Supporting Information for

Dipole Preserving and Polarization Consistent Charges

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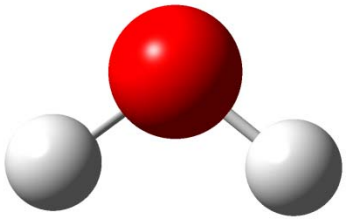
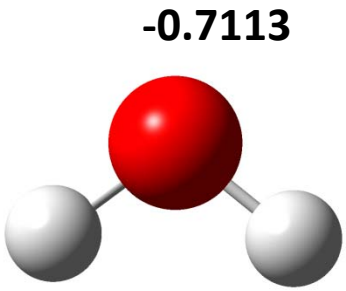
Partial atomic charges obtained from Mulliken population analysis, the present dipole preserving charge (DPC) analysis (polarization is absent for a single molecule in the gas phase), and the class IV CM2 model using the Austin Model 1 (AM1) Hamiltonian. All calculations are performed at the optimized geometry using AM1 at the conformation as illustrated in this supporting information. Atomic coordinates are not listed since the calculations can be repeated with little efforts.

Alcohols and water

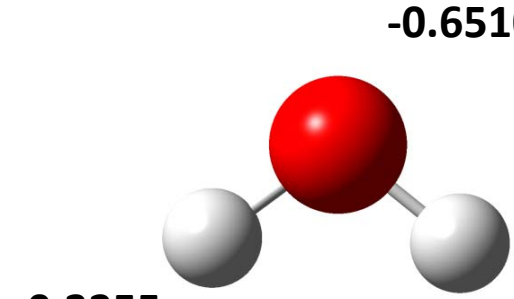
Water



Mulliken



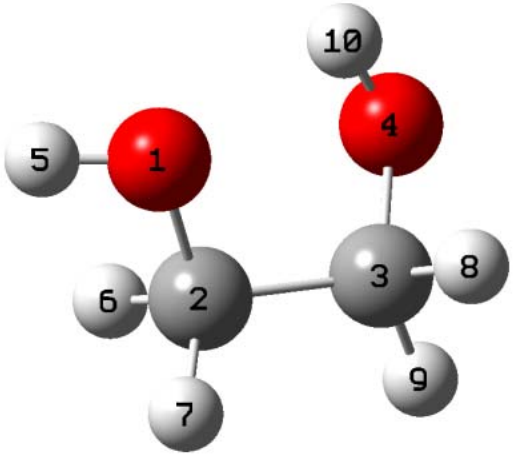
CM2 Charge



DPPC

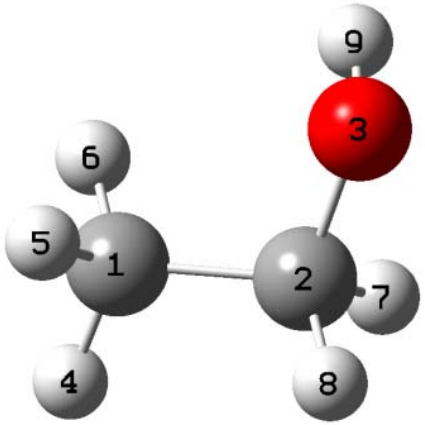
*All the calculations are using AM1 wave function

1,2-ethanediol



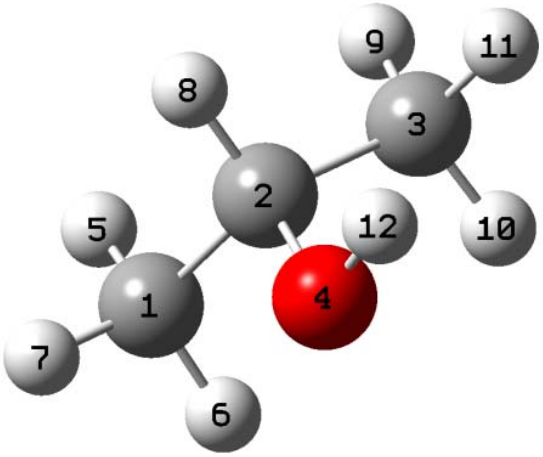
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.3389	-0.4731	-0.537193
2	C	-0.0640	0.0033	0.014506
3	C	-0.0181	0.0534	0.060906
4	O	-0.3274	-0.4917	-0.525138
5	H	0.2054	0.3047	0.361812
6	H	0.0762	0.0792	0.058008
7	H	0.0702	0.0618	0.052104
8	H	0.0770	0.0645	0.058903
9	H	0.1065	0.0759	0.088369
10	H	0.2132	0.3220	0.367725

ethanol



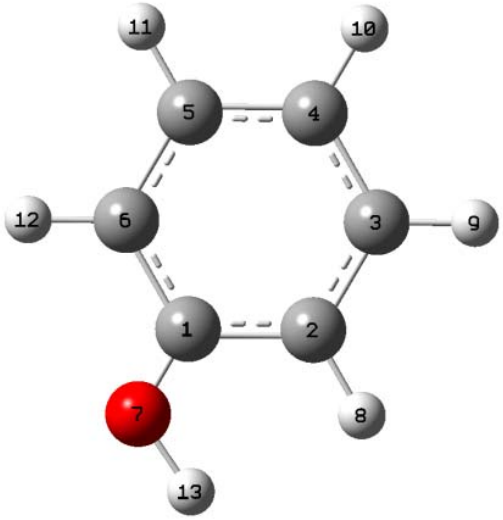
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2538	-0.2442	-0.1965
2	C	-0.0244	0.0547	0.0540
3	O	-0.3270	-0.4891	-0.5264
4	H	0.0842	0.0791	0.0652
5	H	0.0884	0.0865	0.0694
6	H	0.0727	0.0730	0.0536
7	H	0.0607	0.0533	0.0426
8	H	0.1045	0.0782	0.0863
9	H	0.1949	0.3085	0.3518

2-propannol



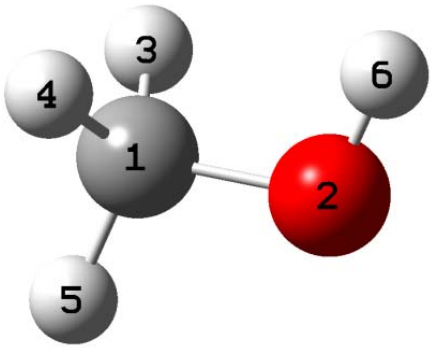
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2091	-0.2085	-0.152102
2	C	0.0276	0.1155	0.086625
3	C	-0.2499	-0.2426	-0.192476
4	O	-0.3291	-0.4878	-0.527778
5	H	0.0766	0.0669	0.05767
6	H	0.0860	0.0799	0.067005
7	H	0.0888	0.0786	0.069802
8	H	0.0679	0.0567	0.05008
9	H	0.0844	0.0796	0.06536
10	H	0.0884	0.0865	0.069424
11	H	0.0720	0.0706	0.0529
12	H	0.1964	0.3047	0.3535

phenol



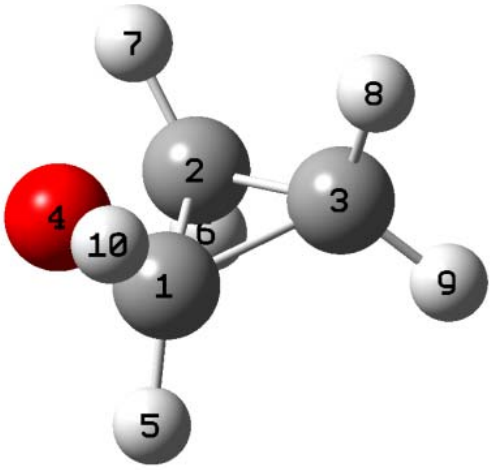
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0779	0.2009	0.1238
2	C	-0.2134	-0.1912	-0.1945
3	C	-0.0916	-0.0611	-0.0734
4	C	-0.1656	-0.1358	-0.1473
5	C	-0.0970	-0.0690	-0.0789
6	C	-0.1566	-0.1420	-0.1381
7	O	-0.2527	-0.4378	-0.4543
8	H	0.1327	0.1015	0.1147
9	H	0.1322	0.0982	0.1141
10	H	0.1333	0.0998	0.1152
11	H	0.1339	0.0997	0.1159
12	H	0.1497	0.1078	0.1318
13	H	0.2173	0.3290	0.3710

methanol



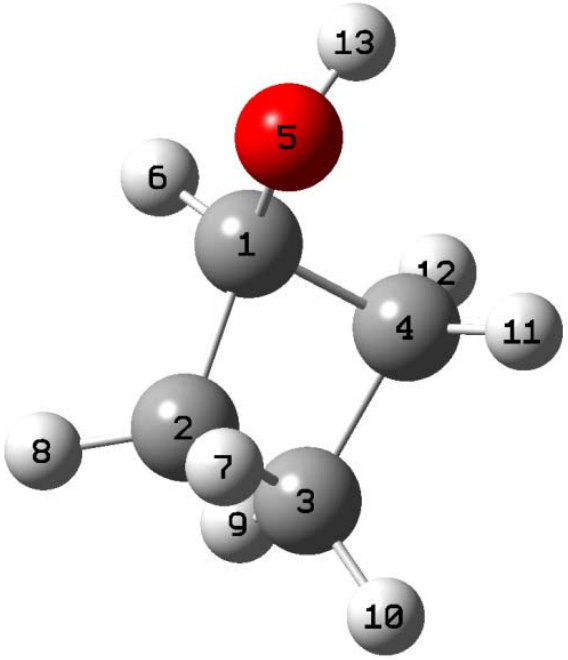
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0733	-0.0136	0.0251
2	O	-0.3260	-0.4774	-0.5263
3	H	0.0529	0.0547	0.0345
4	H	0.0530	0.0547	0.0345
5	H	0.0980	0.0760	0.0795
6	H	0.1954	0.3055	0.3528

cyclopropanol



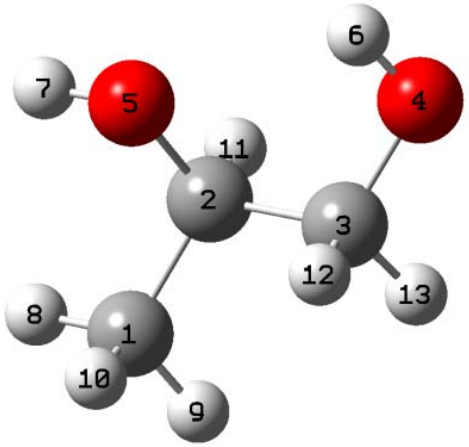
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0407	0.0708	0.1310
2	C	-0.1987	-0.1647	-0.1278
3	C	-0.2487	-0.2216	-0.1843
4	O	-0.2961	-0.4895	-0.6877
5	H	0.1156	0.0796	0.0623
6	H	0.1123	0.0925	0.0740
7	H	0.1248	0.1057	0.0874
8	H	0.1169	0.1021	0.0837
9	H	0.1120	0.0932	0.0747
10	H	0.2026	0.3318	0.4866

cyclobutanol



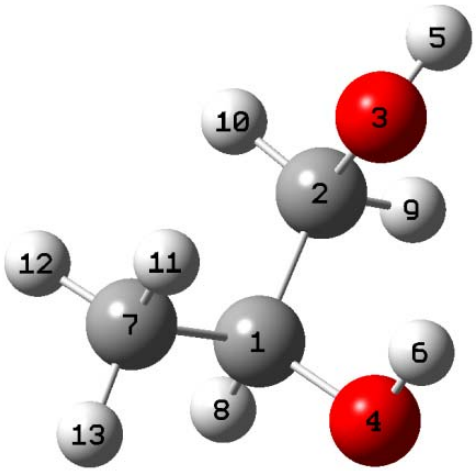
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0073	0.0985	0.0673
2	C	-0.1657	-0.1522	-0.1284
3	C	-0.1685	-0.1493	-0.131
4	C	-0.2092	-0.1913	-0.1714
5	O	-0.3148	-0.4831	-0.5135
6	H	0.0824	0.0638	0.0646
7	H	0.1098	0.0934	0.0912
8	H	0.0916	0.0783	0.0729
9	H	0.0874	0.0760	0.0687
10	H	0.0929	0.0812	0.0742
11	H	0.0975	0.0921	0.0788
12	H	0.0899	0.0795	0.0712
13	H	0.1994	0.3132	0.3553

