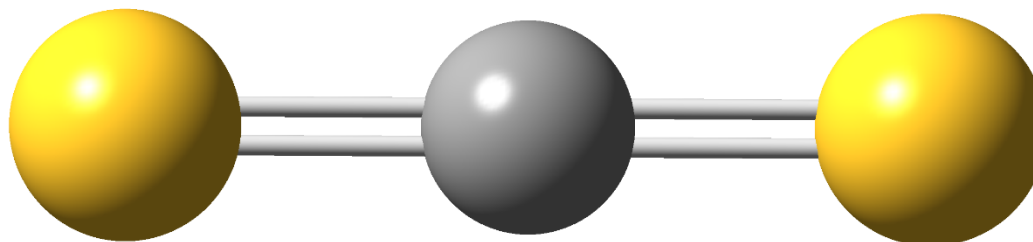
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-2.31911	0.122122	-0.07253
2	No	Show	2	C	1			1.471511			-0.9792	-0.48198	-0.00158
3	No	Show	3	C	2	1		1.516382	111.0872		0.102015	0.578803	-0.07319
4	No	Show	4	S	3	2	1	1.831332	113.2665	179.4834	1.796849	-0.10793	0.025332
5	No	Show	5	H	1	2	3	1.013971	109.2712	-178.701	-3.01944	-0.60763	-0.00081
6	No	Show	6	H	1	2	3	1.0149	108.372	-63.9362	-2.44887	0.709483	0.744903
7	No	Show	7	H	2	1	3	1.090444	108.2394	-119.95	-0.86821	-1.16603	-0.8435
8	No	Show	8	H	2	1	3	1.094447	112.431	122.0706	-0.83399	-1.0701	0.909933
9	No	Show	9	H	3	2	1	1.093776	108.2268	57.4107	-0.05975	1.287872	0.743757
10	No	Show	10	H	3	2	1	1.092173	108.4717	-58.0055	-0.02249	1.137572	-1.00331

2-ACETAMIDOETHANETHIOLATE (no. 195)

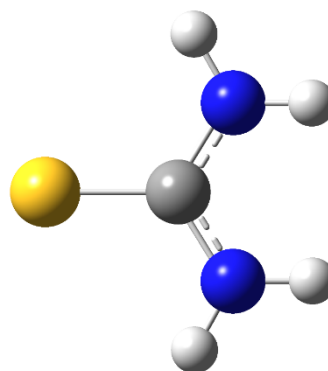
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							3.184489	0.165308	-7.3E-05
2	No	Show	2	O	1			5.466635			-2.14029	1.402596	-9.5E-05
3	No	Show	3	N	2	1		2.249605	42.32919		-0.8632	-0.44937	0.000181
4	No	Show	4	C	3	2	1	1.460694	94.87439	0.005004	0.405413	0.274676	0.000136
5	No	Show	5	C	4	3	2	1.516271	110.5904	-179.987	1.572123	-0.69376	-2.1E-05
6	No	Show	6	C	2	1	5	1.24171	72.59591	0.013094	-2.04669	0.164418	0.000234
7	No	Show	7	C	6	2	1	1.501308	120.9244	-179.969	-3.27277	-0.70199	-0.00017
8	No	Show	8	H	4	3	2	1.090972	109.2088	58.60165	0.45107	0.918864	0.879429
9	No	Show	9	H	4	3	2	1.09097	109.2089	-58.5757	0.450937	0.918991	-0.87907
10	No	Show	10	H	3	2	1	1.008627	146.7807	-179.977	-0.83908	-1.45771	0.000136
11	No	Show	11	H	5	4	3	1.092427	108.4863	-57.9126	1.487202	-1.33854	0.877728
12	No	Show	12	H	5	4	3	1.092427	108.4863	57.91313	1.487075	-1.33841	-0.87785
13	No	Show	13	H	7	6	2	1.087019	112.8574	179.9818	-3.03954	-1.7637	-0.00013
14	No	Show	14	H	7	6	2	1.089347	108.4758	-58.4765	-3.86688	-0.45985	0.880211
15	No	Show	15	H	7	6	2	1.08935	108.478	58.43931	-3.86638	-0.45981	-0.88088

CS

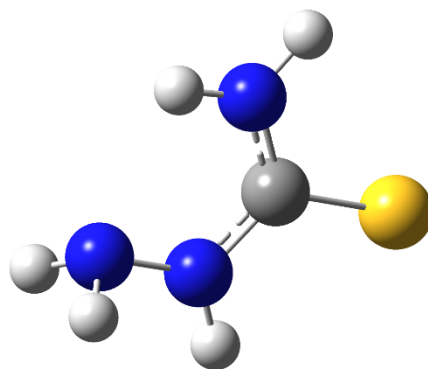
CARBON DISULFIDE (no. 196)



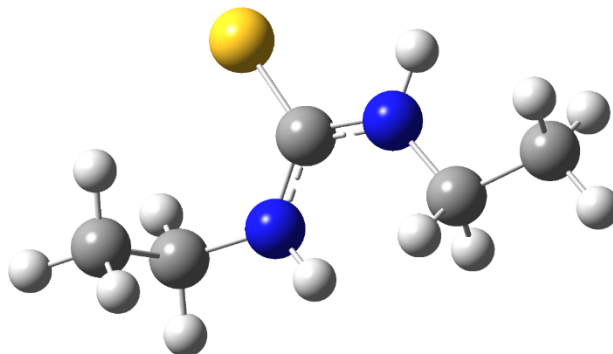
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0	0	1.561259
2	No	Show	2	S	1			3.122518			0	0	-1.56126
3	No	Show	3	C	1	2		1.561259	0		0	0	0

THIOUREA (no. 197)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-1.36553	0.000005	-2.4E-05
2	No	Show	2	N	1			2.66516			1.04352	1.139877	-0.0155
3	No	Show	3	N	2	1		2.279977	64.67595		1.043509	-1.13989	0.015469
4	No	Show	4	C	2	1	3	1.339953	32.97115	-0.01684	0.339312	0.000001	0.000196
5	No	Show	5	H	2	1	4	1.01524	154.2358	-8.41741	2.056688	1.137267	0.04927
6	No	Show	6	H	2	1	4	1.011576	85.751	-176.536	0.545059	2.018767	0.033223
7	No	Show	7	H	3	2	1	1.01524	89.80183	176.3319	2.056663	-1.13727	-0.04952
8	No	Show	8	H	3	2	1	1.011576	150.2349	6.969193	0.545023	-2.01875	-0.03353

THIOSEMICARBAZIDE (no. 198)

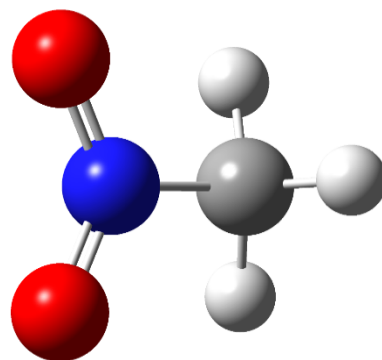
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							1.766626	-0.36033	-4.2E-05
2	No	Show	2	N	1			2.652453			-0.86466	-0.69475	-0.00011
3	No	Show	3	N	2	1		1.397246	154.4897		-2.19149	-0.25679	0.000004
4	No	Show	4	N	2	1	3	2.281739	65.21866	0.012942	-0.17708	1.480925	-6.3E-05
5	No	Show	5	C	4	2	1	1.334885	31.83469	-0.03394	0.152558	0.187381	0.000345
6	No	Show	6	H	2	1	5	1.016397	83.70928	-179.961	-0.6268	-1.68292	0.000006
7	No	Show	7	H	3	2	1	1.022622	108.4697	122.3655	-2.66189	-0.64811	-0.81935
8	No	Show	8	H	3	2	1	1.022626	108.4692	-122.356	-2.66183	-0.64837	0.819275
9	No	Show	9	H	4	2	1	1.010936	150.7014	0.010186	0.560306	2.172485	-0.00013
10	No	Show	10	H	4	2	1	1.015615	87.36688	-179.997	-1.15852	1.742159	-2.6E-05

N,N'-DIETHYLTHIOUREA (no. 199)

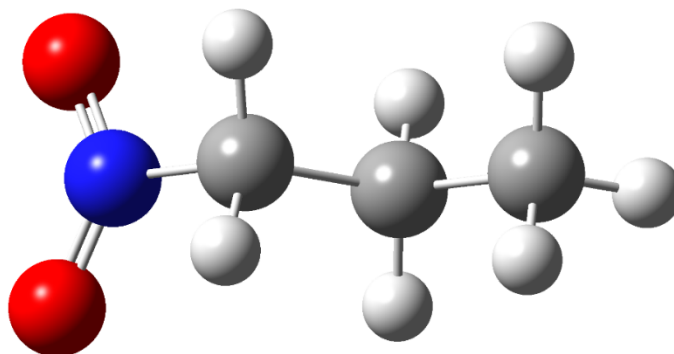
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.9013	1.873722	0.00942
2	No	Show	2	N	1			2.696088			-0.60899	-0.76596	-0.45484
3	No	Show	3	N	2	1		2.287079	63.77683		1.292666	0.380447	0.093071
4	No	Show	4	C	2	1	3	1.456494	92.64332	174.0185	-2.04524	-0.97101	-0.58333
5	No	Show	5	C	3	2	1	1.456648	93.66658	-177.395	2.151287	-0.78677	-0.05596
6	No	Show	6	C	2	1	3	1.345677	31.96686	0.658207	-0.03577	0.404725	-0.12051
7	No	Show	7	C	4	2	1	1.520925	112.9487	-84.8412	-2.73617	-1.18236	0.755006
8	No	Show	8	C	5	3	2	1.516078	109.8681	178.2869	3.594626	-0.40094	0.201729
9	No	Show	9	H	4	2	1	1.096637	107.7809	37.55815	-2.46341	-0.09788	-1.09849
10	No	Show	10	H	4	2	1	1.097706	106.7854	153.4314	-2.18379	-1.8464	-1.23099
11	No	Show	11	H	5	3	2	1.102633	109.6369	-60.6738	1.837491	-1.57058	0.653242
12	No	Show	12	H	5	3	2	1.102644	109.6503	56.90241	2.041452	-1.20057	-1.07209
13	No	Show	13	H	2	1	6	1.01606	149.402	11.28685	-0.03585	-1.60372	-0.40961
14	No	Show	14	H	3	2	1	1.014402	147.3777	-5.48009	1.722949	1.278269	0.287451
15	No	Show	15	H	7	4	2	1.100015	110.8258	-59.9087	-2.32946	-2.06519	1.270007
16	No	Show	16	H	7	4	2	1.099489	110.1477	60.53225	-2.595	-0.30129	1.397398
17	No	Show	17	H	7	4	2	1.099741	110.1264	-179.735	-3.81449	-1.33676	0.603962
18	No	Show	18	H	8	5	3	1.099583	110.6712	-60.3885	3.925203	0.365626	-0.51394
19	No	Show	19	H	8	5	3	1.099507	110.6759	60.05221	3.714622	-0.00464	1.220289
20	No	Show	20	H	8	5	3	1.097522	109.9806	179.8327	4.242927	-1.2798	0.092837

NITRO

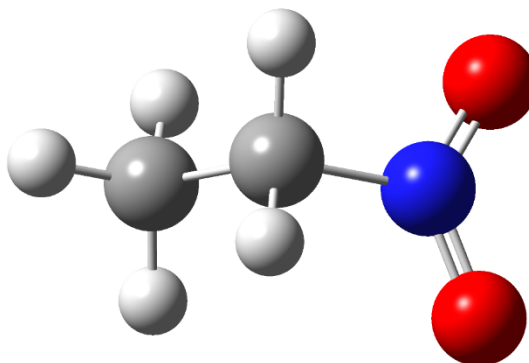
NITROMETHANE (no. 200)



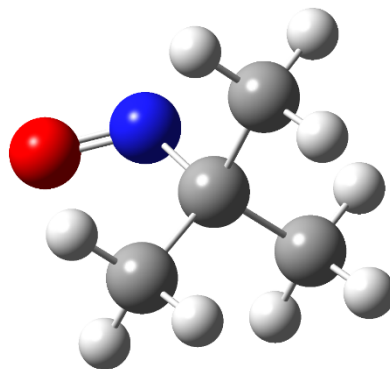
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.7273	1.073179	0.002304
2	No	Show	2	O	1			2.140418			-0.7388	-1.06721	0.002343
3	No	Show	3	N	2	1		1.213157	28.1092		-0.16161	-0.00023	-0.00985
4	No	Show	4	C	3	2	1	1.484327	118.198	178.319	1.322696	-0.00564	-0.00309
5	No	Show	5	H	4	3	2	1.082974	107.6506	149.2476	1.656728	0.872631	-0.54151
6	No	Show	6	H	4	3	2	1.08245	107.8402	26.68624	1.652982	-0.93381	-0.45154
7	No	Show	7	H	4	3	2	1.087641	105.7938	-92.2502	1.614163	0.048865	1.043352

1-NITROPROPANE (no. 201)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.70513	1.070369	-0.14406
2	No	Show	2	O	1			2.141174			-1.70444	-1.07081	-0.14318
3	No	Show	3	N	1	2		1.213994	28.13103		-1.18325	0.000048	0.092242
4	No	Show	4	C	3	1	2	2.449231	111.627	137.7757	1.189806	-0.00055	-0.51383
5	No	Show	5	C	3	1	2	1.493109	118.1005	177.0383	0.203825	0.000688	0.644865
6	No	Show	6	C	4	3	1	1.521108	144.9457	108.4323	2.612461	0.000183	0.02452
7	No	Show	7	H	4	3	1	1.090124	89.03487	-125.656	1.013864	-0.88409	-1.12765
8	No	Show	8	H	4	3	1	1.090127	89.03121	-17.4739	1.013718	0.881548	-1.12968
9	No	Show	9	H	5	3	1	1.085451	106.1104	31.94064	0.287214	0.899069	1.248323
10	No	Show	10	H	5	3	1	1.085458	106.1092	150.7682	0.287252	-0.8964	1.250249
11	No	Show	11	H	6	4	3	1.090174	110.884	-60.1008	2.796185	0.883922	0.635854
12	No	Show	12	H	6	4	3	1.090175	110.8839	60.11497	2.796361	-0.88218	0.637788
13	No	Show	13	H	6	4	3	1.088727	110.3699	-179.993	3.328124	-0.00064	-0.79594