Anti-1,2-propanediol



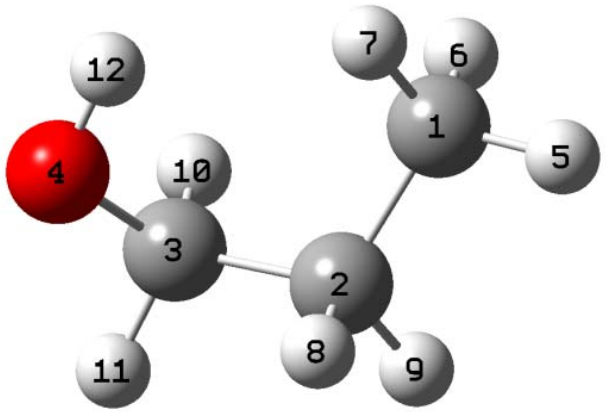
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2474	-0.2415	-0.1900
2	C	-0.0154	0.0671	0.0440
3	C	-0.0114	0.0570	0.0678
4	O	-0.3268	-0.4917	-0.5244
5	O	-0.3399	-0.4689	-0.5373
6	H	0.2151	0.3191	0.3692
7	H	0.2056	0.2992	0.3614
8	H	0.0767	0.0742	0.0577
9	H	0.0880	0.0817	0.0690
10	H	0.0900	0.0863	0.0711
11	H	0.0854	0.0805	0.0675
12	H	0.0747	0.0626	0.0567
13	H	0.1053	0.0747	0.0872

Gauche-1,2-propanediol



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0332	0.1224	0.0933
2	C	-0.0574	0.0053	0.0212
3	O	-0.3378	-0.4571	-0.5361
4	O	-0.3256	-0.4956	-0.5225
5	H	0.2054	0.2962	0.3618
6	H	0.213	0.3197	0.3671
7	C	-0.2456	-0.2411	-0.1883
8	H	0.1119	0.0762	0.0941
9	H	0.0744	0.0739	0.0562
10	H	0.07	0.0602	0.0519
11	H	0.0912	0.0840	0.0723
12	H	0.0785	0.0731	0.0595
13	H	0.0886	0.0828	0.0696

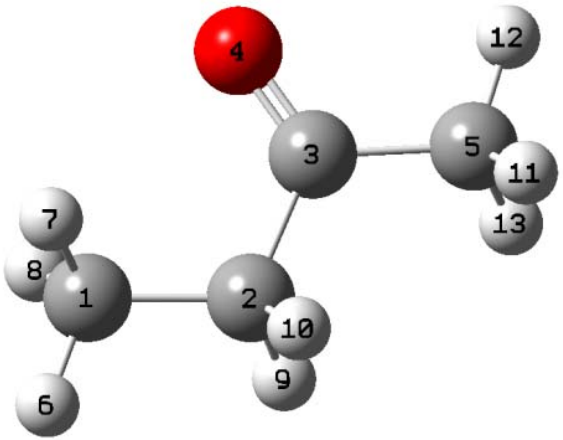
Gauche-propannol



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2151	-0.2046	-0.1580
2	C	-0.2020	-0.1810	-0.1643
3	C	-0.0223	0.0556	0.0563
4	O	-0.3262	-0.4891	-0.5251
5	H	0.0792	0.0738	0.0601
6	H	0.0737	0.0692	0.0546
7	H	0.0688	0.0676	0.0498
8	H	0.0946	0.0891	0.0760
9	H	0.0881	0.0799	0.0695
10	H	0.0612	0.0544	0.0431
11	H	0.1034	0.0760	0.0852
12	H	0.1964	0.3091	0.3526

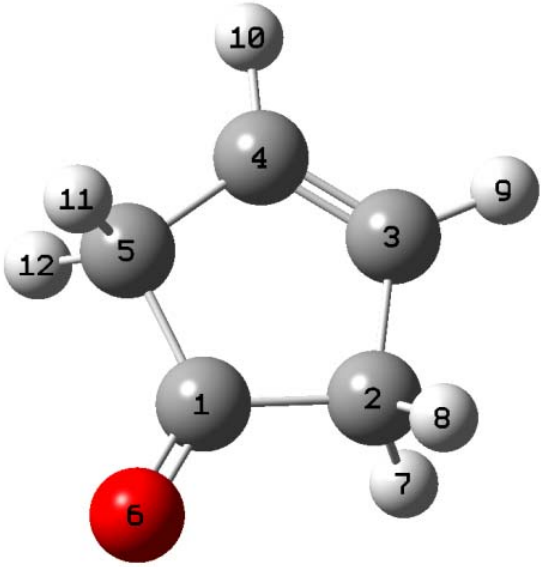
Aldehydes and ketones

2-butanone



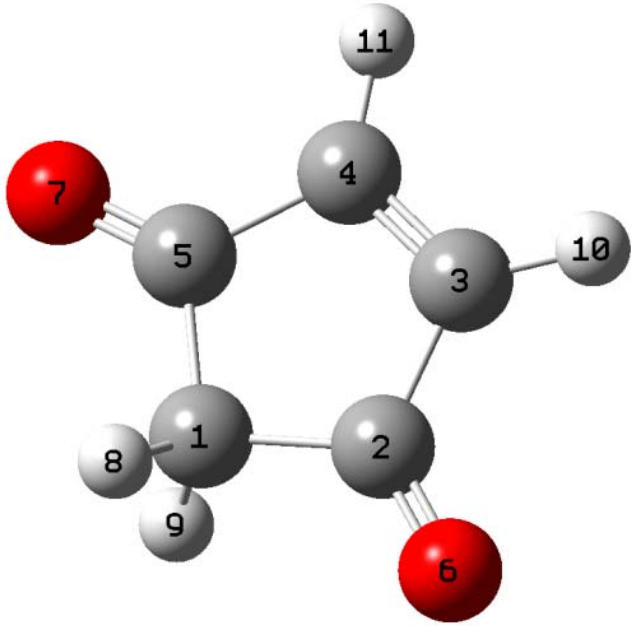
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2058	-0.1979	-0.1488
2	C	-0.2109	-0.1970	-0.1734
3	C	0.2233	0.3489	0.3485
4	O	-0.2897	-0.3793	-0.4169
5	C	-0.2732	-0.2738	-0.2161
6	H	0.0739	0.0653	0.0549
7	H	0.0868	0.0808	0.0678
8	H	0.0866	0.0806	0.0676
9	H	0.1014	0.0926	0.0832
10	H	0.1016	0.0928	0.0834
11	H	0.0995	0.0942	0.0809
12	H	0.1069	0.0986	0.088
13	H	0.0995	0.0942	0.0809

3-cyclopentenenone



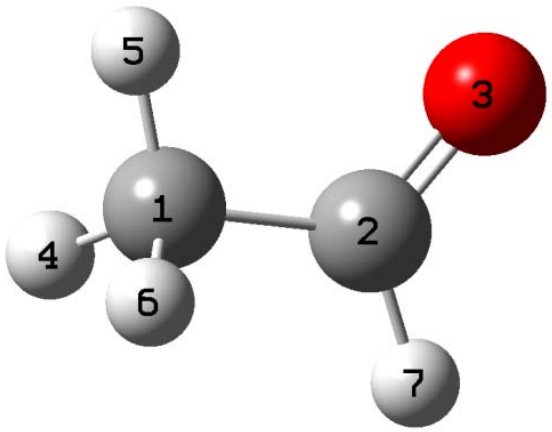
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2293	0.3508	0.3558
2	C	-0.1973	-0.1899	-0.1606
3	C	-0.1703	-0.1337	-0.1523
4	C	-0.1703	-0.1337	-0.1524
5	C	-0.1973	-0.1899	-0.1605
6	O	-0.2812	-0.3731	-0.41
7	H	0.1242	0.1100	0.1063
8	H	0.1242	0.1099	0.1064
9	H	0.1451	0.1149	0.1273
10	H	0.1451	0.1149	0.1273
11	H	0.1242	0.1100	0.1064
12	H	0.1242	0.1100	0.1063

4-cyclopentene-1,3-dinone



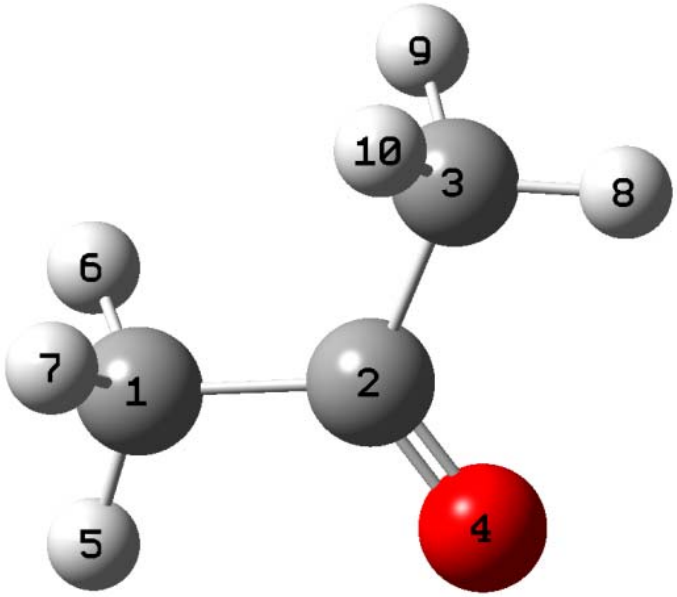
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2777	-0.2837	-0.2402
2	C	0.2448	0.3642	0.3718
3	C	-0.1739	-0.1489	-0.1546
4	C	-0.1739	-0.1490	-0.1547
5	C	0.2448	0.3643	0.3718
6	O	-0.2512	-0.3480	-0.381
7	O	-0.2512	-0.3481	-0.381
8	H	0.1492	0.1358	0.1315
9	H	0.1492	0.1358	0.1315
10	H	0.17	0.1388	0.1524
11	H	0.1699	0.1388	0.1523

acetaldehyde



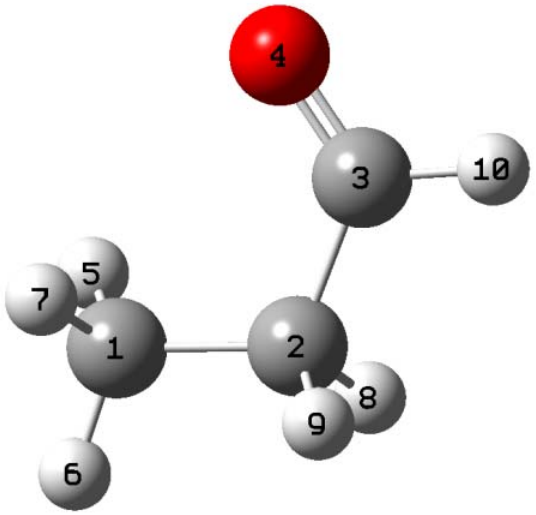
ATOMNO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2893	-0.2847	-0.2324
2	C	0.1804	0.2906	0.3256
3	O	-0.2867	-0.3639	-0.4169
4	H	0.1028	0.0985	0.0843
5	H	0.107	0.1027	0.0881
6	H	0.1026	0.0982	0.0841
7	H	0.0832	0.0586	0.0672

acetone



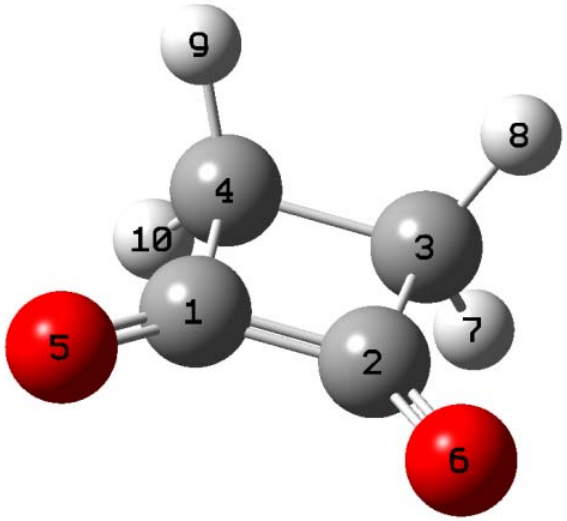
ATOM NO.	TYPE	MULLIKEN	TOTAL	CM2
1	C	-0.2724	-0.2729	-0.2154
2	C	0.2241	0.3523	0.3489
3	C	-0.2724	-0.2729	-0.2154
4	O	-0.2922	-0.3815	-0.4190
5	H	0.107	0.0987	0.0881
6	H	0.0998	0.0945	0.0813
7	H	0.0997	0.0943	0.0811
8	H	0.107	0.0987	0.0880
9	H	0.0998	0.0945	0.0812
10	H	0.0998	0.0944	0.0812

Cis propanal



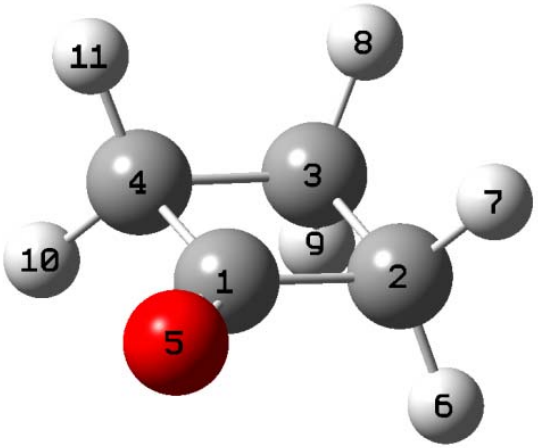
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2063	-0.1970	-0.1493
2	C	-0.2276	-0.2078	-0.1903
3	C	0.18	0.2897	0.3256
4	O	-0.2844	-0.3625	-0.415
5	H	0.0863	0.0807	0.0673
6	H	0.0751	0.0668	0.0561
7	H	0.0864	0.0808	0.0674
8	H	0.1043	0.0966	0.0862
9	H	0.1043	0.0966	0.0862
10	H	0.0818	0.0560	0.0658

Cyclobutane-1,2-dione



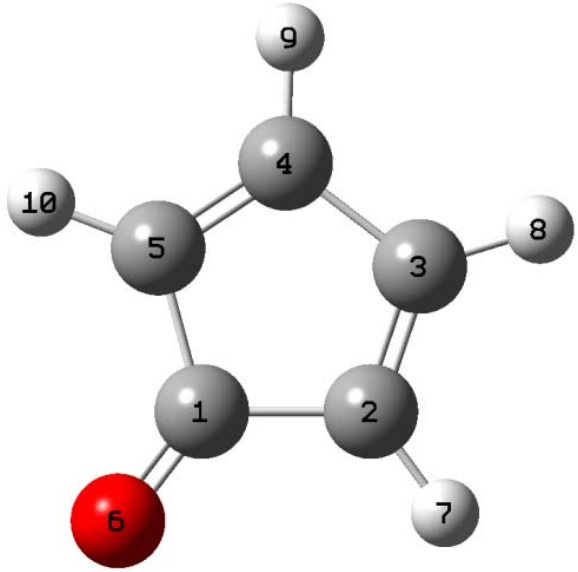
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.1788	0.2897	0.3134
2	C	0.1788	0.2897	0.3135
3	C	-0.2231	-0.2177	-0.1854
4	C	-0.2233	-0.2179	-0.1856
5	O	-0.2081	-0.3007	-0.3442
6	O	-0.2081	-0.3007	-0.3442
7	H	0.1262	0.1144	0.1081
8	H	0.1263	0.1144	0.1082
9	H	0.1263	0.1144	0.1081
10	H	0.1262	0.1144	0.1081

cyclobutanone



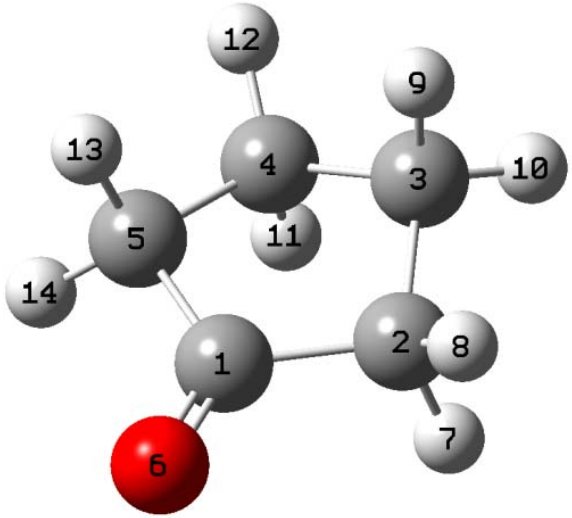
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2286	0.3576	0.3575
2	C	-0.2306	-0.2226	-0.1929
3	C	-0.1679	-0.1529	-0.1304
4	C	-0.2306	-0.2226	-0.1929
5	O	-0.2606	-0.3590	-0.3920
6	H	0.1169	0.1079	0.0987
7	H	0.117	0.1079	0.0987
8	H	0.0966	0.0841	0.0780
9	H	0.0966	0.0841	0.0779
10	H	0.1169	0.1079	0.0987
11	H	0.117	0.1079	0.0987

cyclopentadienone



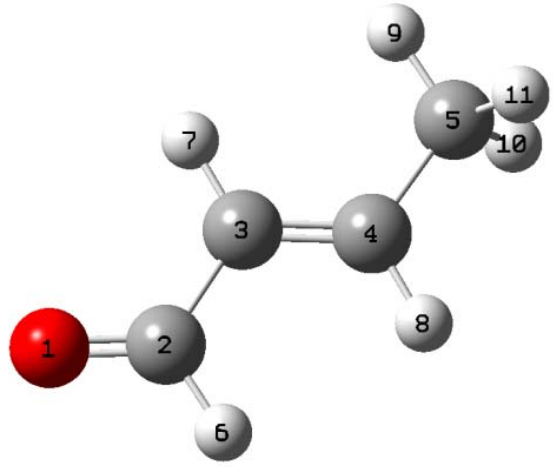
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2659	0.3842	0.3936
2	C	-0.2264	-0.2072	-0.2078
3	C	-0.1073	-0.0717	-0.0888
4	C	-0.1073	-0.0717	-0.0888
5	C	-0.2264	-0.2072	-0.2078
6	O	-0.2372	-0.3350	-0.3681
7	H	0.1662	0.1343	0.1485
8	H	0.1532	0.1200	0.1354
9	H	0.1531	0.1200	0.1354
10	H	0.1662	0.1343	0.1485

cyclopentanenone



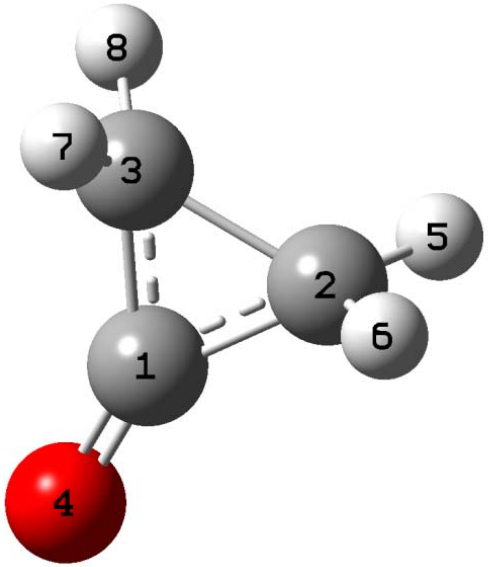
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2338	0.3585	0.3591
2	C	-0.2186	-0.2094	-0.1814
3	C	-0.1578	-0.1399	-0.1203
4	C	-0.1579	-0.1399	-0.1204
5	C	-0.2186	-0.2093	-0.1813
6	O	-0.2903	-0.3809	-0.4179
7	H	0.1154	0.1049	0.0971
8	H	0.1157	0.1046	0.0975
9	H	0.0864	0.0754	0.0675
10	H	0.0872	0.0756	0.0689
11	H	0.0863	0.0753	0.0674
12	H	0.0873	0.0756	0.0688
13	H	0.1154	0.1049	0.0973
14	H	0.1157	0.1046	0.0975

E-2-butenal



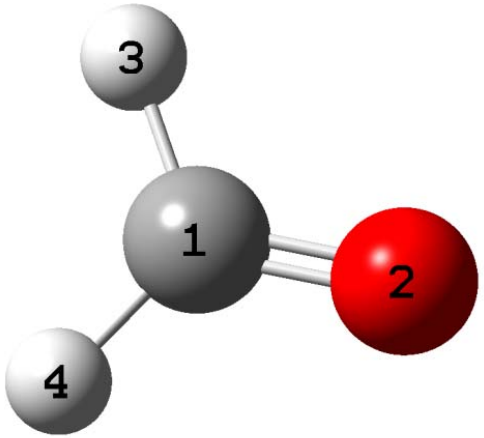
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.287	-0.3681	-0.4155
2	C	0.2092	0.3101	0.3518
3	C	-0.2596	-0.2301	-0.2408
4	C	-0.0885	-0.0450	-0.0697
5	C	-0.2029	-0.1964	-0.1469
6	H	0.083	0.0531	0.0669
7	H	0.1487	0.1273	0.1309
8	H	0.1218	0.1009	0.1039
9	H	0.0887	0.0803	0.0697
10	H	0.0934	0.0841	0.0749
11	H	0.0932	0.0838	0.0747

cyclopropanone



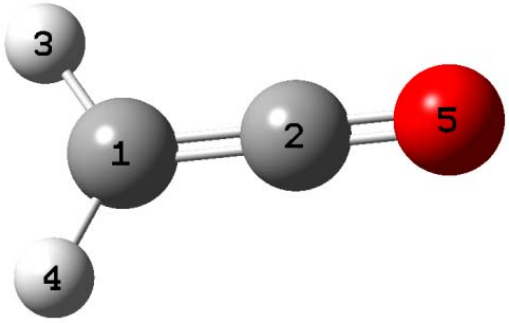
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.224	0.3654	0.3542
2	C	-0.2723	-0.2521	-0.2348
3	C	-0.2724	-0.2522	-0.2349
4	O	-0.2128	-0.3287	-0.3461
5	H	0.1334	0.1169	0.1154
6	H	0.1334	0.1169	0.1154
7	H	0.1334	0.1169	0.1154
8	H	0.1334	0.1169	0.1154

formaldehyde



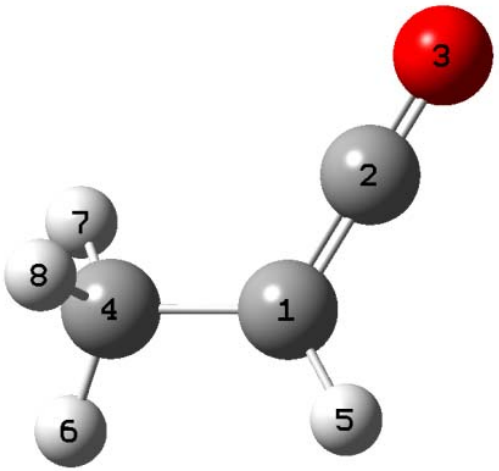
ATOM NO.	TYPE	MULLIKEN	TOTAL	CM2
1	C	0.1384	0.2285	0.3054
2	O	-0.2759	-0.3395	-0.4106
3	H	0.0688	0.0555	0.0526
4	H	0.0687	0.0555	0.0525

Ketene



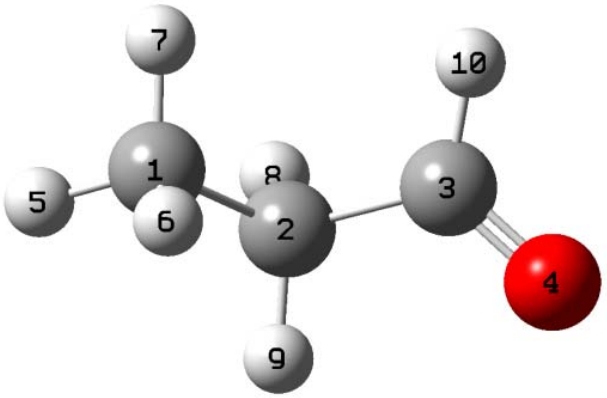
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.4414	-0.4446	-0.4030
2	C	0.2559	0.4344	0.3937
3	H	0.1764	0.1423	0.1595
4	H	0.1764	0.1423	0.1595
5	O	-0.1673	-0.2743	-0.3097

methylketene



ATOM NO.	TYPE	MULLIKEN	TOTAL	CM2
1	C	-0.3703	-0.3785	-0.3493
2	C	0.2492	0.3924	0.3881
3	O	-0.1611	-0.2563	-0.3045
4	C	-0.1284	-0.1539	-0.0716
5	H	0.1761	0.1595	0.1594
6	H	0.08	0.0631	0.0613
7	H	0.0737	0.1115	0.0546
8	H	0.0807	0.0622	0.062