NITROETHANE (no. 202)

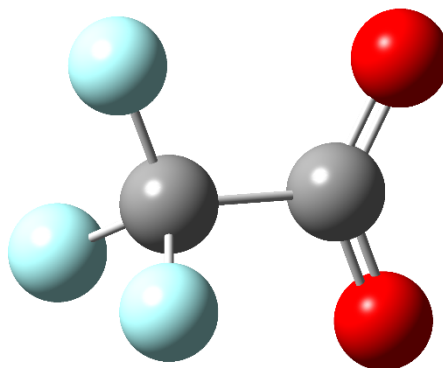
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.154087	-1.06028	-0.18321
2	No	Show	2	O	1			2.141143			1.124996	1.080529	-0.15922
3	No	Show	3	N	1	2		1.213607	28.1013		0.628159	0.000284	0.084073
4	No	Show	4	C	3	1	2	1.496513	118.1116	177.2002	-0.73816	-0.02411	0.694096
5	No	Show	5	C	4	3	1	1.515983	108.3037	-89.8782	-1.75997	0.00494	-0.4254
6	No	Show	6	H	4	3	1	1.08433	105.8129	30.94042	-0.7859	-0.93815	1.275482
7	No	Show	7	H	4	3	1	1.084545	105.7659	149.3903	-0.79362	0.854211	1.32791
8	No	Show	8	H	5	4	3	1.088285	110.7395	-60.9995	-1.65919	0.913665	-1.01568
9	No	Show	9	H	5	4	3	1.08834	110.7503	60.90974	-1.65039	-0.86499	-1.07014
10	No	Show	10	H	5	4	3	1.087977	108.1242	179.9551	-2.75189	-0.01369	0.021179

2-METHYL-2-NITROSOPROPANE (no. 203)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.95763	-0.00206	-0.19438
2	No	Show	2	N	1			1.194846			-0.92831	-0.00864	-0.80111
3	No	Show	3	C	2	1		1.493638	115.461		0.309677	0.000384	0.034512
4	No	Show	4	C	3	2	1	1.525831	104.4697	121.9603	1.063206	-1.25774	-0.38678
5	No	Show	5	C	3	2	1	1.525817	104.4662	-122.092	1.064772	1.247256	-0.41633
6	No	Show	6	C	3	2	1	1.511825	112.9213	-0.07052	0.018645	0.018156	1.517954
7	No	Show	7	H	4	3	2	1.089671	111.0091	55.18194	1.2294	-1.2714	-1.46362
8	No	Show	8	H	4	3	2	1.089664	108.6345	174.5185	2.030793	-1.26826	0.114248
9	No	Show	9	H	4	3	2	1.090217	110.8549	-66.152	0.512466	-2.15408	-0.10074
10	No	Show	10	H	5	3	2	1.090219	110.8592	66.13837	0.515125	2.150834	-0.15173
11	No	Show	11	H	5	3	2	1.089668	111.0064	-55.1947	1.231104	1.235172	-1.49316
12	No	Show	12	H	5	3	2	1.089667	108.6325	-174.528	2.032323	1.268414	0.084441
13	No	Show	13	H	6	3	2	1.089756	111.2082	60.58354	-0.54752	-0.86291	1.819206
14	No	Show	14	H	6	3	2	1.08948	108.7265	179.9968	0.963817	0.02385	2.059787
15	No	Show	15	H	6	3	2	1.089749	111.2064	-60.5915	-0.54615	0.906974	1.798236

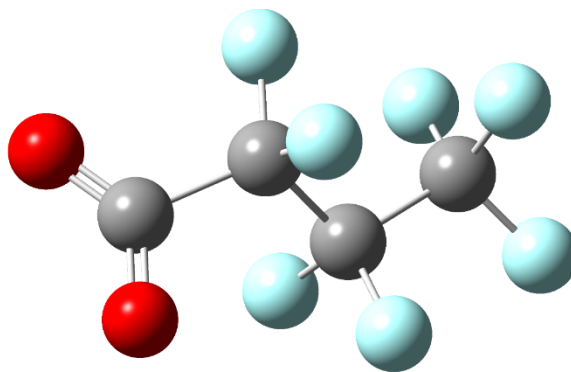
PFAS

TRIFLUOROACETATE (no. 204)



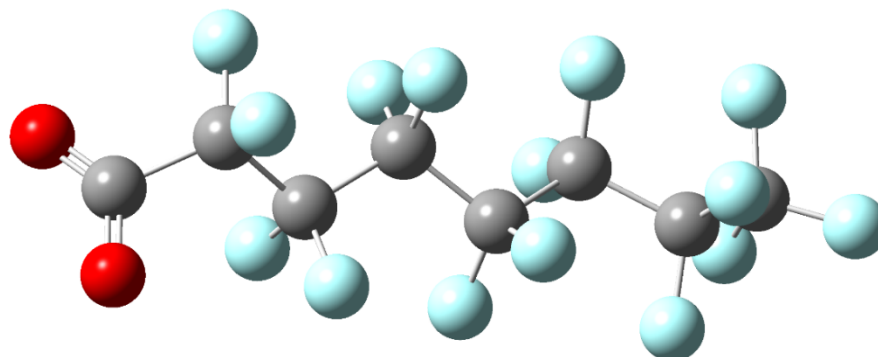
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							-1.05359	1.246161	0.000088
2	No	Show	2	F	1			2.160033			-1.01574	-0.62483	-1.07867
3	No	Show	3	F	2	1		2.157166	60.04542		-1.01596	-0.62509	1.078498
4	No	Show	4	O	2	1	3	2.800023	88.98026	-64.2536	1.516662	-1.13804	0.000066
5	No	Show	5	O	4	2	1	2.26309	80.86151	-28.4131	1.577689	1.124228	0.000134
6	No	Show	6	C	4	2	1	2.344402	28.64416	17.57747	-0.52454	0.015098	0.000027
7	No	Show	7	C	5	4	2	1.243974	24.74701	22.93849	1.026671	0.008948	-0.00017

PERFLUOROBUTANOIC ACID (no. 205)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							0.338468	-1.60151	0.695868
2	No	Show	2	F	1			2.188451			0.08015	-0.9515	-1.37779
3	No	Show	3	F	1	2		2.568868	93.79987		-0.7964	0.486429	1.671398
4	No	Show	4	F	3	1	2	2.184515	93.547	-19.1627	-0.52686	1.65293	-0.15582
5	No	Show	5	F	3	1	2	2.757164	65.26949	-82.9654	1.867241	0.811129	1.037731
6	No	Show	6	F	5	3	1	2.164506	103.5694	74.6276	1.863818	0.934228	-1.12327
7	No	Show	7	F	6	5	3	2.157786	59.99909	-108.294	2.63942	-0.82521	-0.14405
8	No	Show	8	O	4	3	1	2.627656	85.62332	90.49334	-2.87859	0.716507	-0.86082
9	No	Show	9	O	8	4	3	2.263111	91.35801	-32.8617	-2.48819	-1.23103	0.223785
10	No	Show	10	C	9	8	4	2.899063	84.39471	-23.1968	0.304579	-0.53108	-0.1155
11	No	Show	11	C	10	9	8	1.537508	53.64352	43.46505	-0.82703	0.417082	0.313897
12	No	Show	12	C	10	9	8	1.540175	166.6922	63.52439	1.701318	0.117364	-0.08758
13	No	Show	13	C	8	4	3	1.241631	66.71069	-32.4023	-2.22192	-0.07709	-0.16754

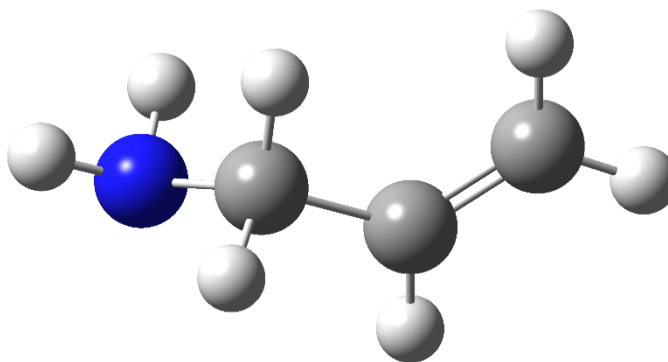
PERFLUOROCTANOIC ACID (no. 206)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	F							0.451591	-1.27009	1.119839
2	No	Show	2	F	1			2.187506			0.255382	-1.22582	-1.0584
3	No	Show	3	F	1	2		2.569948	93.6688		-0.98363	0.834924	1.457042
4	No	Show	4	F	3	1	2	2.188128	93.57895	-18.0011	-0.76758	1.482032	-0.62202
5	No	Show	5	F	2	1	3	2.573706	93.52256	71.22896	1.768157	0.840919	-1.31147
6	No	Show	6	F	5	2	1	2.185515	93.62986	-17.7989	1.578449	1.409443	0.790256
7	No	Show	7	F	4	3	1	2.568934	93.76123	71.34062	-2.27521	-0.38574	-1.53739
8	No	Show	8	F	7	4	3	2.188598	93.53628	-17.9575	-2.10284	-1.59919	0.275844
9	No	Show	9	F	6	5	2	2.56284	93.73092	71.5509	3.022225	-0.53831	1.620863
10	No	Show	10	F	9	6	5	2.184973	93.9039	-18.3526	2.801314	-1.68526	-0.22571
11	No	Show	11	F	4	3	1	2.702207	66.80505	134.9931	-3.30413	1.664931	0.291456
12	No	Show	12	F	11	4	3	2.186545	106.0313	-34.3257	-3.5711	-0.00977	1.671697
13	No	Show	13	F	6	5	2	2.752991	68.90289	133.2643	4.206127	1.495706	-0.02634
14	No	Show	14	F	13	6	5	2.164287	103.4746	-29.7207	4.304442	-0.01802	-1.57007
15	No	Show	15	F	14	13	6	2.159413	60.05099	-108.815	5.259704	-0.35882	0.336344
16	No	Show	16	O	12	11	4	2.785424	88.86482	-101.271	-4.93404	-1.37592	-0.33695
17	No	Show	17	O	16	12	11	2.26387	81.3146	-27.4948	-5.39576	0.741965	-0.99002
18	No	Show	18	C	16	12	11	5.38435	52.05847	74.07454	0.359662	-0.46939	0.045416
19	No	Show	19	C	18	16	12	1.548479	45.56829	-48.185	-0.90428	0.414387	0.183931
20	No	Show	20	C	18	16	12	1.547777	155.4109	-77.9605	1.654609	0.371985	-0.05857
21	No	Show	21	C	19	18	16	1.546835	112.5873	-6.74078	-2.20105	-0.34026	-0.19234
22	No	Show	22	C	20	18	16	1.546132	112.2554	-177.179	2.916813	-0.45046	0.289217
23	No	Show	23	C	21	19	18	1.540608	113.452	161.0819	-3.47802	0.322676	0.358441
24	No	Show	24	C	22	20	18	1.543029	112.5748	160.1414	4.209379	0.186158	-0.26299
25	No	Show	25	C	17	16	12	1.241211	24.5684	23.14453	-4.7484	-0.14524	-0.41175

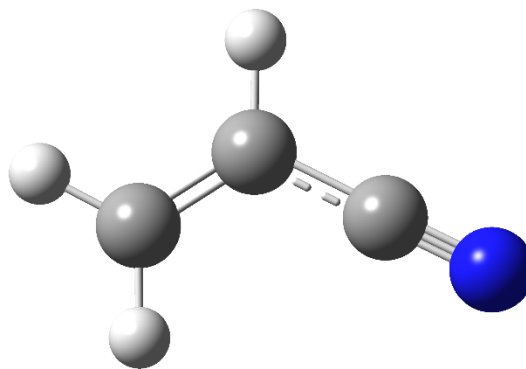
ALKENE

ALLYLAMINE (no. 207)



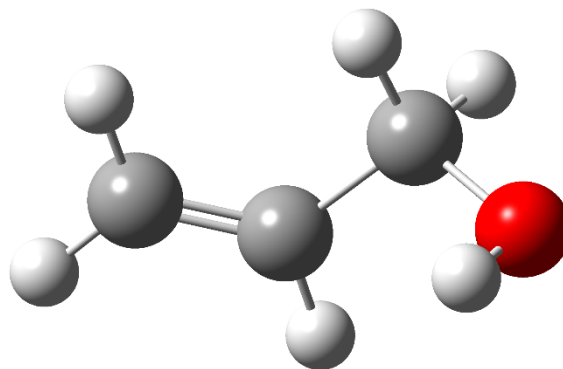
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							-1.68168	-0.34109	-0.21125
2	No	Show	2	C	1			1.4667			-0.57268	0.489422	0.269971
3	No	Show	3	C	2	1		1.498948	110.3033		0.692087	-0.31315	0.325615
4	No	Show	4	C	3	2	1	1.333136	124.4678	126.7161	1.838096	0.043467	-0.25468
5	No	Show	5	H	2	1	3	1.101889	107.6582	-118.253	-0.82202	0.821234	1.290699
6	No	Show	6	H	2	1	3	1.10504	114.292	123.2149	-0.39425	1.400907	-0.32875
7	No	Show	7	H	3	2	1	1.096366	115.5396	-52.7021	0.629737	-1.25563	0.882273
8	No	Show	8	H	1	2	3	1.023049	107.2949	-69.9001	-1.51118	-0.53196	-1.20177
9	No	Show	9	H	1	2	3	1.022026	107.7154	178.3261	-2.52606	0.234708	-0.20691
10	No	Show	10	H	4	3	2	1.092282	121.6055	179.5504	2.735261	-0.57483	-0.17793
11	No	Show	11	H	4	3	2	1.094429	120.9826	-0.13469	1.915215	0.974756	-0.82435

ACRYLONITRILE (no. 208)



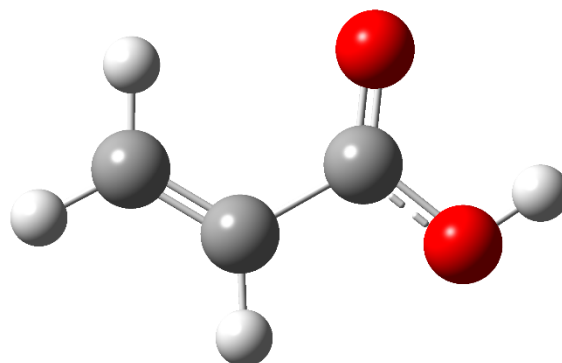
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							0.465078	-1.84797	0
2	No	Show	2	C	1			2.597495			-0.58995	0.525614	0
3	No	Show	3	C	2	1		1.335449	121.4695		0.167723	1.625321	0
4	No	Show	4	C	1	2	3	1.160915	0.348022	0	0	-0.78428	0
5	No	Show	5	H	2	1	4	1.091065	115.7204	180	-1.6805	0.559045	0
6	No	Show	6	H	3	2	1	1.090779	120.0885	180	-0.29921	2.611104	0
7	No	Show	7	H	3	2	1	1.091436	121.4362	0	1.257531	1.565731	0

ALLYL ALCOHOL (no. 209)



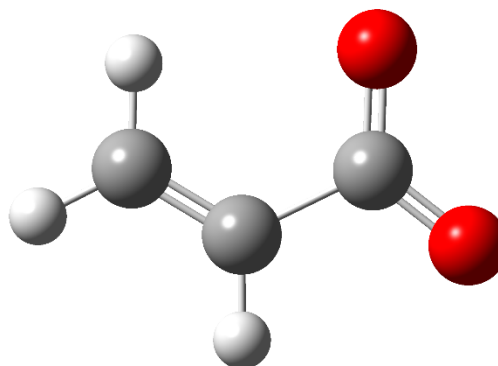
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.70837	-0.25057	0.220836
2	No	Show	2	C	1			1.422332			0.595548	0.489178	-0.26643
3	No	Show	3	C	2	1		1.499684	112.0586		-0.65643	-0.33559	-0.3033
4	No	Show	4	C	3	2	1	1.332715	123.9026	128.8957	-1.81527	0.047926	0.231614
5	No	Show	5	H	2	1	3	1.103897	111.611	123.7539	0.425078	1.404795	0.326169
6	No	Show	6	H	2	1	3	1.100873	105.5458	-119.444	0.869538	0.796029	-1.28755
7	No	Show	7	H	3	2	1	1.095893	115.6204	-51.276	-0.57196	-1.30274	-0.81169
8	No	Show	8	H	4	3	2	1.092093	121.6353	178.9804	-2.70944	-0.57593	0.168901
9	No	Show	9	H	4	3	2	1.09432	120.9329	-0.59821	-1.90627	1.009059	0.74686
10	No	Show	10	H	1	2	3	0.969225	106.7803	-60.1576	1.483022	-0.53575	1.119327

ACRYLIC ACID (no. 210)

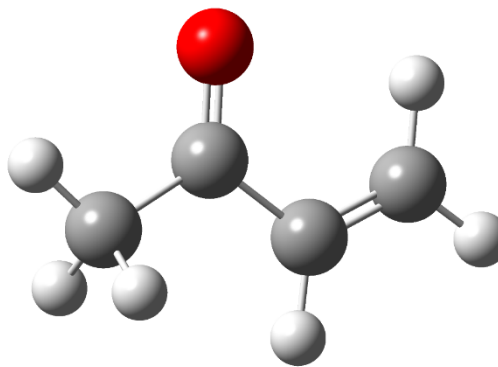


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.526443	-0.75027	-6E-06
2	No	Show	2	O	1			2.24367			0.604439	1.2952	0.000003
3	No	Show	3	C	1	2		2.341271	63.05063		-0.81226	-0.64057	0.000007
4	No	Show	4	C	2	1	3	1.21495	30.18483	0	0.479104	0.086732	0.000004
5	No	Show	5	C	3	1	4	1.332696	151.9607	0.001893	-1.95788	0.040333	-4E-06
6	No	Show	6	H	3	1	4	1.090437	85.05045	-179.999	-0.76918	-1.73015	0.000016
7	No	Show	7	H	5	3	1	1.090884	121.3764	179.9986	-2.92198	-0.4701	-6E-06
8	No	Show	8	H	5	3	1	1.092667	120.2887	-0.00099	-1.94956	1.132968	-1.8E-05
9	No	Show	9	H	1	4	2	0.975885	107.8304	0.000283	2.339856	-0.2111	-9E-06

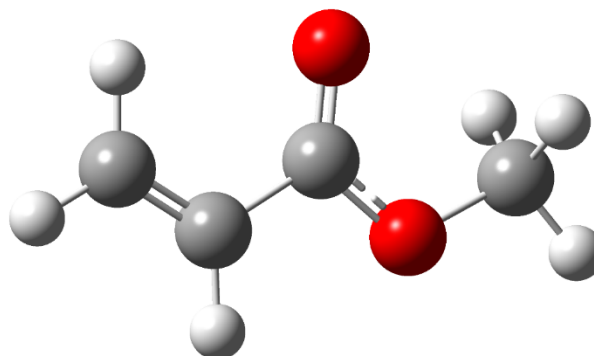
ACRYLATE (no. 211)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.591745	-0.74653	-0.00006
2	No	Show	2	O	1			2.24587			0.644403	1.289756	0.000038
3	No	Show	3	C	1	2		2.354846	62.34105		-0.76047	-0.63521	0.00012
4	No	Show	4	C	2	1	3	1.259494	26.93274	-0.00373	0.60081	0.031017	-1.2E-05
5	No	Show	5	C	3	1	4	1.332719	151.7007	0.020342	-1.90272	0.051374	-4.1E-05
6	No	Show	6	H	3	1	4	1.094156	87.12634	179.9964	-0.75734	-1.72936	0.000092
7	No	Show	7	H	5	3	1	1.092353	122.0349	179.9752	-2.8764	-0.4438	-0.00016
8	No	Show	8	H	5	3	1	1.093097	119.8786	-0.01857	-1.88116	1.144258	-0.00017

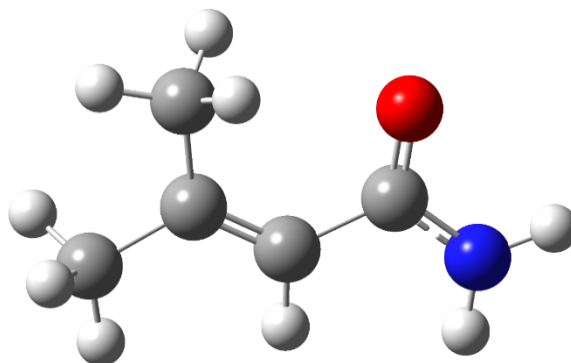
METHYL VINYL KETONE (no. 212)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.39587	1.380568	-0.0001
2	No	Show	2	C	1			2.387144			-1.74463	-0.58903	-0.00015
3	No	Show	3	C	1	2		1.222253	32.084		-0.44533	0.159316	0.000492
4	No	Show	4	C	3	1	2	1.492797	121.4585	179.9188	0.795495	-0.67063	0.000107
5	No	Show	5	C	4	3	1	1.334368	120.8983	0.039828	2.001631	-0.09986	-0.00011
6	No	Show	6	H	2	1	3	1.100847	120.7141	-69.1267	-1.78337	-1.24394	-0.88416
7	No	Show	7	H	2	1	3	1.100848	120.7362	69.06077	-1.78421	-1.24385	0.883881
8	No	Show	8	H	2	1	3	1.095282	85.08154	179.968	-2.59194	0.105012	-0.00058
9	No	Show	9	H	4	3	1	1.09227	117.3067	-179.962	0.672404	-1.75594	0.000034
10	No	Show	10	H	5	4	3	1.091261	121.6962	179.9975	2.917052	-0.69388	-0.00035
11	No	Show	11	H	5	4	3	1.093055	120.1727	-0.00149	2.094014	0.989282	-0.00003

METHYL ACRYLATE (no. 213)

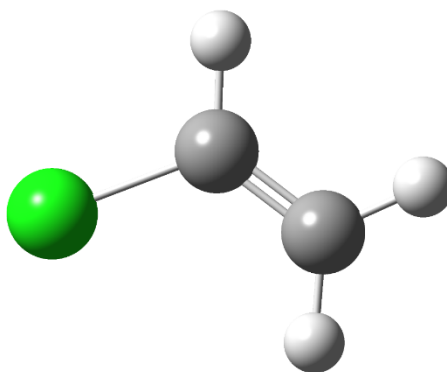
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.013796	-0.72191	0.000002
2	No	Show	2	O	1			2.245677			0.061613	1.311905	0
3	No	Show	3	C	1	2		1.432866	88.37441		2.293727	-0.0778	-5E-06
4	No	Show	4	C	2	1	3	1.215361	29.96591	-179.999	-0.04174	0.100946	0.000011
5	No	Show	5	C	4	2	1	1.482361	125.4181	-179.998	-1.31846	-0.6523	0.000001
6	No	Show	6	C	5	4	2	1.332697	119.9786	-0.00084	-2.47859	0.003573	-5E-06
7	No	Show	7	H	3	1	4	1.09394	105.7599	180	3.032406	-0.88468	-8E-06
8	No	Show	8	H	3	1	4	1.097823	110.2548	60.54724	2.405577	0.545421	0.896824
9	No	Show	9	H	3	1	4	1.097822	110.2548	-60.5477	2.405568	0.545419	-0.89684
10	No	Show	10	H	5	4	2	1.090445	117.0032	179.9993	-1.25119	-1.74067	0.000001
11	No	Show	11	H	6	5	4	1.090857	121.3526	-180	-3.43114	-0.52805	-0.00001
12	No	Show	12	H	6	5	4	1.092632	120.2978	0	-2.49416	1.096094	-4E-06

SENECIOIC ACID AMIDE (no. 214)

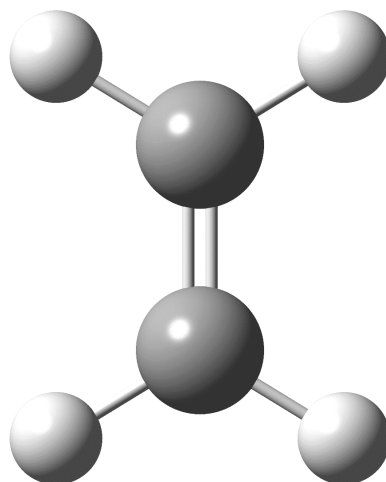


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.440725	1.249123	-0.03809
2	No	Show	2	N	1			2.258693			2.418859	-0.78592	0.021639
3	No	Show	3	C	1	2		2.94616	88.02919		-1.1694	-0.1167	0.00228
4	No	Show	4	C	3	1	2	1.499796	173.4438	-12.9006	-2.41203	-0.95639	-0.01118
5	No	Show	5	C	3	1	2	1.506082	71.11869	177.0322	-1.39765	1.371687	0.032369
6	No	Show	6	C	3	1	2	1.346252	53.5745	-1.78258	0.040949	-0.70591	-0.01422
7	No	Show	7	C	1	2	6	1.239427	30.67682	0.225453	1.332412	0.014771	-0.00942
8	No	Show	8	H	4	3	1	1.101898	109.7348	-112.011	-3.03386	-0.68682	-0.88
9	No	Show	9	H	4	3	1	1.097423	112.3758	9.678757	-2.19002	-2.03056	-0.04588
10	No	Show	10	H	4	3	1	1.101814	109.7783	131.4094	-3.01772	-0.74033	0.883499
11	No	Show	11	H	5	3	1	1.098043	111.2642	-55.8639	-0.87016	1.83851	0.874706
12	No	Show	12	H	5	3	1	1.09942	110.824	62.39429	-1.00829	1.845334	-0.8802
13	No	Show	13	H	5	3	1	1.097707	110.3193	-177.156	-2.47014	1.591306	0.112946
14	No	Show	14	H	6	3	1	1.092867	118.8147	-178.841	0.095296	-1.79727	-0.0324
15	No	Show	15	H	2	1	7	1.013945	91.07888	-178.68	3.340343	-0.36352	0.044728
16	No	Show	16	H	2	1	7	1.012468	149.3306	-3.5316	2.331052	-1.79306	0.076858

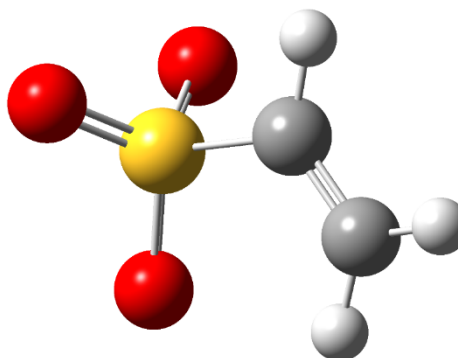
VINYL CHLORIDE (no. 215)



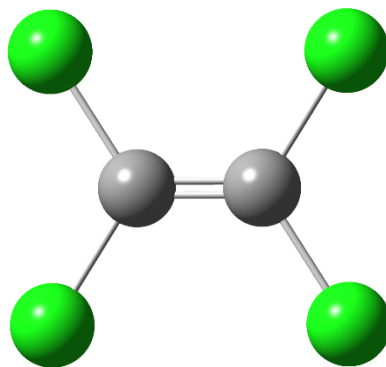
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.06182	-0.09978	-2E-06
2	No	Show	2	C	1			1.749325			0.577347	0.511169	0.000009
3	No	Show	3	C	2	1		1.325688	122.3229		1.632798	-0.291	0.000002
4	No	Show	4	H	2	1	3	1.090332	112.8067	179.998	0.622346	1.600572	-1.3E-05
5	No	Show	5	H	3	2	1	1.091592	118.7722	179.9978	2.630078	0.152855	-2.7E-05
6	No	Show	6	H	3	2	1	1.09132	122.2356	-0.00081	1.537681	-1.37817	0.000002

ETHYLENE (no. 216)