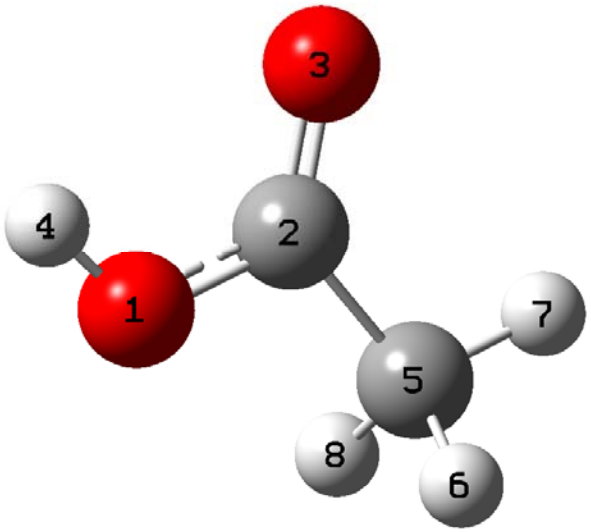
Trans-propanal



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2054	-0.1963	-0.1525
2	C	-0.2304	-0.2167	-0.1957
3	C	0.1867	0.2953	0.3279
4	O	-0.2794	-0.3567	-0.4189
5	H	0.0823	0.0756	0.064
6	H	0.08	0.0748	0.0604
7	H	0.0744	0.0697	0.0565
8	H	0.1043	0.0981	0.0928
9	H	0.1088	0.1022	0.0951
10	H	0.0788	0.0540	0.0703

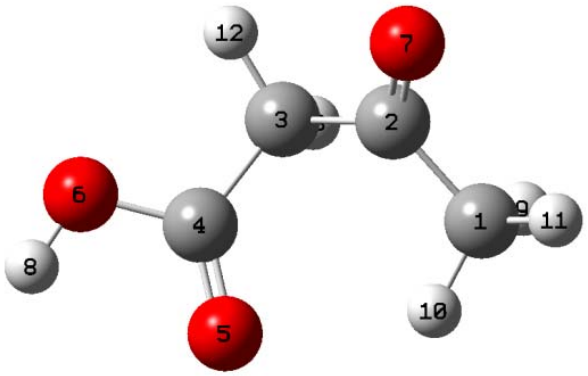
Acids

acetic acid



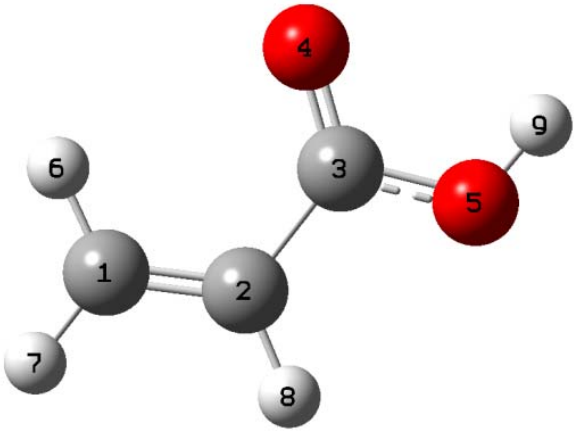
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.3212	-0.4873	-0.5134
2	C	0.3058	0.5052	0.4634
3	O	-0.3614	-0.4463	-0.4746
4	H	0.2433	0.3501	0.3899
5	C	-0.2174	-0.2259	-0.1605
6	H	0.1169	0.1022	0.0984
7	H	0.1167	0.0989	0.0980
8	H	0.1172	0.1030	0.0988

Acetoacetic acid



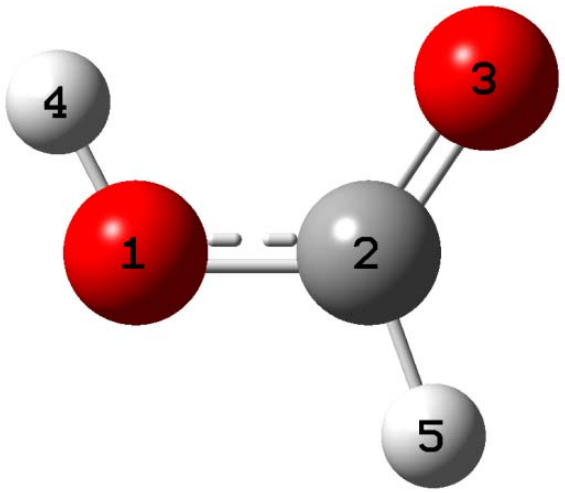
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2775	-0.2814	-0.2211
2	C	0.2382	0.3604	0.3653
3	C	-0.2229	-0.2297	-0.1848
4	C	0.3193	0.5171	0.4775
5	O	-0.3612	-0.4503	-0.474
6	O	-0.3084	-0.4715	-0.5009
7	O	-0.2724	-0.3638	-0.4015
8	H	0.2481	0.3516	0.394
9	H	0.1042	0.0987	0.0858
10	H	0.1329	0.1198	0.1147
11	H	0.1116	0.1025	0.0928
12	H	0.1486	0.1229	0.1304
13	H	0.1394	0.1237	0.1217

Cis-acrylic acid



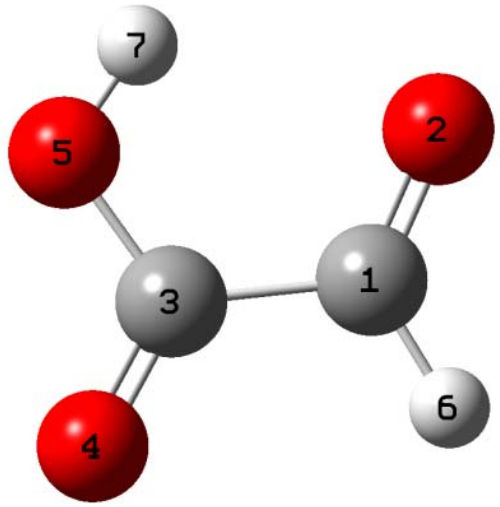
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1263	-0.1115	-0.0892
2	C	-0.1932	-0.1695	-0.1743
3	C	0.3344	0.5238	0.4899
4	O	-0.3651	-0.4551	-0.4766
5	O	-0.314	-0.4752	-0.5068
6	H	0.1377	0.1200	0.1196
7	H	0.1264	0.1077	0.1082
8	H	0.156	0.1148	0.1383
9	H	0.2441	0.3450	0.3910

Cis-formicacid



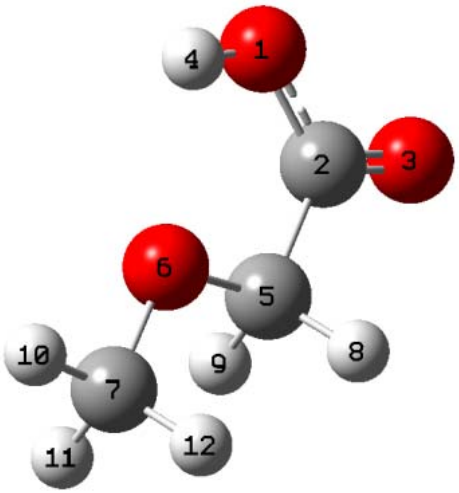
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.3245	-0.4865	-0.5168
2	C	0.2605	0.4286	0.4386
3	O	-0.3571	-0.4280	-0.4732
4	H	0.2418	0.3542	0.3877
5	H	0.1793	0.1317	0.1638

Formylformic acid



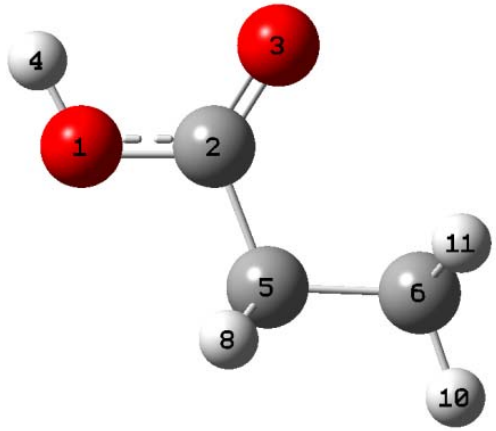
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.1572	0.2427	0.3076
2	O	-0.2453	-0.3189	-0.3792
3	C	0.2299	0.4192	0.3956
4	O	-0.2647	-0.3655	-0.3838
5	O	-0.2684	-0.4502	-0.4641
6	H	0.1461	0.1108	0.1301
7	H	0.2451	0.3619	0.3937

Methoxyethanoic acid



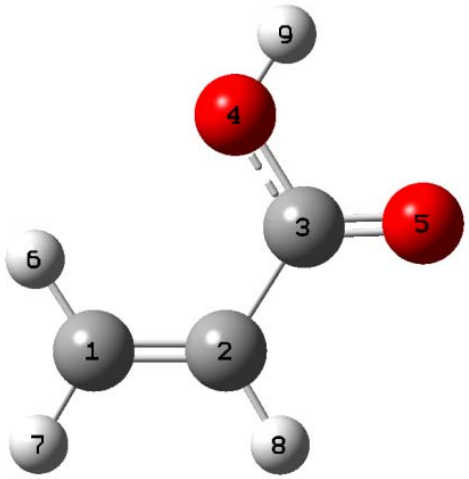
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.2806	-0.4656	-0.4753
2	C	0.3039	0.4965	0.4661
3	O	-0.3062	-0.4136	-0.4232
4	H	0.2476	0.3434	0.3952
5	C	-0.0699	-0.0225	0.008
6	O	-0.3003	-0.3175	-0.3813
7	C	-0.0665	-0.0259	0.0292
8	H	0.112	0.0969	0.0943
9	H	0.1119	0.0973	0.0942
10	H	0.1084	0.0864	0.0901
11	H	0.0698	0.0624	0.0513
12	H	0.0699	0.0621	0.0514

Propanoic acid



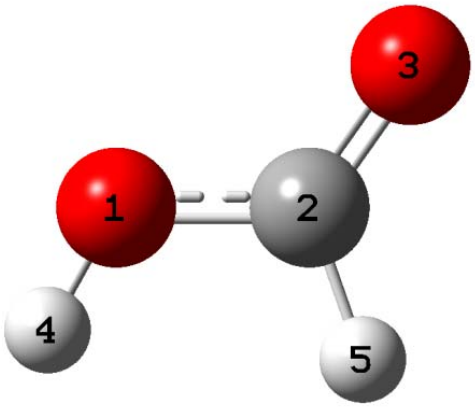
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.3232	-0.4866	-0.5153
2	C	0.3039	0.4995	0.4617
3	O	-0.3596	-0.4450	-0.4732
4	H	0.2428	0.3483	0.3894
5	C	-0.1548	-0.1498	-0.1173
6	C	-0.2118	-0.2079	-0.1548
7	H	0.1189	0.1002	0.1007
8	H	0.1189	0.1003	0.1008
9	H	0.0911	0.0843	0.0721
10	H	0.0826	0.0723	0.0636
11	H	0.0913	0.0845	0.0724

Trans-acrylic acid



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1618	-0.1422	-0.0876
2	C	-0.2201	-0.1917	-0.1747
3	C	0.3226	0.5235	0.4914
4	O	-0.2885	-0.4823	-0.5134
5	O	-0.2902	-0.3978	-0.4715
6	H	0.1188	0.1132	0.1184
7	H	0.1332	0.1101	0.1064
8	H	0.1637	0.1318	0.1393
9	H	0.2224	0.3353	0.3917