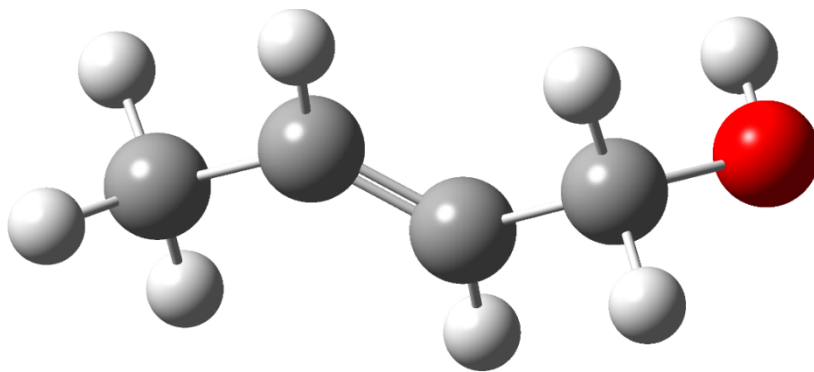
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0	0.665627	0
2	No	Show	2	C	1			1.331254			0	-0.66563	0
3	No	Show	3	H	1	2		1.093192	121.489		0.932209	1.23664	0
4	No	Show	4	H	1	2	3	1.093193	121.489	180	-0.93221	1.236639	0
5	No	Show	5	H	2	1	3	1.093192	121.489	180	-0.93221	-1.23664	0
6	No	Show	6	H	2	1	3	1.093193	121.4891	0	0.932209	-1.23664	0

ETHENESULFONATE (no. 217)

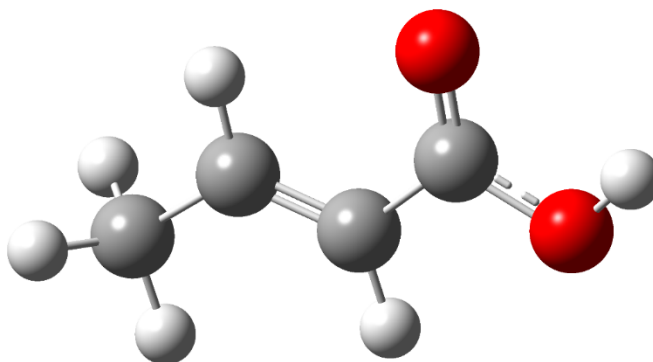
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							-0.45765	-0.03134	0.000002
2	No	Show	2	O	1			1.497044			-0.26722	-1.51622	-0.00047
3	No	Show	3	O	1	2		1.498114	113.2863		-1.11107	0.482351	-1.2464
4	No	Show	4	O	1	2	3	1.497887	113.2761	129.8059	-1.11268	0.481018	1.245836
5	No	Show	5	C	1	2	4	1.781801	106.7453	115.111	1.169424	0.694906	0.000985
6	No	Show	6	C	5	1	2	1.327829	121.8046	0.056644	2.268402	-0.05033	0.000072
7	No	Show	7	H	5	1	2	1.093221	113.801	-179.942	1.164605	1.788115	0.002406
8	No	Show	8	H	6	5	1	1.09226	120.9923	179.9877	3.259404	0.40896	0.000491
9	No	Show	9	H	6	5	1	1.092192	120.5111	-0.01743	2.199237	-1.14033	-0.00104

TETRACHLOROETHYLENE (no. 218)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							0	1.454634	1.589744
2	No	Show	2	Cl	1			2.909268			0	-1.45463	1.589744
3	No	Show	3	Cl	2	1		3.179488	90		0	-1.45463	-1.58974
4	No	Show	4	Cl	3	2	1	2.909268	90	0	0	1.454634	-1.58974
5	No	Show	5	C	1	2	3	1.720552	32.28026	0	0	0	0.670864
6	No	Show	6	C	5	1	2	1.341728	122.2803	180	0	0	-0.67086

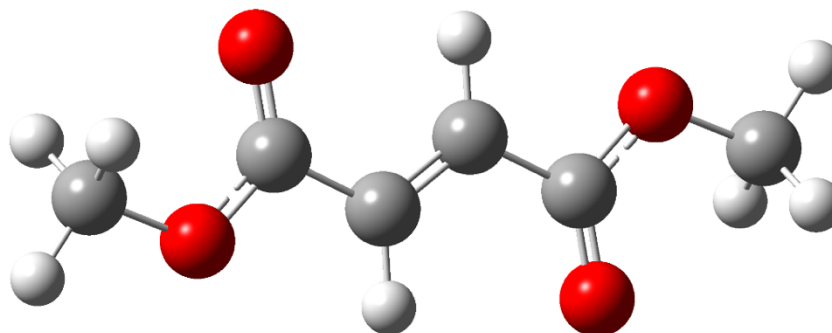
CROTONYL ALCOHOL (no. 219)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.30878	-0.44804	-0.22146
2	No	Show	2	C	1			1.424537			1.339055	0.502366	0.209444
3	No	Show	3	C	2	1		1.498741	112.1792		-0.01766	-0.1112	0.37995
4	No	Show	4	C	3	2	1	1.335577	123.923	-125.88	-1.12386	0.350457	-0.2091
5	No	Show	5	C	4	3	2	1.496577	125.0703	-179.35	-2.49234	-0.23304	-0.0462
6	No	Show	6	H	2	1	3	1.100883	105.3058	119.8861	1.710202	0.878824	1.17509
7	No	Show	7	H	2	1	3	1.104131	111.3807	-123.655	1.279341	1.359288	-0.48426
8	No	Show	8	H	3	2	1	1.097088	116.0991	54.07037	-0.07085	-0.99098	1.033226
9	No	Show	9	H	4	3	2	1.097249	118.3246	0.394408	-1.03826	1.227519	-0.86285
10	No	Show	10	H	5	4	3	1.101333	110.8068	120.0557	-3.18711	0.51056	0.374836
11	No	Show	11	H	5	4	3	1.101223	110.7621	-121.894	-2.90711	-0.53365	-1.02103
12	No	Show	12	H	5	4	3	1.098939	111.3883	-0.85403	-2.4777	-1.11066	0.615042
13	No	Show	13	H	1	2	3	0.969242	106.6553	58.83066	1.990058	-0.80807	-1.06301

CROTONIC ACID (no. 220)

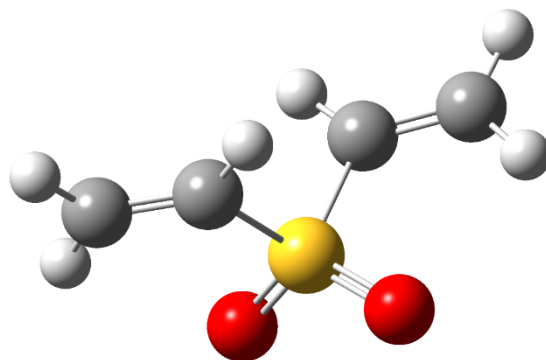
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.041248	-0.88822	0.000305
2	No	Show	2	O	1			2.242645			1.379711	1.25463	0.0002
3	No	Show	3	C	2	1		2.867686	87.97122		-1.32871	0.312245	-5.4E-05
4	No	Show	4	C	3	2	1	1.488425	178.7462	179.2779	-2.74483	-0.14601	0.000223
5	No	Show	5	C	3	2	1	1.338097	56.33954	-0.02018	-0.26223	-0.49592	-0.00033
6	No	Show	6	C	2	1	5	1.217217	30.46186	-0.07663	1.099578	0.070087	-0.00075
7	No	Show	7	H	3	2	1	1.095407	61.39275	-179.998	-1.14938	1.392874	-9.1E-05
8	No	Show	8	H	4	3	2	1.097487	111.8466	-179.275	-2.81977	-1.24094	0.000398
9	No	Show	9	H	4	3	2	1.101007	110.0124	-57.7274	-3.26984	0.253099	0.881868
10	No	Show	10	H	4	3	2	1.101012	110.0119	59.17901	-3.27008	0.25281	-0.88141
11	No	Show	11	H	5	3	2	1.091342	122.3779	179.9768	-0.35311	-1.58347	-0.00029
12	No	Show	12	H	1	6	2	0.975389	107.6725	-0.05758	2.911669	-0.44805	0.000917

DIMETHYL FUMARATE (no. 221)

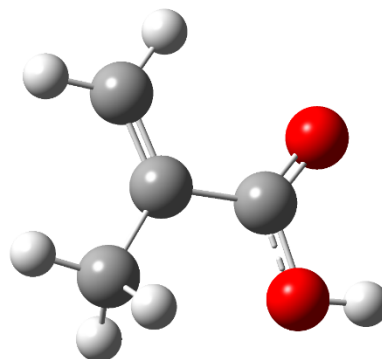


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.844553	0.723045	0.000003
2	No	Show	2	O	1			5.870025			-2.84456	-0.72304	0.000008
3	No	Show	3	O	1	2		2.247152	57.08862		2.125957	-1.40611	-9E-06
4	No	Show	4	O	2	1	3	2.247154	57.0882	-179.999	-2.12595	1.40611	-4E-06
5	No	Show	5	C	1	3	2	2.328472	63.14339	-0.00245	0.539927	0.390658	-8.2E-05
6	No	Show	6	C	5	1	3	1.332871	152.3193	0.007713	-0.53992	-0.39067	-3.4E-05
7	No	Show	7	C	3	1	5	1.213587	29.54679	0.008499	1.896533	-0.21441	-0.00012
8	No	Show	8	C	4	2	1	1.213588	29.54691	0.00135	-1.89653	0.214404	-1.1E-05
9	No	Show	9	C	1	7	3	1.434436	115.2706	0.007523	4.192049	0.231252	0.0001
10	No	Show	10	C	2	1	7	1.434436	145.6874	-179.994	-4.19205	-0.23124	0.000063
11	No	Show	11	H	5	1	7	1.09089	85.81439	-179.993	0.463425	1.478862	-0.0001
12	No	Show	12	H	6	5	1	1.09089	121.8663	-0.00848	-0.46342	-1.47887	-1.4E-05
13	No	Show	13	H	9	1	7	1.097569	110.0945	60.54655	4.372594	-0.37412	-0.89745
14	No	Show	14	H	9	1	7	1.097569	110.0941	-60.5544	4.372474	-0.37407	0.897701
15	No	Show	15	H	9	1	7	1.093645	105.7077	179.9962	4.831137	1.118735	0.000119
16	No	Show	16	H	10	2	1	1.097569	110.094	60.55677	-4.37258	0.374073	-0.89753
17	No	Show	17	H	10	2	1	1.097569	110.0945	-60.5441	-4.37249	0.374145	0.897621
18	No	Show	18	H	10	2	1	1.093645	105.7077	-179.994	-4.83115	-1.11872	0.000132

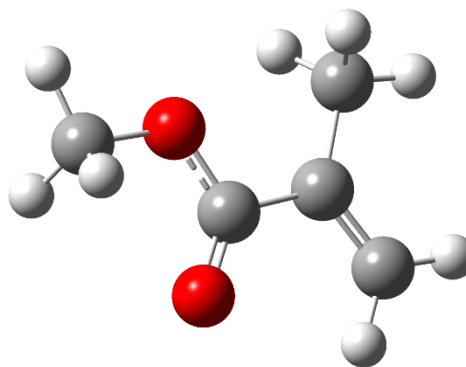
DIVINYLSULFONE (no. 222)



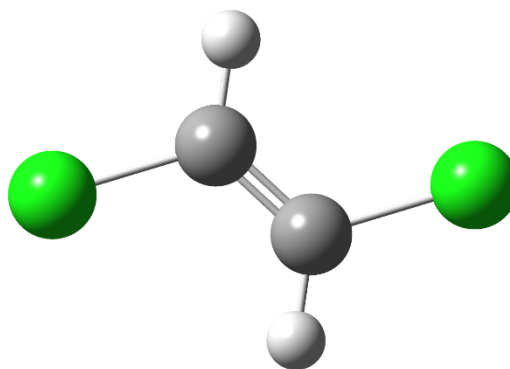
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	S							0	0	0.369359
2	No	Show	2	O	1			1.48596			1.15081	-0.55515	1.127988
3	No	Show	3	O	1	2		1.48596	118.6016		-1.15081	0.555154	1.127988
4	No	Show	4	C	1	3	2	1.772108	108.7821	-123.749	0.619409	1.250047	-0.72338
5	No	Show	5	C	1	3	2	1.772108	107.9177	124.1743	-0.61941	-1.25005	-0.72338
6	No	Show	6	C	4	1	3	1.327512	119.3567	-3.10888	0	2.422369	-0.78882
7	No	Show	7	C	5	1	3	1.327512	119.3567	-133.003	0	-2.42237	-0.78882
8	No	Show	8	H	4	1	3	1.091784	114.0697	175.8038	1.515622	0.956381	-1.27343
9	No	Show	9	H	5	1	3	1.091784	114.0697	45.90946	-1.51562	-0.95638	-1.27343
10	No	Show	10	H	6	4	1	1.091695	120.3294	178.6449	0.380822	3.211478	-1.44004
11	No	Show	11	H	6	4	1	1.092131	120.9436	-1.01827	-0.89314	2.619689	-0.19207
12	No	Show	12	H	7	5	1	1.091695	120.3294	178.6449	-0.38082	-3.21148	-1.44004
13	No	Show	13	H	7	5	1	1.092131	120.9436	-1.01827	0.893137	-2.61969	-0.19207

METHACRYLIC ACID (no. 223)

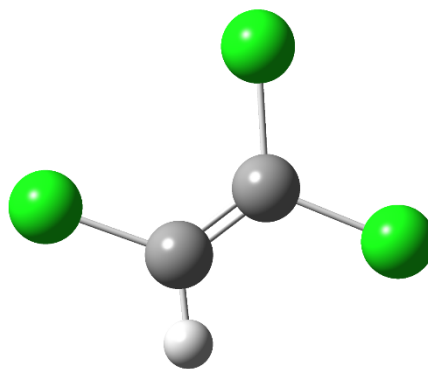
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.238941	-1.16422	-1.4E-05
2	No	Show	2	O	1			2.239012			1.513701	1.057871	0.000008
3	No	Show	3	C	1	2		2.356293	63.22682		-0.7186	0.147329	0.000004
4	No	Show	4	C	3	1	2	1.499837	86.41193	-179.999	-1.47381	-1.1485	0.000007
5	No	Show	5	C	2	1	3	1.215152	30.40153	0.001219	0.774799	0.093185	0.000013
6	No	Show	6	C	3	1	5	1.336306	148.8511	0.003331	-1.28396	1.358147	-1.1E-05
7	No	Show	7	H	4	3	1	1.099798	110.7545	59.30365	-1.21646	-1.74957	0.884334
8	No	Show	8	H	4	3	1	1.096937	110.3448	180	-2.55445	-0.96011	0.000016
9	No	Show	9	H	4	3	1	1.099798	110.7545	-59.3038	-1.21648	-1.74956	-0.88433
10	No	Show	10	H	6	3	1	1.091583	120.9127	179.998	-2.36979	1.470043	-1.9E-05
11	No	Show	11	H	6	3	1	1.091074	120.6048	-0.00205	-0.66807	2.258772	-1.5E-05
12	No	Show	12	H	1	5	2	0.975641	107.651	0.000944	2.21357	-1.1198	-2.1E-05

METHYL METHACRYLATE (no. 224)

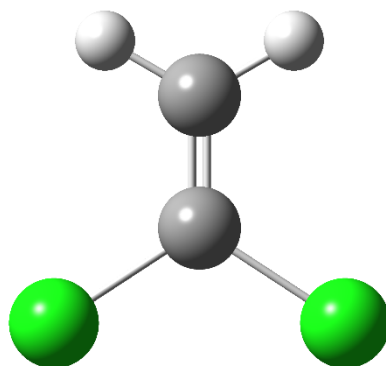
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.07726	0.656727	0.000003
2	No	Show	2	O	1			2.240919			-0.63633	-1.54039	-3E-06
3	No	Show	3	C	1	2		2.349839	63.33066		1.189061	0.035808	0.000001
4	No	Show	4	C	3	1	2	1.499897	86.50363	179.9997	1.496434	1.503872	-2E-06
5	No	Show	5	C	2	1	3	1.215724	30.16558	0.000464	-0.24419	-0.38964	0.000005
6	No	Show	6	C	3	1	5	1.336403	148.8903	0	2.110139	-0.93248	0.000001
7	No	Show	7	C	1	5	2	1.433015	115.4279	0.000366	-2.473	0.331998	-1E-06
8	No	Show	8	H	4	3	1	1.099751	110.7652	-59.2943	1.062394	1.993106	-0.88415
9	No	Show	9	H	4	3	1	1.099751	110.7652	59.29529	1.062411	1.993105	0.884152
10	No	Show	10	H	4	3	1	1.096976	110.3156	-180	2.581388	1.665831	-1.2E-05
11	No	Show	11	H	6	3	1	1.091567	120.8962	180	3.175116	-0.69302	-2E-06
12	No	Show	12	H	6	3	1	1.091029	120.5942	0	1.812391	-1.9821	0.000003
13	No	Show	13	H	7	1	5	1.09385	105.7528	180	-3.0008	1.290085	-1E-06
14	No	Show	14	H	7	1	5	1.097683	110.207	60.52975	-2.72745	-0.24753	0.896834
15	No	Show	15	H	7	1	5	1.097684	110.207	-60.5299	-2.72744	-0.24753	-0.89684

TRANS-1,2-DICHLOROETHYLENE (no. 225)

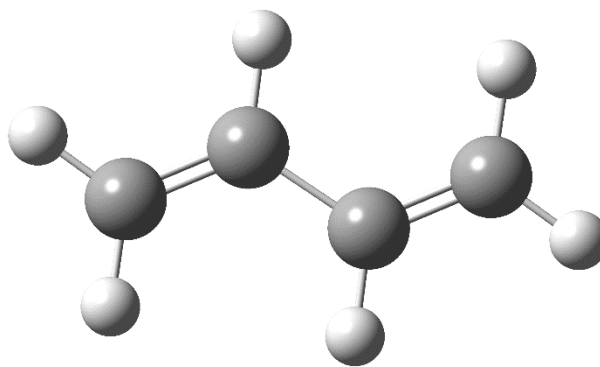
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-2.1501	-0.04997	-8.8E-05
2	No	Show	2	Cl	1			4.301367			2.150103	0.049969	-8.8E-05
3	No	Show	3	C	1	2		1.73638	15.41954		-0.4874	0.450475	0.00023
4	No	Show	4	C	3	1	2	1.32739	120.5039	-	0.487404	-0.45048	0.00023
5	No	Show	5	H	3	1	4	1.089868	114.9031	0.03186	-0.33286	1.52933	0.000111
6	No	Show	6	H	4	3	1	1.089867	124.593	-	0.332856	-1.52933	0.000111
										0.00458			

TRICHLOROETHYLENE (no. 226)

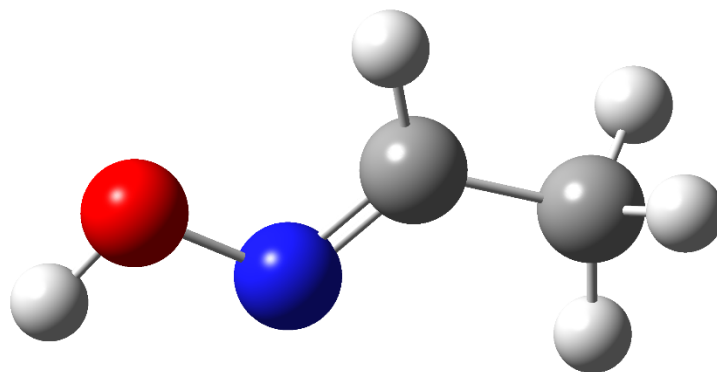
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							2.029259	-0.76867	-0.00017
2	No	Show	2	Cl	1			2.919027			0.328049	1.603379	-1.5E-05
3	No	Show	3	Cl	2	1		3.23594	88.57423		-2.25379	-0.34737	-0.00016
4	No	Show	4	C	2	1	3	1.723461	32.40488	0.0427	0.425543	-0.11732	0.000558
5	No	Show	5	C	4	2	1	1.332912	124.2244	-179.943	-0.63239	-0.92814	0.000387
6	No	Show	6	H	5	4	2	1.089756	121.4828	179.9577	-0.51877	-2.01196	0.000083

CIS-1,2-DICHLOROETHYLENE (no. 227)

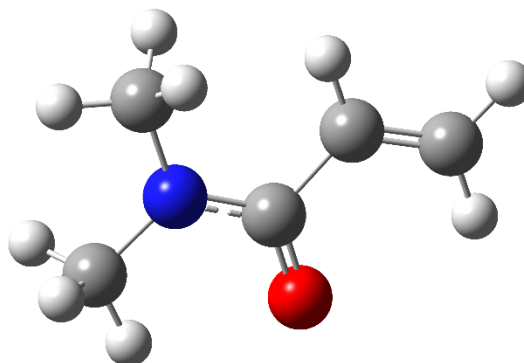
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	Cl							-1.4556	-0.52054	-6.3E-05
2	No	Show	2	Cl	1			2.9112			1.455597	-0.52057	-6.3E-05
3	No	Show	3	C	1	2		1.737657	33.10956		-8.3E-05	0.428628	0.000545
4	No	Show	4	C	3	1	2	1.325823	123.1151	179.9268	0.000061	1.754451	-2.4E-05
5	No	Show	5	H	4	3	1	1.089881	120.0457	0.025775	-0.94331	2.300247	-0.00049
6	No	Show	6	H	4	3	1	1.089873	120.0471	-179.946	0.94353	2.30006	-0.00049

1,3-BUTADIENE (no. 228)

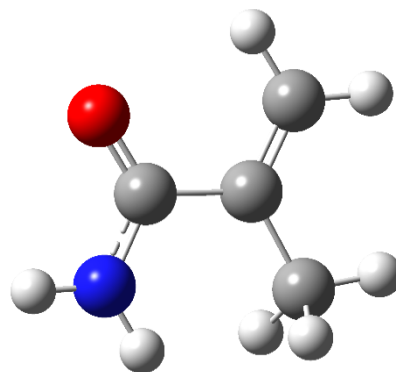
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	C							0.608003	-0.40667	0.000001
2	No	Show	2	C	1			1.462937			-0.608	0.406668	0.000001
3	No	Show	3	C	1	2		1.338436	123.4395		1.842006	0.111646	0
4	No	Show	4	C	2	1	3	1.338437	123.4394	180	-1.84201	-0.11165	0
5	No	Show	5	H	1	3	2	1.095415	120.0754	180	0.468972	-1.49322	0.000001
6	No	Show	6	H	2	1	3	1.095415	116.4852	0	-0.46897	1.493224	0.000001
7	No	Show	7	H	3	1	2	1.091402	121.4562	-180	2.727646	-0.52616	-1E-06
8	No	Show	8	H	3	1	2	1.093776	120.924	0	1.996882	1.194401	-1E-06
9	No	Show	9	H	4	2	1	1.091401	121.4562	-180	-2.72765	0.526161	-1E-06
10	No	Show	10	H	4	2	1	1.093776	120.9239	0	-1.99688	-1.1944	-1E-06

ACETALDEHYDE OXIME (no. 229)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.76943	0.175052	-1E-06
2	No	Show	2	N	1			1.394907			-0.53689	-0.4781	0.000002
3	No	Show	3	C	2	1		2.402823	142.8347		1.834724	-0.09205	-1E-06
4	No	Show	4	C	2	1	3	1.275497	110.6381	0	0.419262	0.366105	0.000002
5	No	Show	5	H	3	2	1	1.100118	121.7829	-71.2076	2.358231	0.298373	-0.88531
6	No	Show	6	H	3	2	1	1.097112	83.58291	-179.999	1.888858	-1.18783	-7E-06
7	No	Show	7	H	3	2	1	1.100118	121.7827	71.20883	2.358232	0.298364	0.885309
8	No	Show	8	H	4	2	1	1.098395	119.8099	0	0.197797	1.441942	-1E-06
9	No	Show	9	H	1	2	4	0.968937	103.7348	180	-2.41342	-0.5489	-4E-06

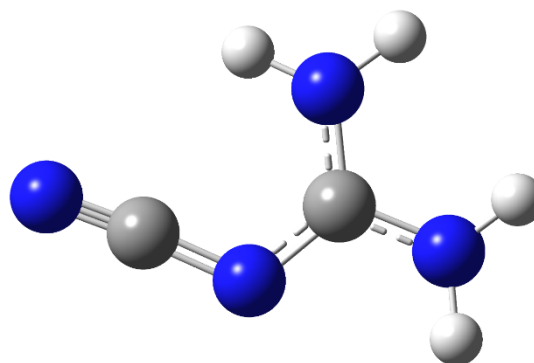
N,N-DIMETHYLACRYLAMIDE (no. 230)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.537435	-1.5867	0.000146
2	No	Show	2	N	1			2.274001			-0.96203	0.122895	0.000316
3	No	Show	3	C	2	1		1.4548	92.77763		-2.10094	-0.78226	-0.00025
4	No	Show	4	C	2	1	3	1.460643	150.7544	-179.938	-1.26591	1.551577	-7.7E-05
5	No	Show	5	C	1	2	3	1.240817	30.06663	179.9757	0.296703	-0.36946	0.000205
6	No	Show	6	C	5	1	2	1.496203	120.5621	179.9992	1.412973	0.62682	0.000172
7	No	Show	7	C	6	5	1	1.333549	119.6786	0.017524	2.677073	0.202081	-0.00028
8	No	Show	8	H	3	2	1	1.100001	110.1522	-120.185	-2.72046	-0.61129	-0.89298
9	No	Show	9	H	3	2	1	1.099998	110.1522	120.2474	-2.72149	-0.61109	0.891727
10	No	Show	10	H	3	2	1	1.092828	109.3244	0.031609	-1.74242	-1.81461	0.000088
11	No	Show	11	H	4	2	1	1.098414	111.7622	-61.3342	-0.87148	2.052071	0.894599
12	No	Show	12	H	4	2	1	1.095297	107.7879	180	-2.35564	1.661882	0.000491
13	No	Show	13	H	4	2	1	1.09843	111.7678	61.3273	-0.87242	2.051488	-0.89551
14	No	Show	14	H	6	5	1	1.089351	119.7884	-179.985	1.187217	1.692521	0.000476
15	No	Show	15	H	7	6	5	1.091006	121.2182	179.9987	3.510263	0.906416	-0.00033
16	No	Show	16	H	7	6	5	1.092099	120.4441	-0.00044	2.901741	-0.86666	-0.00061

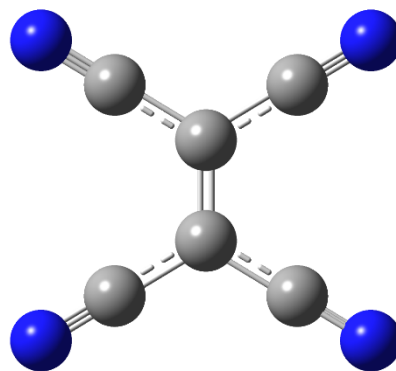
METHACRYLAMIDE (no. 231)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.46841	1.141553	0.000137
2	No	Show	2	N	1			2.255358			-1.35395	-1.1109	0.000109
3	No	Show	3	C	1	2		2.404585	62.45092		0.717226	0.139044	-8.8E-05
4	No	Show	4	C	3	1	2	1.502204	145.1189	-0.0141	1.479175	-1.15558	0.000038
5	No	Show	5	C	1	2	3	1.235799	30.43663	0.045189	-0.78911	0.109205	-0.00043
6	No	Show	6	C	3	1	5	1.335838	91.46829	179.9652	1.305087	1.338578	0.000058
7	No	Show	7	H	4	3	1	1.101232	111.095	-59.6604	1.233125	-1.76021	0.886941
8	No	Show	8	H	4	3	1	1.101232	111.095	59.72688	1.233653	-1.76007	-0.88711
9	No	Show	9	H	4	3	1	1.096868	110.4146	-179.967	2.559165	-0.9639	0.000364
10	No	Show	10	H	6	3	1	1.091678	120.9794	179.9864	2.392822	1.431278	0.000252
11	No	Show	11	H	6	3	1	1.090675	120.5421	-0.01544	0.705492	2.249653	-4.4E-05
12	No	Show	12	H	2	1	5	1.012307	150.2219	0.040484	-0.80725	-1.96289	0.000007
13	No	Show	13	H	2	1	5	1.01463	90.85394	-179.958	-2.36639	-1.17749	0.000269

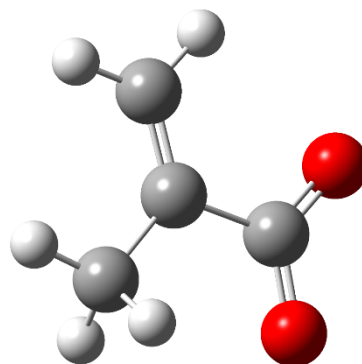
CYANOGUANIDINE (no. 232)