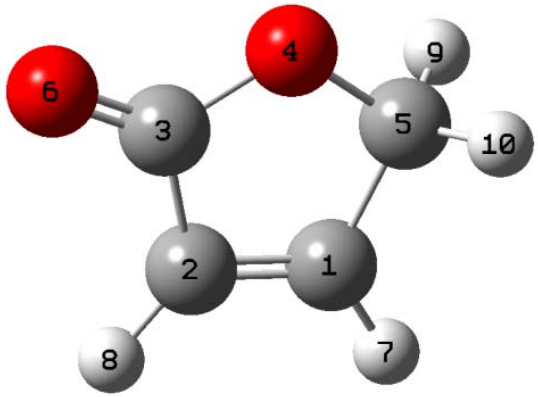
Trans-formicacid



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.3014	-0.4555	-0.4993
2	C	0.2459	0.4055	0.4276
3	O	-0.2939	-0.3857	-0.4155
4	H	0.2231	0.3291	0.3762
5	H	0.1263	0.1066	0.111

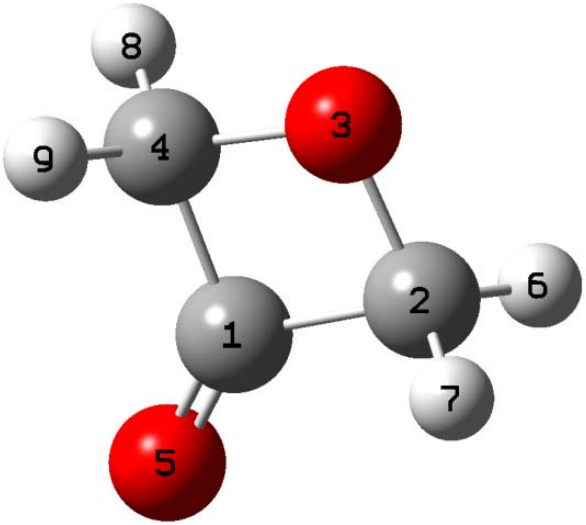
Ester and lactone

2-furanone



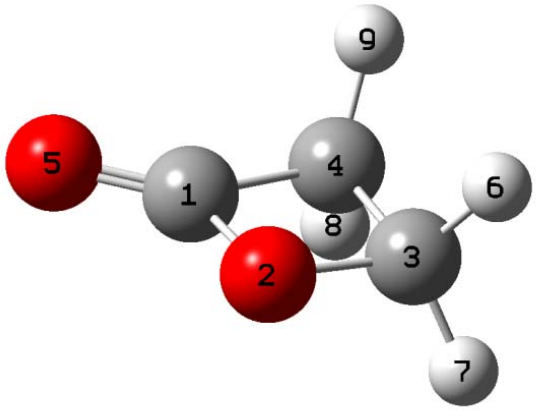
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1424	-0.1041	-0.1238
2	C	-0.2077	-0.1839	-0.1885
3	C	0.3164	0.5022	0.4758
4	O	-0.2547	-0.3454	-0.3367
5	C	-0.0266	0.0402	0.049
6	O	-0.2758	-0.3855	-0.3962
7	H	0.1656	0.1345	0.1479
8	H	0.1798	0.1416	0.1624
9	H	0.1228	0.1003	0.1051
10	H	0.1227	0.1002	0.1051

3-oxetanone



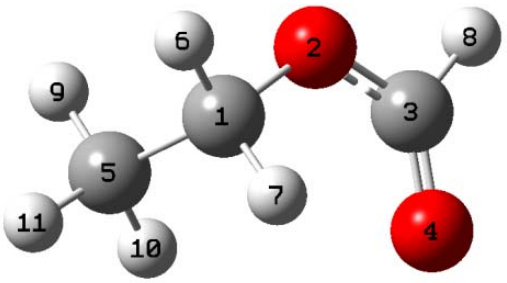
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.1985	0.3204	0.3306
2	C	-0.0972	-0.0513	-0.0199
3	O	-0.2654	-0.3302	-0.3467
4	C	-0.0972	-0.0513	-0.0199
5	O	-0.2324	-0.3294	-0.3668
6	H	0.1234	0.1105	0.1056
7	H	0.1235	0.1105	0.1057
8	H	0.1234	0.1105	0.1056
9	H	0.1235	0.1105	0.1057

Beta-propiolactone



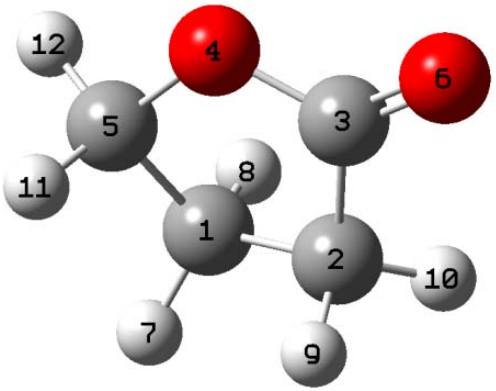
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.3001	0.4856	0.4641
2	O	-0.2653	-0.3274	-0.3468
3	C	-0.0409	0.0082	0.0353
4	C	-0.2235	-0.2230	-0.1851
5	O	-0.2596	-0.3693	-0.384
6	H	0.1135	0.0947	0.0953
7	H	0.1135	0.0947	0.0953
8	H	0.1311	0.1183	0.1129
9	H	0.1311	0.1183	0.1129

Cis-ethylformate



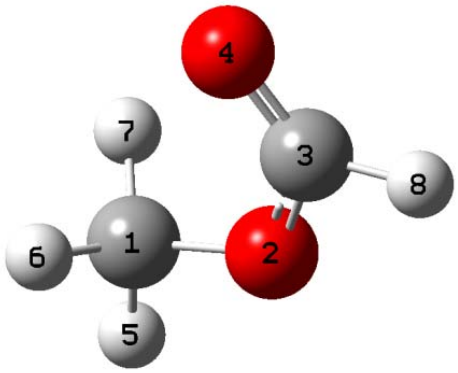
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0158	0.0597	0.0582
2	O	-0.2876	-0.3543	-0.3704
3	C	0.2577	0.4223	0.4346
4	O	-0.3517	-0.4274	-0.4684
5	C	-0.2442	-0.2366	-0.1871
6	H	0.1048	0.0720	0.0868
7	H	0.0986	0.0913	0.0804
8	H	0.1714	0.1215	0.156
9	H	0.0848	0.0813	0.0658
10	H	0.0952	0.0914	0.0763
11	H	0.0866	0.0788	0.0678

Gamma-butyrolactone



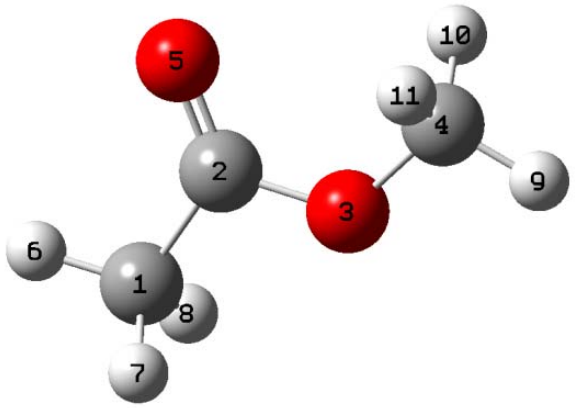
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1936	-0.1746	-0.156
2	C	-0.2011	-0.1916	-0.163
3	C	0.2976	0.4924	0.4584
4	O	-0.2508	-0.3442	-0.3335
5	C	-0.0308	0.0426	0.0454
6	O	-0.2893	-0.3947	-0.4093
7	H	0.1027	0.0901	0.0841
8	H	0.1027	0.0901	0.084
9	H	0.1284	0.1119	0.1103
10	H	0.1284	0.1119	0.1102
11	H	0.1029	0.0831	0.0847
12	H	0.1028	0.0830	0.0846

methyformate



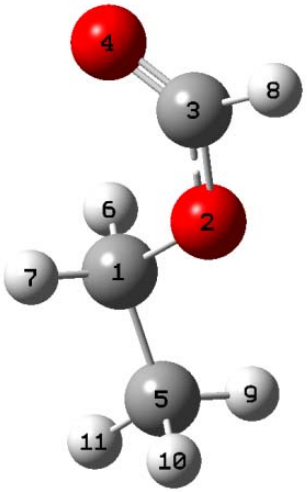
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0678	-0.0104	0.0265
2	O	-0.2859	-0.3477	-0.3693
3	C	0.2546	0.4172	0.4317
4	O	-0.3481	-0.4237	-0.4652
5	H	0.1032	0.0742	0.0847
6	H	0.0851	0.0823	0.0665
7	H	0.0849	0.0820	0.0663
8	H	0.1742	0.1262	0.1587

methylacetate



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.2176	-0.2264	-0.1606
2	C	0.2995	0.4915	0.4563
3	O	-0.2825	-0.3513	-0.3651
4	C	-0.0634	-0.0073	0.031
5	O	-0.3516	-0.4402	-0.466
6	H	0.1153	0.0974	0.0966
7	H	0.1152	0.1015	0.0967
8	H	0.1152	0.1014	0.0967
9	H	0.1013	0.0724	0.0829
10	H	0.0845	0.0807	0.0659
11	H	0.0842	0.0804	0.0657

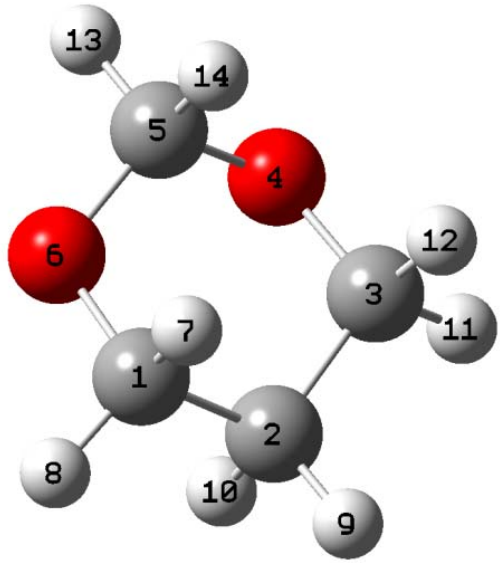
Trans-ethylformate



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0153	0.0508	0.0586
2	O	-0.2884	-0.3529	-0.3712
3	C	0.2569	0.4186	0.434
4	O	-0.352	-0.4286	-0.4685
5	C	-0.2181	-0.2179	-0.1612
6	H	0.0908	0.0838	0.0726
7	H	0.0908	0.0837	0.0726
8	H	0.1725	0.1249	0.157
9	H	0.088	0.0812	0.069
10	H	0.0881	0.0813	0.0691
11	H	0.0868	0.0751	0.068

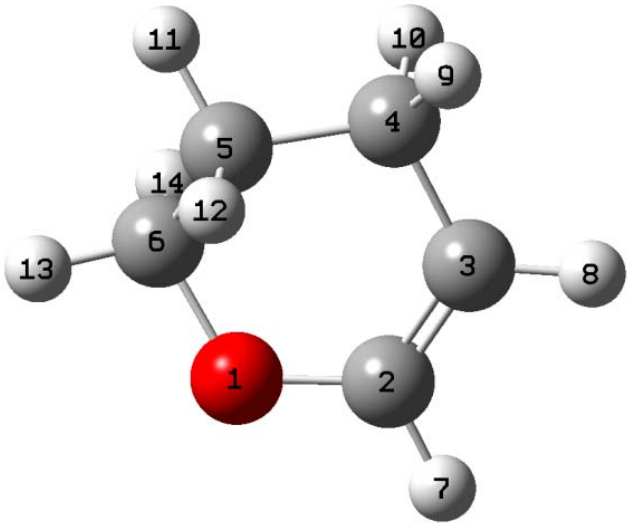
Ethers

1,3-dioxanel



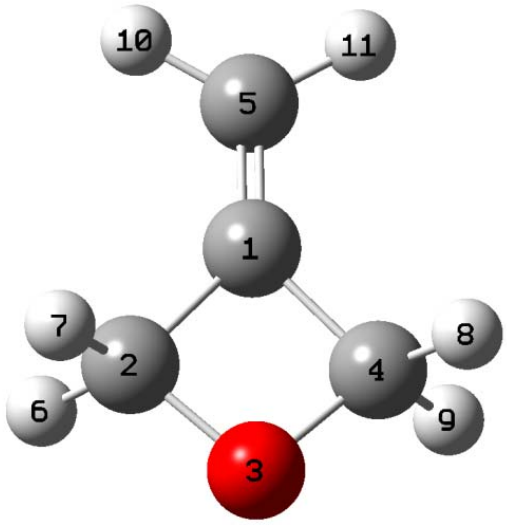
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0224	0.0545	0.0543
2	C	-0.2263	-0.2043	-0.1885
3	C	-0.0223	0.0546	0.0543
4	O	-0.2902	-0.3633	-0.3708
5	C	0.0927	0.2169	0.2073
6	O	-0.2902	-0.3632	-0.3708
7	H	0.0672	0.0566	0.049
8	H	0.1111	0.0823	0.093
9	H	0.0946	0.0809	0.0761
10	H	0.106	0.0992	0.0874
11	H	0.1111	0.0823	0.093
12	H	0.0672	0.0566	0.0491
13	H	0.1368	0.0924	0.1195
14	H	0.0647	0.0545	0.0473

3,4-dihydro-2,4-pyran



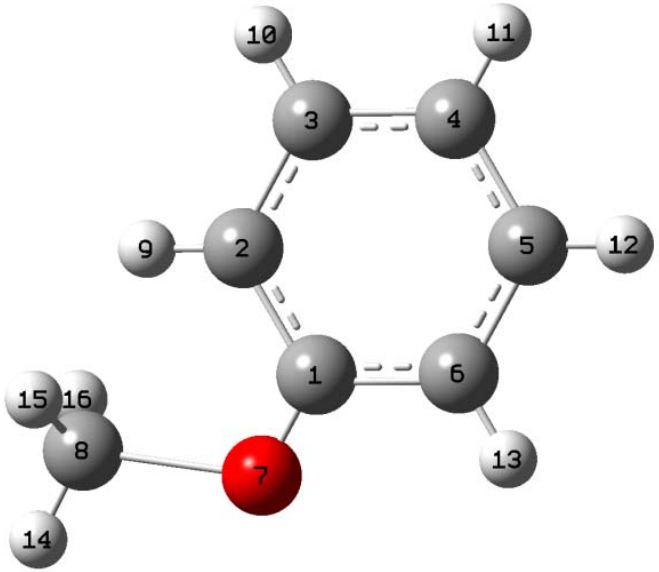
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.221	-0.3085	-0.3075
2	C	-0.0129	0.0945	0.0494
3	C	-0.2765	-0.2365	-0.2570
4	C	-0.1157	-0.0966	-0.0789
5	C	-0.1914	-0.1706	-0.1539
6	C	-0.0257	0.0544	0.0500
7	H	0.1606	0.1084	0.1435
8	H	0.1372	0.1065	0.1193
9	H	0.0906	0.0727	0.0722
10	H	0.0852	0.0719	0.0669
11	H	0.091	0.0767	0.0723
12	H	0.0947	0.0875	0.0761
13	H	0.1051	0.0758	0.0870
14	H	0.0789	0.0637	0.0607

3-methylene-oxetane



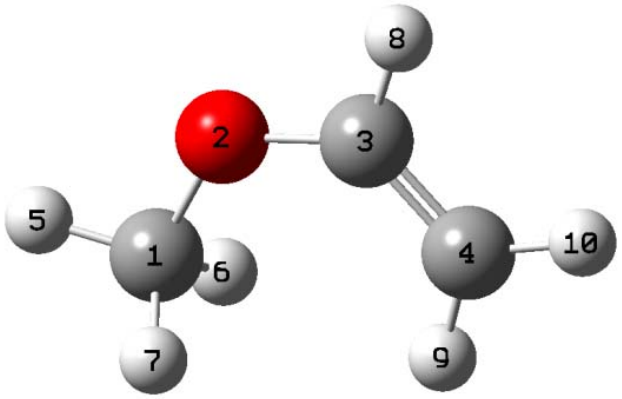
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1769	-0.1098	-0.1767
2	C	-0.0065	0.0466	0.0699
3	C	-0.2826	-0.3513	-0.3639
4	O	-0.0064	0.0467	0.0700
5	C	-0.1885	-0.1765	-0.1520
6	H	0.1037	0.0848	0.0857
7	H	0.1039	0.0850	0.0859
8	H	0.1039	0.0849	0.0860
9	H	0.1034	0.0846	0.0855
10	H	0.1230	0.1025	0.1048
11	H	0.1230	0.1025	0.1049

anisole



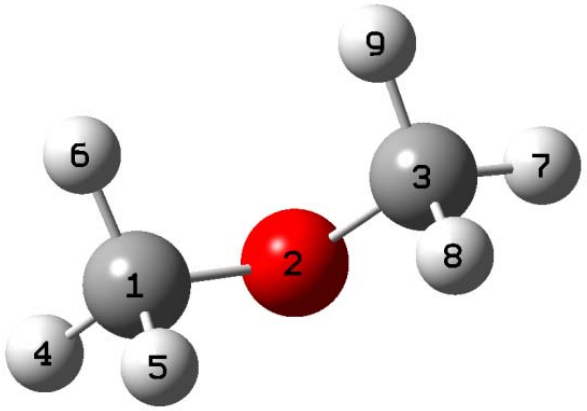
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0776	0.1912	0.1219
2	C	-0.2036	-0.1835	-0.1848
3	C	-0.0958	-0.0660	-0.0776
4	C	-0.1648	-0.1350	-0.1465
5	C	-0.0998	-0.0717	-0.0816
6	C	-0.1558	-0.1413	-0.1374
7	O	-0.2117	-0.3004	-0.2984
8	C	-0.0758	-0.0169	0.0200
9	H	0.1360	0.1031	0.1181
10	H	0.1308	0.0972	0.1128
11	H	0.1324	0.0990	0.1143
12	H	0.1330	0.0989	0.1150
13	H	0.1481	0.1073	0.1303
14	H	0.1051	0.0767	0.0867
15	H	0.0721	0.0707	0.0536
16	H	0.0720	0.0706	0.0536

Cis-vinylmethyl



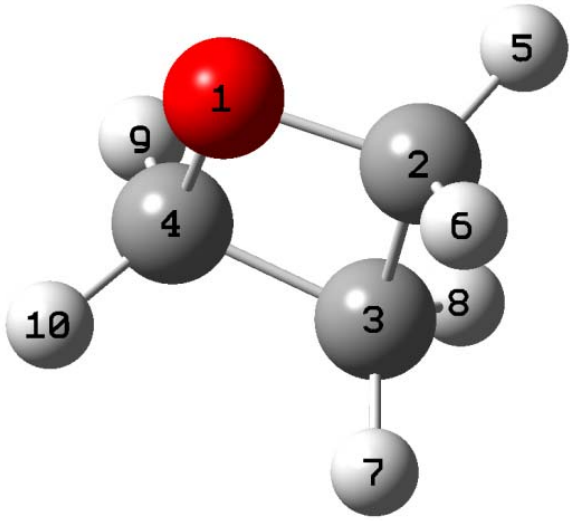
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0804	-0.0206	0.0153
2	O	-0.2225	-0.3011	-0.3096
3	C	-0.0108	0.0995	0.0514
4	C	-0.3375	-0.3218	-0.2993
5	H	0.1023	0.0746	0.0839
6	H	0.0711	0.0709	0.0526
7	H	0.0711	0.0708	0.0526
8	H	0.1583	0.1123	0.1412
9	H	0.1207	0.1076	0.1024
10	H	0.1276	0.1079	0.1094

Dimethylether



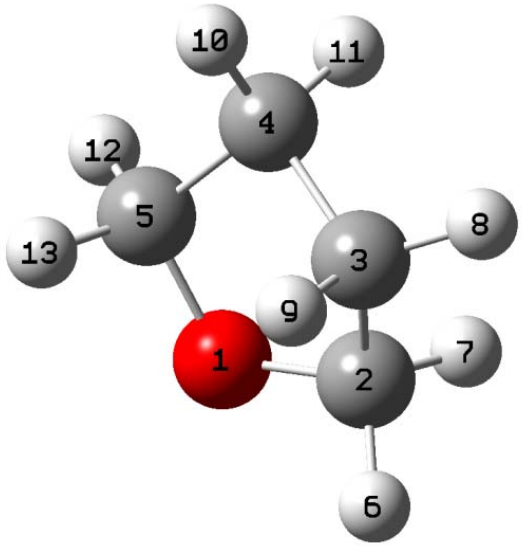
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0759	-0.0202	0.0209
2	O	-0.2765	-0.3403	-0.3593
3	C	-0.0759	-0.0202	0.0209
4	H	0.098	0.0766	0.0795
5	H	0.0581	0.0569	0.0397
6	H	0.0581	0.0568	0.0396
7	H	0.098	0.0767	0.0795
8	H	0.0581	0.0569	0.0397
9	H	0.0581	0.0568	0.0396

oxetane



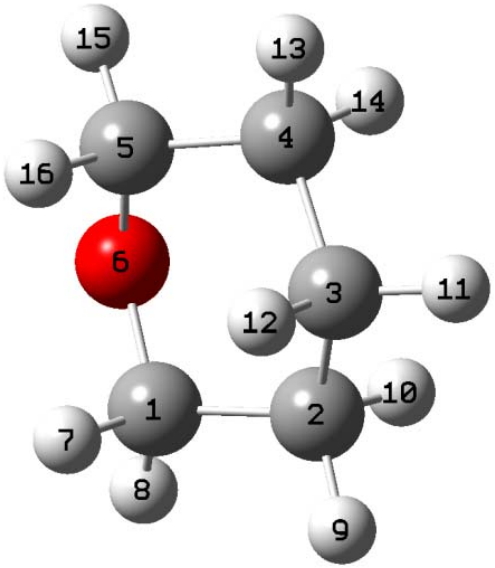
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.2837	-0.3437	-0.3652
2	C	-0.0384	0.0242	0.0388
3	C	-0.2185	-0.2005	-0.181
4	C	-0.0384	0.0242	0.0388
5	H	0.0946	0.0792	0.0764
6	H	0.0946	0.0791	0.0764
7	H	0.1002	0.0896	0.0815
8	H	0.1002	0.0896	0.0816
9	H	0.0946	0.0792	0.0764
10	H	0.0946	0.0791	0.0764

tetrahydrofuran



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	O	-0.2838	-0.3772	-0.365
2	C	-0.0228	0.0563	0.0539
3	C	-0.1854	-0.1634	-0.148
4	C	-0.1854	-0.1634	-0.1475
5	C	-0.0228	0.0563	0.0535
6	H	0.0846	0.0673	0.0647
7	H	0.0834	0.0664	0.0673
8	H	0.0911	0.0809	0.0724
9	H	0.0911	0.0810	0.072
10	H	0.0911	0.0810	0.0727
11	H	0.091	0.0809	0.0724
12	H	0.0834	0.0664	0.0679
13	H	0.0846	0.0673	0.0638

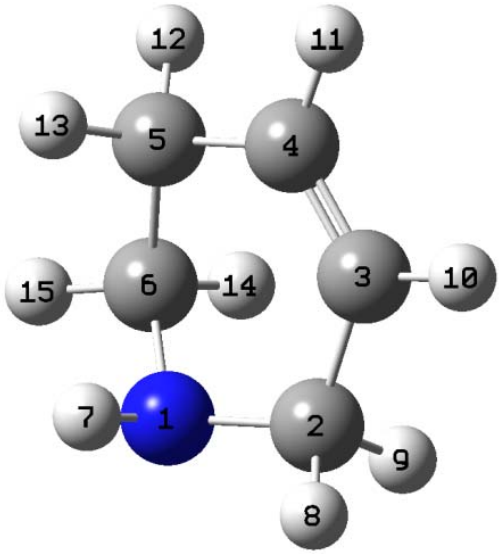
tetrahydropyran



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0232	0.0542	0.0538
2	C	-0.1911	-0.1701	-0.1534
3	C	-0.156	-0.1330	-0.1186
4	C	-0.191	-0.1700	-0.1534
5	C	-0.0231	0.0542	0.0538
6	O	-0.2731	-0.3550	-0.3552
7	H	0.0657	0.0553	0.0476
8	H	0.1035	0.0745	0.0854
9	H	0.0865	0.0737	0.0678
10	H	0.092	0.0854	0.0733
11	H	0.0835	0.0713	0.0648
12	H	0.0789	0.0706	0.0602
13	H	0.0864	0.0737	0.0678
14	H	0.0919	0.0853	0.0733
15	H	0.1035	0.0745	0.0854
16	H	0.0657	0.0553	0.0475