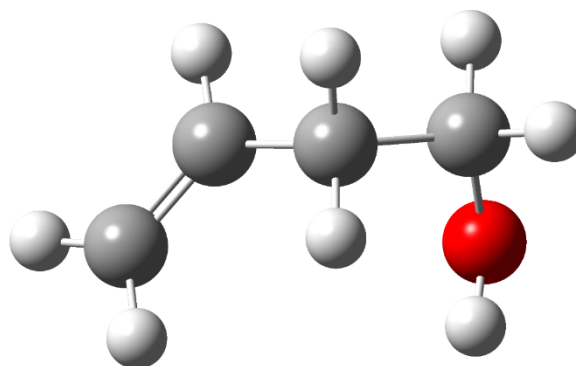
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.986369	-0.54979	-0.04999
2	No	Show	2	N	1			2.303008			0.634127	1.31197	0.045525
3	No	Show	3	N	1	2		2.289586	61.98604		-0.28046	-0.86839	-0.00313
4	No	Show	4	N	3	1	2	2.491404	149.1454	3.740825	-2.57651	0.098661	0.003374
5	No	Show	5	C	3	1	2	1.332788	31.27473	0.049247	0.751592	-0.02506	-0.00207
6	No	Show	6	C	4	3	1	1.1723	1.995287	-1.62436	-1.48095	-0.31848	0.000023
7	No	Show	7	H	1	5	3	1.014012	117.0841	-13.6947	2.072818	-1.54398	0.12986
8	No	Show	8	H	1	5	3	1.014414	119.3025	-166.592	2.785209	0.041153	0.154149
9	No	Show	9	H	2	1	5	1.014802	88.95294	-170.627	1.450927	1.890815	-0.1206
10	No	Show	10	H	2	1	5	1.015154	148.2407	-22.3552	-0.27751	1.726123	-0.1216

TETRACYANOETHYLENE (no. 233)

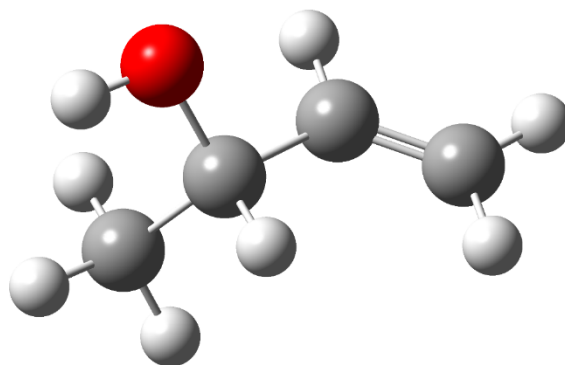
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							2.216554	-2.02131	0.000057
2	No	Show	2	N	1			4.433893			-2.21734	-2.02061	-3.1E-05
3	No	Show	3	N	2	1		4.042129	89.99684		-2.21648	2.021523	0.00006
4	No	Show	4	N	1	2	3	4.04171	90.00299	-0.00237	2.217405	2.020402	-1.9E-05
5	No	Show	5	C	2	1	4	2.592118	31.21103	0.000501	-0.00018	-0.67774	-2.4E-05
6	No	Show	6	C	5	2	1	1.355482	121.2149	-179.999	0.000125	0.677739	-3.1E-05
7	No	Show	7	C	1	5	2	1.157732	0.000594	115.5604	1.226485	-1.42122	0.00001
8	No	Show	8	C	2	1	7	1.157731	31.22064	-0.00274	-1.22718	-1.42067	-0.00001
9	No	Show	9	C	3	2	1	1.157732	58.77908	0.003307	-1.22654	1.421214	0.000009
10	No	Show	10	C	4	1	7	1.157731	58.78805	0.00072	1.227122	1.420668	-3.1E-05

METHACRYLATE (no. 234)

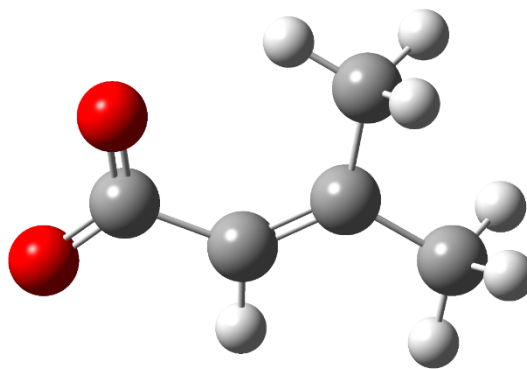
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.630824	0.91257	0.000046
2	No	Show	2	O	1			2.240182			1.205275	-1.28682	-6.1E-05
3	No	Show	3	C	2	1		2.370044	62.59159		-0.65317	0.183995	0.000033
4	No	Show	4	C	3	2	1	1.501072	88.02996	-179.998	-1.5437	-1.02438	0.000037
5	No	Show	5	C	1	2	3	1.259264	27.22945	0.000896	0.85243	-0.0773	0.000013
6	No	Show	6	C	3	2	1	1.336576	148.7699	0.012019	-1.1193	1.436655	-4.4E-05
7	No	Show	7	H	4	3	2	1.100576	110.5062	-58.6576	-1.34082	-1.65283	-0.8804
8	No	Show	8	H	4	3	2	1.098329	111.529	179.982	-2.60529	-0.74271	0.000399
9	No	Show	9	H	4	3	2	1.100567	110.507	58.6175	-1.34027	-1.65324	0.880041
10	No	Show	10	H	6	3	2	1.093139	121.5452	179.9907	-2.19186	1.64775	-6.8E-05
11	No	Show	11	H	6	3	2	1.091336	120.2938	-0.0089	-0.42814	2.281232	-9.1E-05

3-BUTEN-1-OL (no. 235)

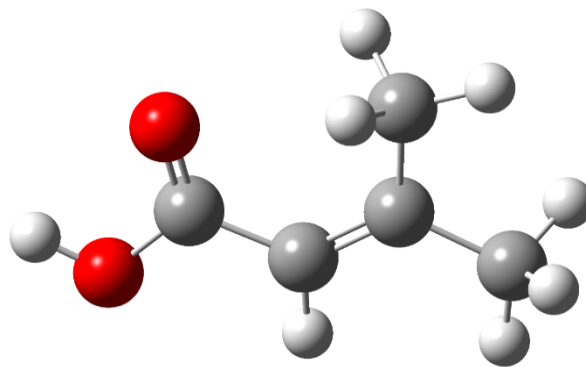
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.486772	-1.02384	-0.08018
2	No	Show	2	C	1			2.446422			0.021627	0.883548	0.367268
3	No	Show	3	C	1	2		1.419562	35.22349		1.372742	0.389888	-0.13961
4	No	Show	4	C	2	1	3	1.499758	93.11547	127.9743	-1.12009	0.292207	-0.40479
5	No	Show	5	C	4	2	1	1.333437	124.6624	90.4346	-2.0637	-0.4917	0.117845
6	No	Show	6	H	2	1	3	1.102644	140.3869	0.716159	0.008033	1.982756	0.281359
7	No	Show	7	H	2	1	3	1.102899	93.15601	-121.922	-0.07949	0.632918	1.436542
8	No	Show	8	H	3	1	2	1.100716	106.0627	-120.23	1.500316	0.661471	-1.19864
9	No	Show	9	H	3	1	2	1.103683	111.1003	123.0911	2.18187	0.878088	0.430553
10	No	Show	10	H	4	2	1	1.096916	116.0181	-88.2821	-1.145	0.520394	-1.47742
11	No	Show	11	H	1	3	2	0.969547	106.8474	-55.3994	1.306595	-1.28198	0.836836
12	No	Show	12	H	5	4	2	1.092238	121.5503	-179.326	-2.86804	-0.90433	-0.49515
13	No	Show	13	H	5	4	2	1.094339	120.9993	0.942859	-2.06198	-0.74226	1.183112

3-BUTEN-2-OL (no. 236)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.0892	1.238838	-0.05663
2	No	Show	2	C	1			1.428228			-0.38086	0.053607	0.308488
3	No	Show	3	C	2	1		1.522695	110.4648		-1.18148	-1.18405	-0.07337
4	No	Show	4	C	2	1	3	1.502016	106.7798	120.9671	0.933808	0.093341	-0.41686
5	No	Show	5	C	4	2	1	1.331832	124.2716	128.1507	2.119153	-0.06275	0.169972
6	No	Show	6	H	2	1	4	1.104837	110.1785	118.0307	-0.1878	0.044843	1.396292
7	No	Show	7	H	3	2	1	1.101144	110.0198	-59.2988	-2.15788	-1.17326	0.43561
8	No	Show	8	H	3	2	1	1.100693	110.0973	60.2656	-1.3539	-1.20247	-1.16032
9	No	Show	9	H	3	2	1	1.099175	110.7941	-179.17	-0.64775	-2.0995	0.218624
10	No	Show	10	H	4	2	1	1.096648	115.0825	-53.5021	0.862037	0.236075	-1.50181
11	No	Show	11	H	1	2	4	0.969354	106.891	170.908	-1.98953	1.147159	0.290732
12	No	Show	12	H	5	4	2	1.091927	121.4726	177.7339	3.045784	-0.0618	-0.40766
13	No	Show	13	H	5	4	2	1.09408	121.0454	-1.92233	2.198948	-0.20266	1.252131

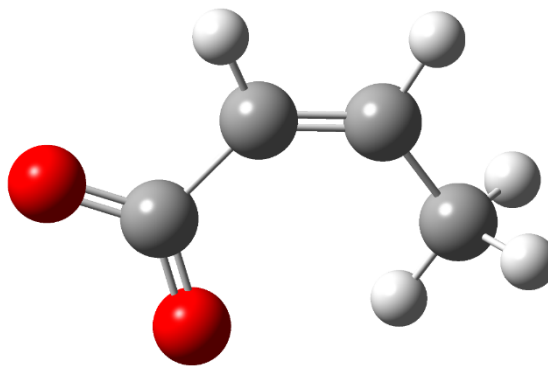
3-METHYLBUT-2-ENOATE (no. 237)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.61952	1.179317	0.108494
2	No	Show	2	O	1			2.237766			-2.41435	-0.90257	-0.09539
3	No	Show	3	C	1	2		3.020879	85.83043		1.118858	-0.09148	-0.00139
4	No	Show	4	C	3	1	2	1.504952	170.4444	-26.1084	2.368931	-0.9287	0.034166
5	No	Show	5	C	3	1	2	1.502753	75.21376	171.1646	1.378401	1.386482	-0.08224
6	No	Show	6	C	3	1	2	1.345383	50.94945	-5.37427	-0.08912	-0.68272	0.034584
7	No	Show	7	C	1	2	6	1.262516	27.63094	0.40987	-1.47001	-0.07061	0.012204
8	No	Show	8	H	4	3	1	1.102369	110.2086	-104.443	3.003137	-0.63013	0.884964
9	No	Show	9	H	4	3	1	1.102207	110.3673	138.2894	2.968582	-0.76153	-0.87541
10	No	Show	10	H	4	3	1	1.09804	112.0597	16.85414	2.145258	-2.00038	0.118758
11	No	Show	11	H	5	3	1	1.102876	109.5372	112.7722	1.89551	1.720734	0.832755
12	No	Show	12	H	5	3	1	1.092056	112.3312	-8.72001	0.459191	1.963056	-0.20554
13	No	Show	13	H	5	3	1	1.101944	109.4674	-131.133	2.066445	1.593358	-0.91775
14	No	Show	14	H	6	3	1	1.095083	117.1817	-177.063	-0.10956	-1.77692	0.073373

3,3-DIMETHYLACRYLIC ACID (no. 238)

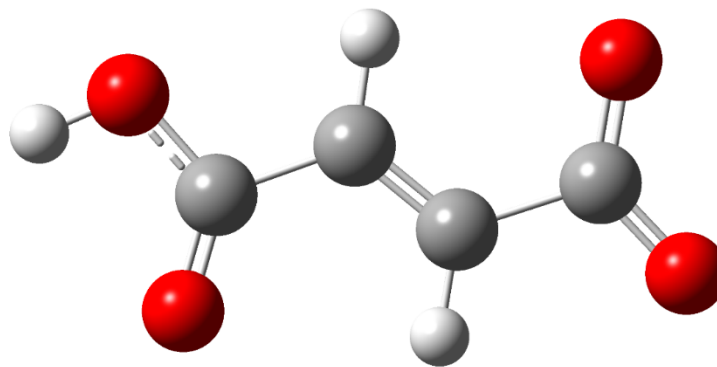
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.35415	-0.88314	0.000095
2	No	Show	2	O	1			2.241136			-1.49045	1.184878	-0.00013
3	No	Show	3	C	2	1		2.95401	86.75522		1.166578	-0.10602	0.000017
4	No	Show	4	C	3	2	1	1.497118	173.3603	0.049953	2.428502	-0.91157	-4.3E-05
5	No	Show	5	C	3	2	1	1.503568	70.87674	-179.99	1.344324	1.38701	0.000102
6	No	Show	6	C	3	2	1	1.348407	53.35859	0.005703	-0.03006	-0.72752	-2.5E-05
7	No	Show	7	C	2	1	6	1.219405	30.93528	-0.0008	-1.3151	-0.02185	-2.1E-05
8	No	Show	8	H	4	3	2	1.10172	109.5504	121.795	3.033925	-0.64827	-0.88204
9	No	Show	9	H	4	3	2	1.097023	112.4198	-0.03737	2.23551	-1.99148	-0.00018
10	No	Show	10	H	4	3	2	1.101719	109.5508	-121.87	3.033875	-0.64849	0.882056
11	No	Show	11	H	5	3	2	1.09715	110.4499	179.9803	2.410437	1.646126	0.000552
12	No	Show	12	H	5	3	2	1.099198	110.8665	-59.0349	0.865922	1.838304	-0.88064
13	No	Show	13	H	5	3	2	1.099188	110.8696	58.98959	0.865114	1.838353	0.880364
14	No	Show	14	H	6	3	2	1.090592	120.1715	179.996	-0.08191	-1.81687	-7.2E-05
15	No	Show	15	H	1	7	2	0.974924	107.3267	0	-3.17163	-0.35192	0.000069

ISOCROTONATE (no. 239)

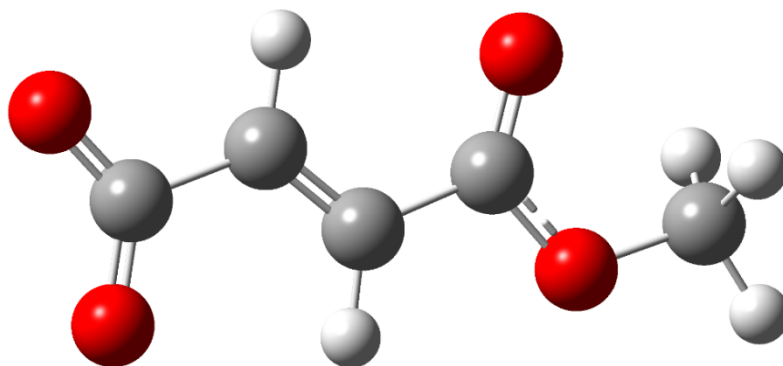


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.76436	-1.32883	0.103947
2	No	Show	2	O	1			2.239447			-2.21949	0.358558	-0.12063
3	No	Show	3	C	1	2		2.992946	86.21393		1.371785	0.766365	0.034671
4	No	Show	4	C	3	1	2	1.497187	77.33587	-169.26	2.154273	-0.5043	-0.08651
5	No	Show	5	C	3	1	2	1.341207	51.79807	6.942379	0.042327	0.938354	0.077057
6	No	Show	6	C	2	1	5	1.261546	27.44645	0.31715	-1.05349	-0.10384	0.014028
7	No	Show	7	H	3	1	6	1.096698	167.6452	23.41186	1.982742	1.675562	0.087943
8	No	Show	8	H	4	3	1	1.102448	109.8453	-112.435	2.760806	-0.65833	0.821116
9	No	Show	9	H	4	3	1	1.092716	112.0901	8.932951	1.507597	-1.37261	-0.23442
10	No	Show	10	H	4	3	1	1.101237	109.7686	131.1918	2.867372	-0.42437	-0.92187
11	No	Show	11	H	5	3	1	1.094239	117.7542	176.6535	-0.33708	1.962444	0.145227

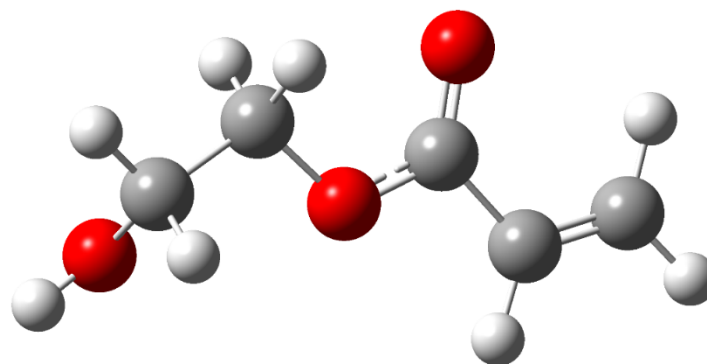
HYDROGEN FUMARATE (no. 240)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-2.73312	0.910183	0.000019
2	No	Show	2	O	1			2.243675			-2.17929	-1.26407	-4.6E-05
3	No	Show	3	O	2	1		5.082706	100.0315		2.889376	-0.8866	0.000019
4	No	Show	4	O	3	2	1	2.248814	77.27585	-0.00332	2.23252	1.264145	-4.5E-05
5	No	Show	5	C	1	2	3	2.336811	63.16156	0	-0.45212	0.402496	0.000029
6	No	Show	6	C	5	1	2	1.334702	153.2042	-0.00407	0.580076	-0.44367	0.000056
7	No	Show	7	C	2	1	5	1.21548	30.25188	0.000343	-1.84505	-0.09545	0
8	No	Show	8	C	3	2	1	1.256224	50.79048	-0.00304	2.02515	0.025108	-1.2E-05
9	No	Show	9	H	5	1	7	1.090686	85.45742	179.9981	-0.30023	1.482553	0.000026
10	No	Show	10	H	6	5	1	1.093722	120.052	0.007142	0.403482	-1.52304	-2.2E-05
11	No	Show	11	H	1	7	2	0.975637	107.8889	0	-3.62744	0.520231	-9E-06

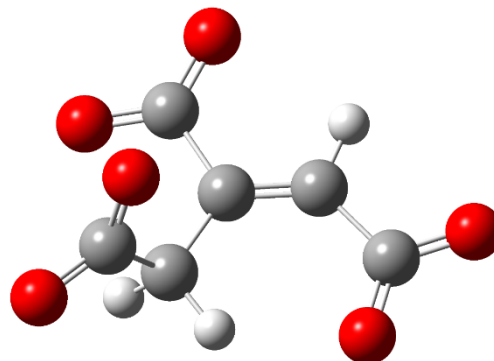
MONOMETHYL FUMARATE (no. 241)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							2.25362	-0.75708	0.000027
2	No	Show	2	O	1			2.244747			1.60349	1.391458	0.000418
3	No	Show	3	O	2	1		5.070401	100.1944		-3.43289	0.805082	-5.4E-05
4	No	Show	4	O	3	2	1	2.249523	77.58964	0.013238	-2.69861	-1.32123	0.000073
5	No	Show	5	C	1	2	3	2.332185	63.23443	-0.00587	-0.04363	-0.3549	0.000161
6	No	Show	6	C	2	1	5	1.215907	30.08391	-0.007	1.324834	0.207912	0.000146
7	No	Show	7	C	5	1	6	1.334747	152.9982	0.08017	-1.11056	0.447105	-0.00058
8	No	Show	8	C	1	6	2	1.432651	115.2433	-0.02354	3.610951	-0.29867	-0.00029
9	No	Show	9	C	4	3	2	1.256459	26.46866	0.00318	-2.53641	-0.07528	0.000087
10	No	Show	10	H	5	1	6	1.090859	85.53176	-179.958	-0.14746	-1.44081	0.000881
11	No	Show	11	H	7	5	1	1.09369	119.9183	-0.07631	-0.97701	1.532611	-0.00076
12	No	Show	12	H	8	1	6	1.097876	110.2711	60.57681	3.809626	0.302445	0.896663
13	No	Show	13	H	8	1	6	1.09786	110.2778	-60.4948	3.808961	0.303533	-0.89664
14	No	Show	14	H	8	1	6	1.093903	105.7956	-179.962	4.229868	-1.20065	-0.00104

2-HYDROXYETHYL ACRYLATE (no. 242)

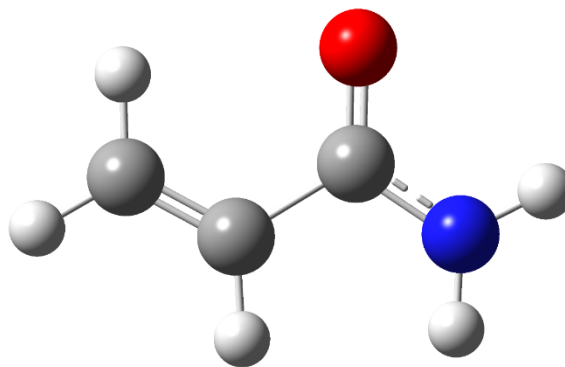
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-0.19671	-0.20081	0.219362
2	No	Show	2	O	1			2.800566			-2.79214	-0.88307	-0.58155
3	No	Show	3	O	1	2		2.245821	136.1999		1.290633	1.400773	-0.29682
4	No	Show	4	C	1	3	2	1.438919	88.75314	-37.3124	-1.24528	0.776645	0.094574
5	No	Show	5	C	2	1	4	1.417664	57.89269	-38.2261	-2.54357	0.091621	0.417434
6	No	Show	6	C	3	1	4	1.215538	29.9292	-179.917	1.043679	0.246668	-0.00598
7	No	Show	7	C	6	3	1	1.482488	125.3411	-179.922	2.048061	-0.83305	0.14631
8	No	Show	8	C	7	6	3	1.332661	119.9524	0.255592	3.341641	-0.56887	-0.03492
9	No	Show	9	H	4	1	6	1.0985	109.4596	-58.0736	-1.05713	1.605976	0.789925
10	No	Show	10	H	4	1	6	1.099719	108.9063	61.10665	-1.25036	1.16437	-0.93452
11	No	Show	11	H	5	2	1	1.103052	111.7084	150.4734	-3.33467	0.859861	0.443718
12	No	Show	12	H	5	2	1	1.103298	111.373	-88.4553	-2.47607	-0.36694	1.418648
13	No	Show	13	H	2	1	6	0.968222	145.2071	165.0517	-3.60419	-1.34853	-0.33384
14	No	Show	14	H	7	6	3	1.090407	117.0038	-179.777	1.674423	-1.82354	0.407695
15	No	Show	15	H	8	7	6	1.09094	121.363	179.9699	4.100173	-1.34565	0.071786
16	No	Show	16	H	8	7	6	1.092602	120.2769	-0.01254	3.666309	0.441224	-0.29584

TRANS-ACONITATE(3-) (no. 243)

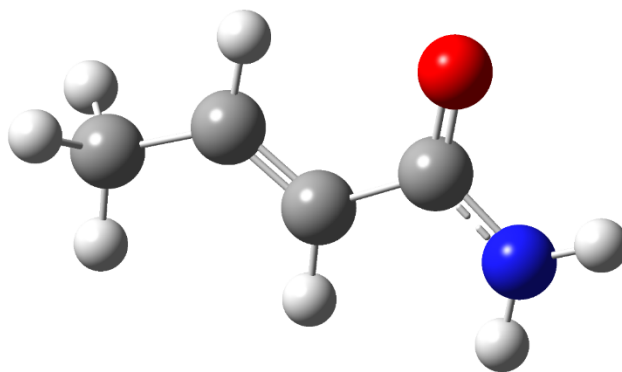


Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.64574	-0.84883	1.461645
2	No	Show	2	O	1			2.24089			-2.60877	-1.99889	-0.20314
3	No	Show	3	O	1	2		3.242204	81.78235		-1.97884	1.586928	-0.65213
4	No	Show	4	O	3	1	2	2.237527	90.77196	-157.989	-0.35573	2.737503	0.371699
5	No	Show	5	O	4	3	1	4.831639	107.7019	57.70176	3.628762	0.004856	0.336609
6	No	Show	6	O	5	4	3	2.236609	84.90326	-10.164	2.267104	-1.62012	-0.37597
7	No	Show	7	C	2	1	3	2.383203	62.58674	55.28175	-0.61903	-0.79003	-0.71231
8	No	Show	8	C	7	2	1	1.498863	138.5887	-31.3432	0.08014	0.460625	-0.2723
9	No	Show	9	C	8	7	2	1.343548	126.7376	133.8442	1.38604	0.592787	0.014547
10	No	Show	10	C	1	2	7	1.259512	27.24191	1.390969	-1.72104	-1.23638	0.265609
11	No	Show	11	C	4	3	1	1.259285	27.38797	50.83516	-0.82066	1.698882	-0.16765
12	No	Show	12	C	6	5	4	1.262187	27.63403	2.004324	2.498834	-0.43208	-0.01821
13	No	Show	13	H	7	2	1	1.095737	100.7224	106.9619	0.099464	-1.61161	-0.80933
14	No	Show	14	H	7	2	1	1.099247	84.29191	-145.196	-1.09834	-0.62767	-1.68814
15	No	Show	15	H	9	8	7	1.092844	116.5422	-179.482	1.71886	1.584903	0.329578

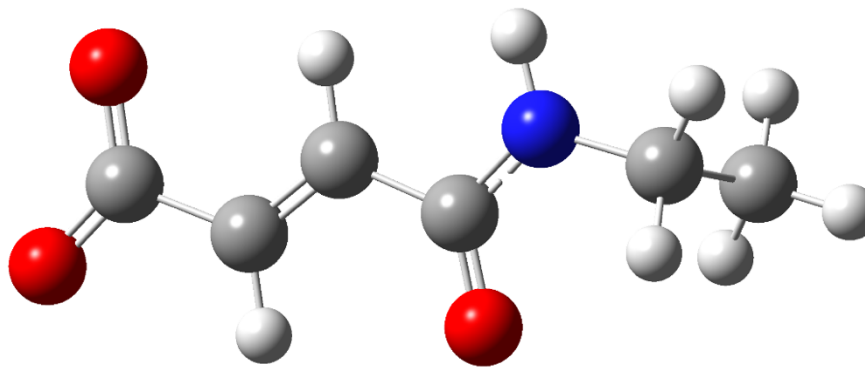
ACRYLAMIDE (no. 244)



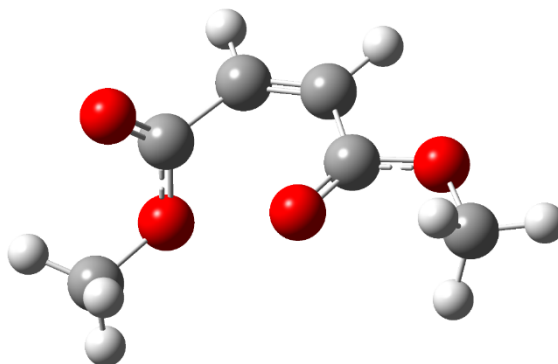
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.508118	1.353903	-0.00003
2	No	Show	2	N	1			2.263412			1.597272	-0.63023	-2.6E-05
3	No	Show	3	C	1	2		1.235409	29.97882		0.481922	0.118772	0.000126
4	No	Show	4	C	3	1	2	1.492724	122.4917	-179.978	-0.79386	-0.65621	0.000018
5	No	Show	5	C	4	3	1	1.331959	120.3065	-0.0114	-1.96533	-0.02235	-2.7E-05
6	No	Show	6	H	4	3	1	1.092549	117.8316	179.9895	-0.72821	-1.74678	-6E-06
7	No	Show	7	H	2	1	3	1.012978	148.5778	0.018918	1.550289	-1.64212	-6.7E-05
8	No	Show	8	H	2	1	3	1.01467	91.9881	-179.991	2.503146	-0.17312	-0.00013
9	No	Show	9	H	5	4	3	1.090944	121.5297	-179.999	-2.90961	-0.56871	-8.2E-05
10	No	Show	10	H	5	4	3	1.092659	120.12	0.000789	-1.99781	1.069824	0.000002