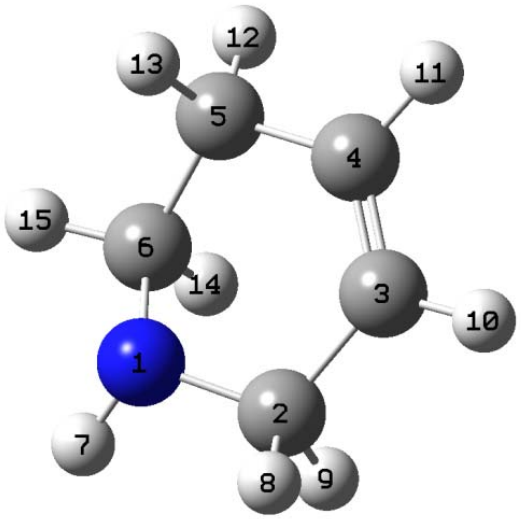
Amines and ammonia

1,2,5,6-tetrahydropydidine(ax)



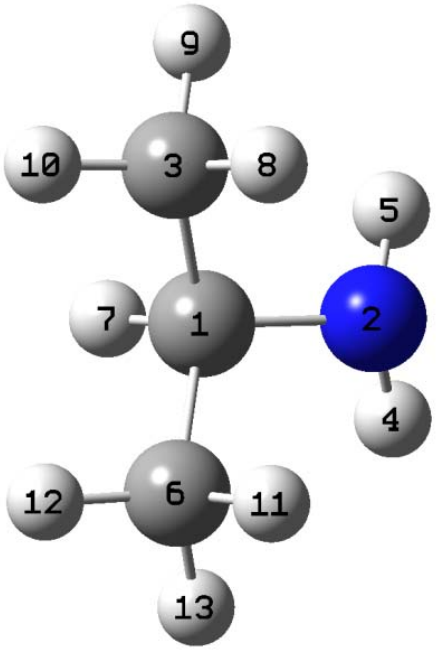
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.2738	-0.6278	-0.6493
2	C	-0.063	0.0751	0.0664
3	C	-0.202	-0.1539	-0.1823
4	C	-0.1629	-0.1171	-0.1446
5	C	-0.17	-0.1426	-0.1313
6	C	-0.087	0.0560	0.0433
7	H	0.1446	0.2858	0.3292
8	H	0.0935	0.0774	0.0753
9	H	0.1019	0.0576	0.0841
10	H	0.1285	0.1044	0.1106
11	H	0.1229	0.0972	0.1049
12	H	0.0946	0.0803	0.0762
13	H	0.088	0.0795	0.0697
14	H	0.0947	0.0624	0.0763
15	H	0.09	0.0658	0.0716

1,2,5,6-tetrahydropydidine(eq)



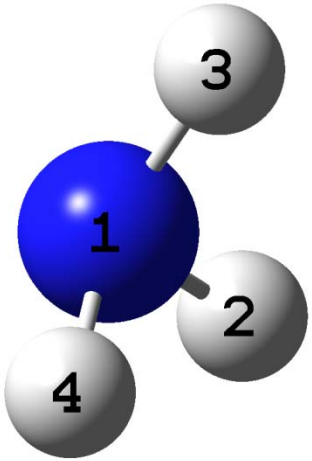
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.2993	-0.5499	-0.6689
2	C	-0.0474	0.0372	0.0811
3	C	-0.1735	-0.1349	-0.1551
4	C	-0.1575	-0.1189	-0.1392
5	C	-0.1310	-0.1165	-0.0940
6	C	-0.0708	0.0056	0.0586
7	H	0.1573	0.2702	0.3400
8	H	0.0980	0.0528	0.0800
9	H	0.0548	0.0755	0.0371
10	H	0.1266	0.0990	0.1086
11	H	0.1233	0.0962	0.1053
12	H	0.0871	0.0683	0.0687
13	H	0.1000	0.0873	0.0818
14	H	0.0450	0.0740	0.0269
15	H	0.0875	0.0541	0.0692

2-aminopropane



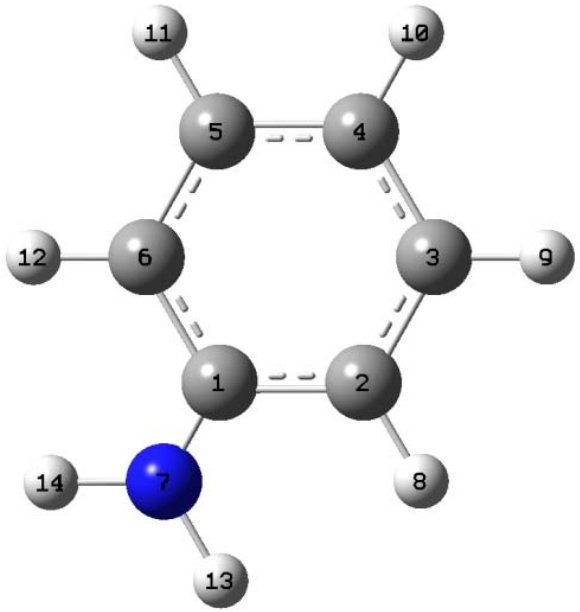
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0281	0.0652	0.0834
2	N	-0.346	-0.7517	-0.8190
3	C	-0.2095	-0.2087	-0.1519
4	H	0.1436	0.2959	0.3327
5	H	0.1436	0.2957	0.3328
6	C	-0.2096	-0.2087	-0.1520
7	H	0.0412	0.0884	0.0234
8	H	0.0882	0.0793	0.0692
9	H	0.0702	0.0654	0.0511
10	H	0.074	0.0672	0.0549
11	H	0.0882	0.0793	0.0692
12	H	0.0741	0.0673	0.0550
13	H	0.0701	0.0654	0.0511

ammonia



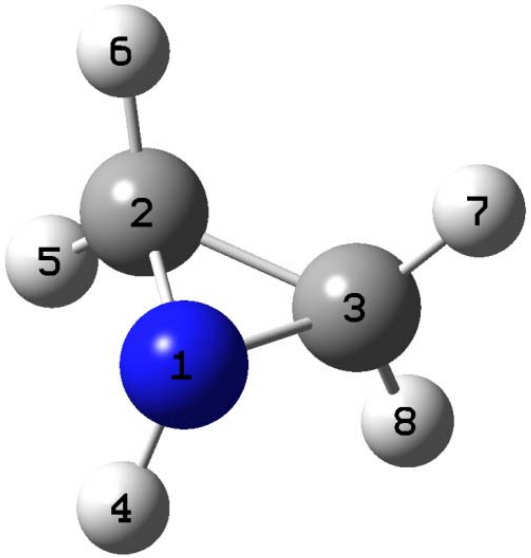
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.3959	-1.1345	-0.9858
2	H	0.132	0.3782	0.3286
3	H	0.132	0.3782	0.3286
4	H	0.132	0.3782	0.3286

aniline



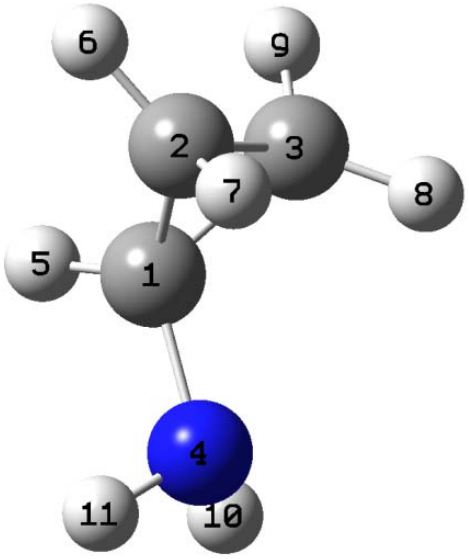
M NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0553	0.3018	0.1579
2	C	-0.1907	-0.2268	-0.1688
3	C	-0.0934	-0.0530	-0.0747
4	C	-0.1729	-0.1446	-0.1533
5	C	-0.0934	-0.0526	-0.0747
6	C	-0.1907	-0.2279	-0.1688
7	N	-0.3276	-0.9282	-0.8014
8	H	0.1302	0.1287	0.1122
9	H	0.1287	0.0953	0.1106
10	H	0.1306	0.0971	0.1126
11	H	0.1286	0.0952	0.1106
12	H	0.1301	0.1291	0.1121
13	H	0.1826	0.3931	0.3628
14	H	0.1825	0.3929	0.3628

aziridine



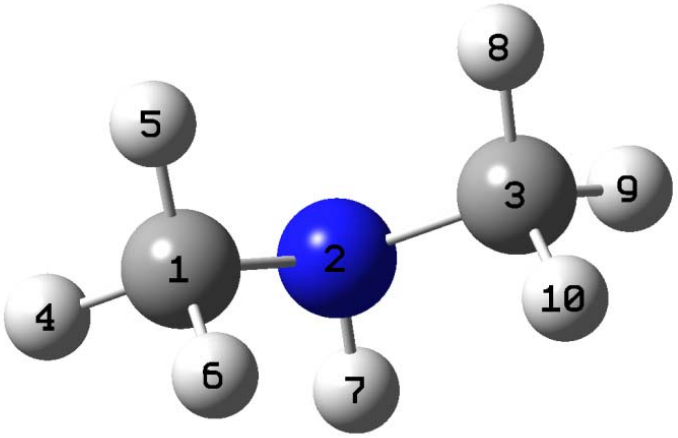
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.2316	-0.5426	-0.6055
2	C	-0.1876	-0.0860	-0.0575
3	C	-0.1876	-0.0860	-0.0575
4	H	0.1441	0.3190	0.3303
5	H	0.1018	0.1025	0.0836
6	H	0.1295	0.0953	0.1115
7	H	0.1296	0.0953	0.1115
8	H	0.1018	0.1025	0.0836

Cyclopropyl amine



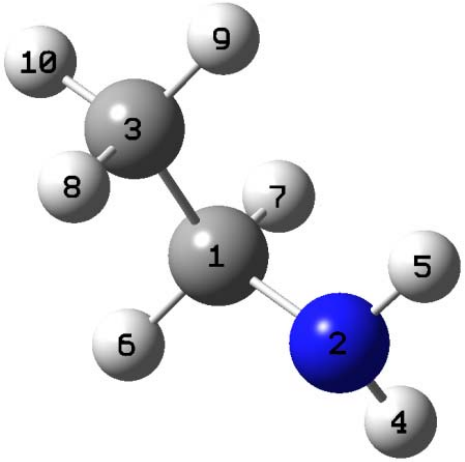
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1062	0.0170	0.0067
2	C	-0.2006	-0.1768	-0.163
3	C	-0.2004	-0.1766	-0.1628
4	N	-0.3254	-0.7407	-0.7971
5	H	0.0828	0.1099	0.0654
6	H	0.1044	0.0843	0.086
7	H	0.1204	0.0985	0.102
8	H	0.1205	0.0986	0.1022
9	H	0.1044	0.0843	0.0859
10	H	0.150	0.3004	0.3374
11	H	0.150	0.3012	0.3373

dimethylamine



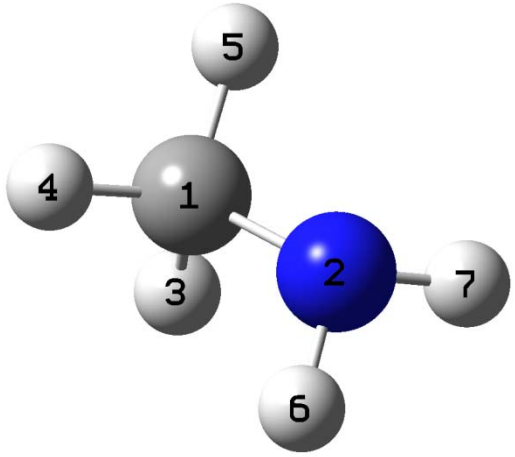
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.125	-0.0503	0.0249
2	N	-0.3078	-0.5532	-0.6788
3	C	-0.125	-0.0503	0.0249
4	H	0.0817	0.0611	0.063
5	H	0.0829	0.0607	0.0642
6	H	0.0378	0.0708	0.0196
7	H	0.153	0.2686	0.3356
8	H	0.0829	0.0607	0.0642
9	H	0.0817	0.0611	0.063
10	H	0.0378	0.0708	0.0196