CROTONAMIDE (no. 245)

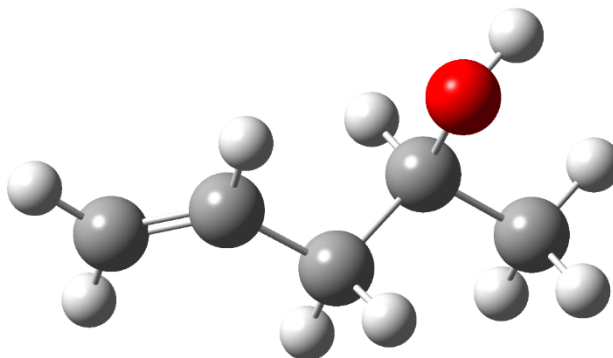
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.318706	1.315155	-6E-06
2	No	Show	2	N	1			2.26155			2.10972	-0.80355	0.000007
3	No	Show	3	C	1	2		2.842106	89.57749		-1.33648	0.301475	0
4	No	Show	4	C	3	1	2	1.336503	57.15159	0.000311	-0.25875	-0.48893	0.000011
5	No	Show	5	C	3	1	2	1.490498	177.6654	-179.992	-2.74945	-0.17297	-6E-06
6	No	Show	6	C	1	2	4	1.237646	30.23384	0.001449	1.108881	0.095425	0.000019
7	No	Show	7	H	3	1	6	1.095324	60.31009	179.999	-1.16902	1.383922	-5E-06
8	No	Show	8	H	4	3	1	1.093639	121.42	-180	-0.35095	-1.57867	0.000017
9	No	Show	9	H	5	3	1	1.101073	110.2151	-58.5901	-3.28159	0.216522	0.881749
10	No	Show	10	H	5	3	1	1.101073	110.215	58.574	-3.28157	0.216508	-0.88178
11	No	Show	11	H	5	3	1	1.097895	111.812	179.9919	-2.81172	-1.2691	0.000002
12	No	Show	12	H	2	1	6	1.012925	148.8494	0.01037	1.922043	-1.79894	-6.7E-05
13	No	Show	13	H	2	1	6	1.014301	91.67334	179.9977	3.069909	-0.47668	-6.4E-05

4-(ETHYLAMINO)-4-OXOBUT-2-ENOATE (no. 246)

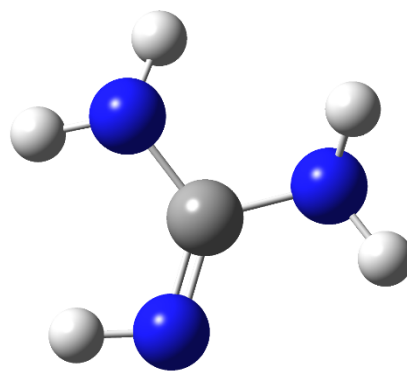
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.074915	-1.42928	0.24734
2	No	Show	2	O	1			5.037206			-3.90792	-0.79907	-0.13688
3	No	Show	3	O	2	1		2.2482	78.08766		-3.16784	1.323577	-0.16924
4	No	Show	4	N	1	2	3	2.264467	102.488	4.400662	1.828731	0.70154	0.38586
5	No	Show	5	C	4	1	2	1.454808	94.1013	-179.073	3.228319	0.312	0.462529
6	No	Show	6	C	5	4	1	1.522267	112.8153	80.54751	3.826723	-0.01056	-0.89952
7	No	Show	7	C	1	4	5	1.239048	30.17731	-176.7	0.848951	-0.21101	0.246993
8	No	Show	8	C	7	1	4	1.489329	122.6648	-179.066	-0.52345	0.351936	0.113893
9	No	Show	9	C	8	7	1	1.334205	121.1105	1.445053	-1.58896	-0.44504	0.01588
10	No	Show	10	C	2	1	7	1.257581	51.44047	3.196058	-3.00681	0.077676	-0.10818
11	No	Show	11	H	5	4	1	1.096673	107.5351	-157.007	3.774046	1.133239	0.942571
12	No	Show	12	H	5	4	1	1.098524	107.619	-41.0803	3.29375	-0.56522	1.120531
13	No	Show	13	H	4	1	7	1.014616	145.9465	-7.24326	1.590035	1.684487	0.306579
14	No	Show	14	H	6	5	4	1.099552	110.3734	-59.8979	3.280541	-0.84038	-1.37078
15	No	Show	15	H	6	5	4	1.099627	110.8251	60.47274	3.77877	0.863841	-1.56458
16	No	Show	16	H	6	5	4	1.09947	110.1447	-179.528	4.879855	-0.30674	-0.78988
17	No	Show	17	H	8	7	1	1.093332	118.5109	-178.853	-0.64295	1.438661	0.102845
18	No	Show	18	H	9	8	7	1.09358	119.7024	-0.04804	-1.45707	-1.53052	0.032321

CIS-DIMETHYL FUMARATE (no. 247)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.82122	-0.39193	-0.78894
2	No	Show	2	O	1			4.521804			2.621394	0.230857	-0.22142
3	No	Show	3	O	1	2		2.24756	87.65175		-2.1123	0.486768	1.259155
4	No	Show	4	O	2	1	3	2.246229	32.6317	61.38079	0.745621	-0.77597	0.495034
5	No	Show	5	C	1	3	4	2.349503	62.55317	-69.3278	-0.67564	1.598144	-0.29152
6	No	Show	6	C	5	1	3	1.333392	113.0038	118.4056	0.649775	1.465281	-0.35118
7	No	Show	7	C	3	1	5	1.210662	29.29825	-1.95472	-1.59473	0.508156	0.164913
8	No	Show	8	C	4	2	1	1.215408	29.63729	-36.4806	1.311166	0.189522	0.02049
9	No	Show	9	C	1	7	3	1.435655	114.9183	-5.66146	-2.64768	-1.49728	-0.39363
10	No	Show	10	C	2	1	7	1.434664	114.2854	121.8692	3.345762	-0.96043	0.116782
11	No	Show	11	H	5	1	7	1.092422	118.3473	-93.5036	-1.15521	2.548208	-0.53806
12	No	Show	12	H	6	5	1	1.089703	121.4529	147.4063	1.290178	2.288799	-0.66607
13	No	Show	13	H	9	1	7	1.097318	110.4257	60.27159	-3.63551	-1.14187	-0.0743
14	No	Show	14	H	9	1	7	1.098155	109.6635	-60.9325	-2.16494	-2.04473	0.426859
15	No	Show	15	H	9	1	7	1.093648	105.6393	179.9023	-2.73482	-2.13202	-1.27996
16	No	Show	16	H	10	2	1	1.097565	110.1031	40.29874	2.967977	-1.81003	-0.46641
17	No	Show	17	H	10	2	1	1.097555	110.0936	-80.7638	3.242953	-1.17274	1.188689
18	No	Show	18	H	10	2	1	1.093591	105.6816	159.7549	4.389353	-0.75375	-0.13648

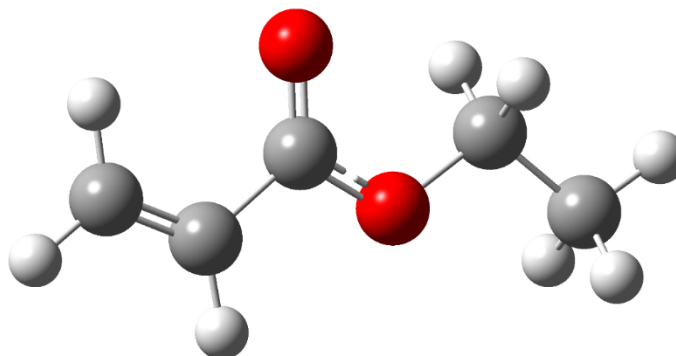
4-PENTEN-2-OL (no. 248)

Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							1.085739	1.348276	0.083572
2	No	Show	2	C	1			1.427849			0.869277	-0.00304	-0.32367
3	No	Show	3	C	2	1		1.526382	106.5716		-0.33498	-0.50826	0.466496
4	No	Show	4	C	2	1	3	1.518558	110.7176	-122.013	2.107901	-0.84484	-0.07228
5	No	Show	5	C	3	2	1	1.500224	112.6759	60.50141	-1.57801	0.287706	0.198215
6	No	Show	6	C	5	3	2	1.333731	124.5565	121.6171	-2.71629	-0.22297	-0.27335
7	No	Show	7	H	2	1	3	1.105676	109.5349	117.2531	0.619731	-0.0292	-1.4005
8	No	Show	8	H	3	2	1	1.104457	107.1497	-60.2604	-0.07337	-0.44086	1.537404
9	No	Show	9	H	3	2	1	1.100282	109.1873	-176.847	-0.50595	-1.56838	0.226637
10	No	Show	10	H	4	2	1	1.100469	110.304	-59.6164	2.964656	-0.44023	-0.632
11	No	Show	11	H	4	2	1	1.10076	110.0358	60.038	2.357036	-0.8384	0.999898
12	No	Show	12	H	4	2	1	1.099537	110.9395	-179.514	1.948121	-1.88447	-0.39263
13	No	Show	13	H	5	3	2	1.09516	116.026	-57.4748	-1.51315	1.362358	0.398943
14	No	Show	14	H	1	2	4	0.968955	107.1783	59.79752	1.831187	1.687329	-0.43433
15	No	Show	15	H	6	5	3	1.092258	121.451	-179.505	-3.5899	0.406167	-0.4578
16	No	Show	16	H	6	5	3	1.094347	121.1556	0.753645	-2.81165	-1.29207	-0.48671

GUANIDINE (no. 249)

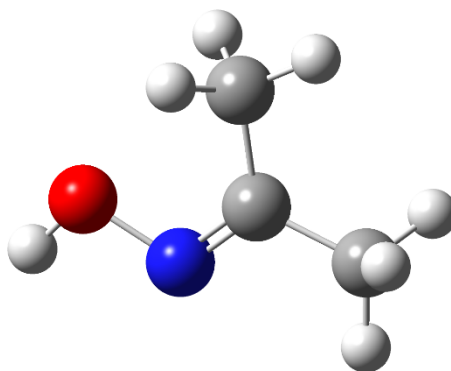
Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	N							1.315322	0.224746	-0.0986
2	No	Show	2	N	1			2.318612			-0.86793	0.981006	0.094935
3	No	Show	3	N	1	2		2.321298	61.8072		-0.38614	-1.35102	0.003373
4	No	Show	4	C	3	1	2	1.286258	30.99887	0.272905	-0.02571	-0.11631	-0.00107
5	No	Show	5	H	1	4	3	1.016985	111.625	-19.8569	1.919224	-0.55094	0.161928
6	No	Show	6	H	1	4	3	1.018043	113.4364	-146.58	1.556516	1.070071	0.414881
7	No	Show	7	H	2	1	4	1.017244	142.8625	-34.3642	-1.82486	0.77562	-0.18233
8	No	Show	8	H	2	1	4	1.01822	84.26626	-152.545	-0.51494	1.809678	-0.37991
9	No	Show	9	H	3	1	4	1.02512	139.2553	7.553781	-1.41049	-1.38969	-0.00614

ETHYL ACRYLATE (no. 250)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							0.578671	-0.4348	-5.6E-05
2	No	Show	2	O	1			2.246026			-0.70584	1.407663	0.000013
3	No	Show	3	C	1	2		1.443193	88.89861		1.746469	0.413172	0.000005
4	No	Show	4	C	3	1	2	1.507963	107.3209	179.9972	2.955601	-0.48791	0.000051
5	No	Show	5	C	2	1	3	1.216252	29.86885	179.9949	-0.59954	0.196066	-9.9E-05
6	No	Show	6	C	5	2	1	1.482973	125.2019	179.987	-1.73195	-0.76145	-2.2E-05
7	No	Show	7	C	6	5	2	1.33261	120.0377	0.006104	-2.98621	-0.31122	0.000062
8	No	Show	8	H	3	1	5	1.099131	108.4682	-58.703	1.710041	1.055984	-0.89081
9	No	Show	9	H	3	1	5	1.099131	108.4683	58.70245	1.709961	1.055969	0.890829
10	No	Show	10	H	4	3	1	1.098389	109.4741	180	3.868012	0.123615	0.000097
11	No	Show	11	H	4	3	1	1.098876	110.7047	-60.4071	2.963754	-1.1271	0.893866
12	No	Show	12	H	4	3	1	1.098876	110.7047	60.40692	2.963834	-1.12708	-0.89377
13	No	Show	13	H	6	5	2	1.090477	116.9886	-179.994	-1.48243	-1.823	-4.3E-05
14	No	Show	14	H	7	6	5	1.09099	121.3738	179.9995	-3.8355	-0.99603	0.000111
15	No	Show	15	H	7	6	5	1.092566	120.3137	-0.00033	-3.18658	0.762811	0.00008

ACETONE OXIME (no. 251)



Row	Highlight	Display	Tag	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	No	Show	1	O							-1.81461	-0.14675	-6E-06
2	No	Show	2	N	1			1.398943			-0.60253	-0.84524	0.000009
3	No	Show	3	C	2	1		1.280146	110.8638		0.38976	-0.03645	-4E-06
4	No	Show	4	C	3	2	1	1.49483	117.4726	-180	1.762218	-0.6288	0.000001
5	No	Show	5	C	3	2	1	1.49884	123.2342	0.001398	0.234432	1.45432	-1E-06
6	No	Show	6	H	4	3	2	1.096695	111.1312	-0.01026	1.719858	-1.72467	0.000199
7	No	Show	7	H	4	3	2	1.100781	109.8641	121.2075	2.318195	-0.28452	-0.88548
8	No	Show	8	H	4	3	2	1.100778	109.8646	-121.23	2.318341	-0.28418	0.885258
9	No	Show	9	H	5	3	2	1.0961	110.9236	-179.99	1.212174	1.949755	-0.00019
10	No	Show	10	H	5	3	2	1.100137	110.1551	-58.7804	-0.33729	1.775871	-0.8832
11	No	Show	11	H	5	3	2	1.100141	110.1542	58.80214	-0.33693	1.775889	0.883428
12	No	Show	12	H	1	2	3	0.968319	103.3058	179.9996	-2.47821	-0.85193	-1E-06