ethylammonia



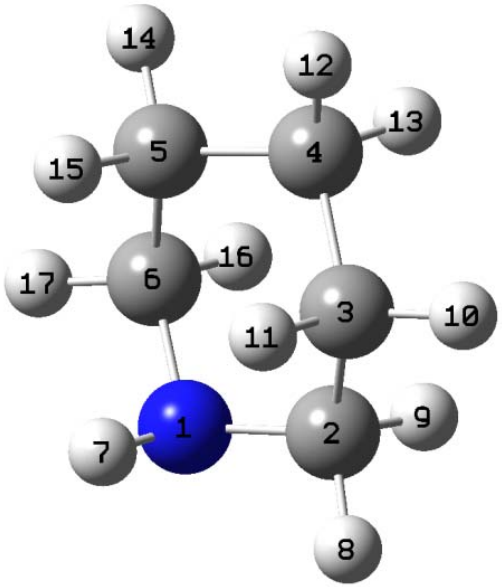
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.0785	0.0234	0.0527
2	N	-0.3491	-0.7493	-0.8226
3	C	-0.2148	-0.2097	-0.1573
4	H	0.1446	0.2967	0.3337
5	H	0.1407	0.2904	0.3298
6	H	0.0873	0.0474	0.0690
7	H	0.0362	0.0852	0.0182
8	H	0.0879	0.0792	0.0690
9	H	0.0697	0.0674	0.0507
10	H	0.0759	0.0692	0.0569

methylammonia



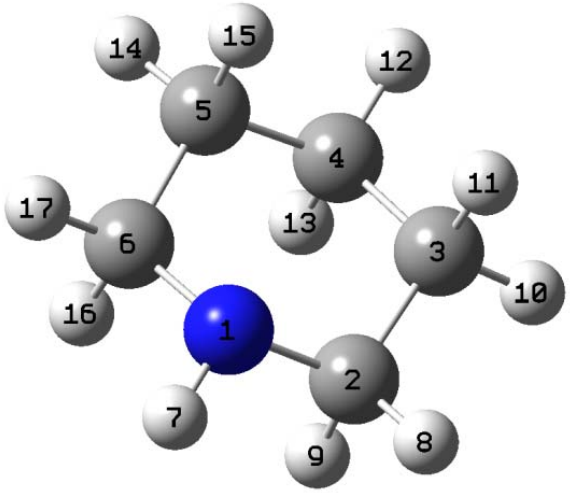
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1287	-0.0301	0.0232
2	N	-0.3515	-0.7606	-0.8257
3	H	0.0309	0.0835	0.0127
4	H	0.0821	0.0553	0.0634
5	H	0.0822	0.0549	0.0635
6	H	0.1425	0.2984	0.3315
7	H	0.1425	0.2986	0.3315

Piperidine(ax)



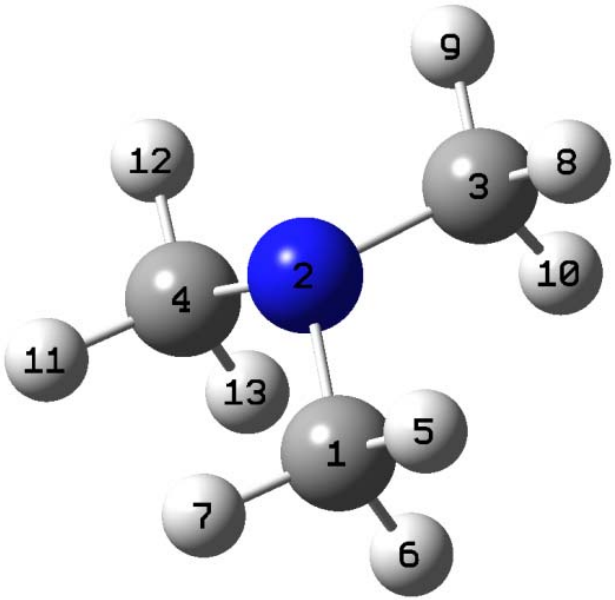
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.2752	-0.6232	-0.6506
2	C	-0.0872	0.0524	0.043
3	C	-0.1932	-0.1639	-0.1538
4	C	-0.1549	-0.1308	-0.1173
5	C	-0.1931	-0.1639	-0.1538
6	C	-0.0872	0.0524	0.0430
7	H	0.1424	0.2842	0.3269
8	H	0.088	0.0675	0.0695
9	H	0.0922	0.0580	0.0738
10	H	0.0861	0.0755	0.0674
11	H	0.078	0.0750	0.0593
12	H	0.0791	0.0676	0.0604
13	H	0.081	0.0731	0.0623
14	H	0.086	0.0755	0.0674
15	H	0.078	0.0750	0.0593
16	H	0.0921	0.0579	0.0737
17	H	0.0879	0.0675	0.0695

Piperidine(eq)



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.2982	-0.5504	-0.668
2	C	-0.0729	0.0056	0.0565
3	C	-0.1558	-0.1393	-0.1181
4	C	-0.1567	-0.1360	-0.1191
5	C	-0.1558	-0.1393	-0.1181
6	C	-0.0729	0.0057	0.0565
7	H	0.1554	0.2716	0.3381
8	H	0.0869	0.0548	0.0686
9	H	0.0424	0.0717	0.0243
10	H	0.0797	0.0659	0.061
11	H	0.0914	0.0805	0.0727
12	H	0.0805	0.0680	0.0618
13	H	0.076	0.0684	0.0573
14	H	0.0797	0.0659	0.061
15	H	0.0913	0.0804	0.0727
16	H	0.0423	0.0717	0.0243
17	H	0.0869	0.0548	0.0686

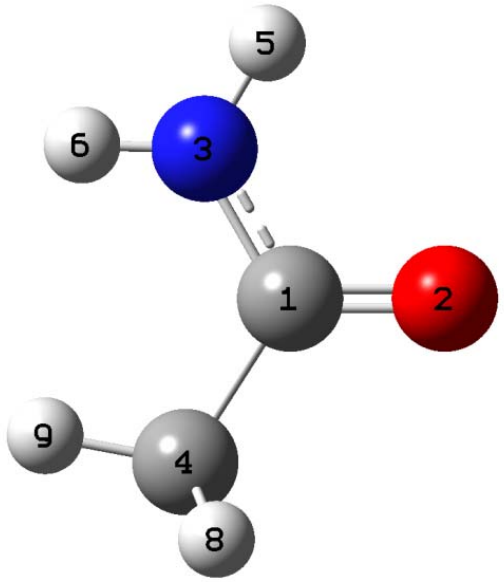
trimethylamine



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1188	-0.0572	0.0293
2	N	-0.2667	-0.4009	-0.5437
3	C	-0.1188	-0.0573	0.0293
4	C	-0.1188	-0.0573	0.0293
5	H	0.0824	0.0629	0.0636
6	H	0.043	0.0648	0.0247
7	H	0.0824	0.0632	0.0636
8	H	0.0824	0.0631	0.0636
9	H	0.0823	0.0630	0.0636
10	H	0.0429	0.0648	0.0247
11	H	0.0824	0.0629	0.0637
12	H	0.0823	0.0632	0.0636
13	H	0.043	0.0648	0.0247

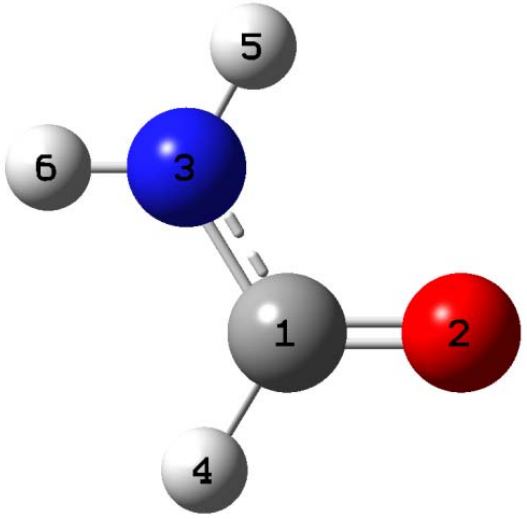
Amides

acetamide



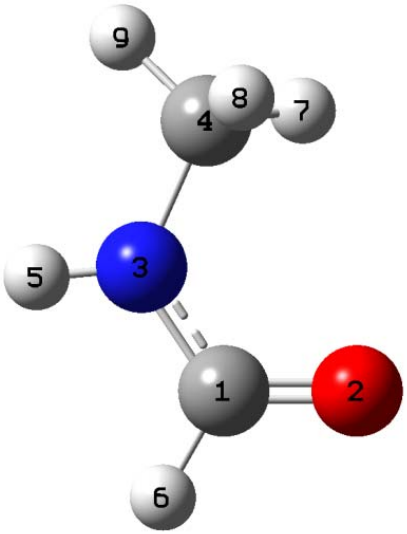
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.3000	0.4195	0.5134
2	O	-0.3744	-0.4761	-0.4992
3	N	-0.4427	-0.4233	-0.8769
4	C	-0.2421	-0.2490	-0.1826
5	H	0.2291	0.2286	0.3986
6	H	0.2176	0.2177	0.3903
7	H	0.0980	0.0894	0.0794
8	H	0.1176	0.1048	0.0987
9	H	0.0970	0.0884	0.0783

formamide



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2575	0.3545	0.4910
2	O	-0.3706	-0.4613	-0.4982
3	N	-0.4483	-0.4218	-0.8815
4	H	0.1190	0.0807	0.1033
5	H	0.2232	0.2275	0.3934
6	H	0.2192	0.2203	0.3919

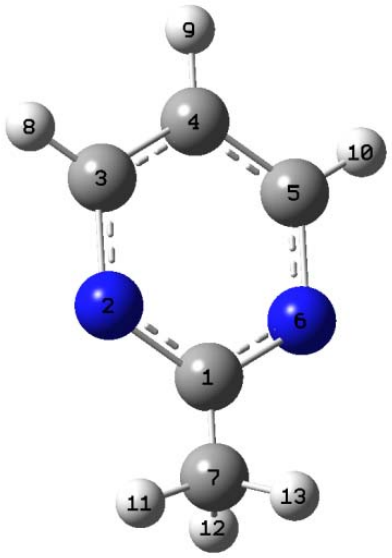
N-methylformamide



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.2541	0.3529	0.4896
2	O	-0.3633	-0.4549	-0.4948
3	N	-0.3977	-0.3422	-0.7437
4	C	-0.0757	-0.0610	0.0625
5	H	0.2224	0.2274	0.3904
6	H	0.1172	0.0794	0.1019
7	H	0.0737	0.0756	0.0976
8	H	0.0939	0.0672	0.0485
9	H	0.0754	0.0556	0.0479

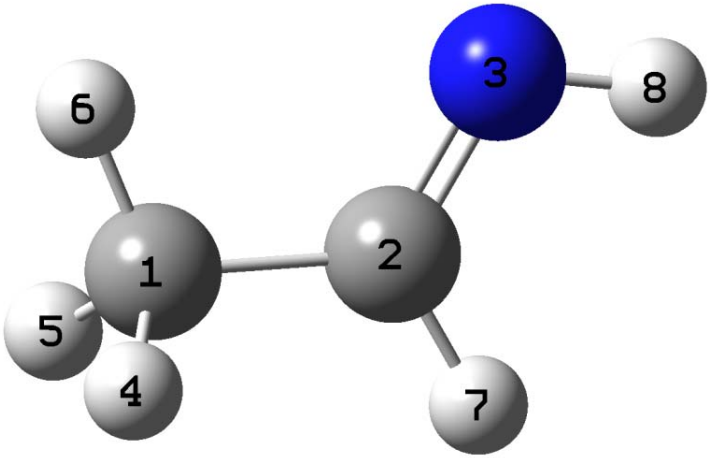
Imines and Naromatics

2-methylpyrimidine



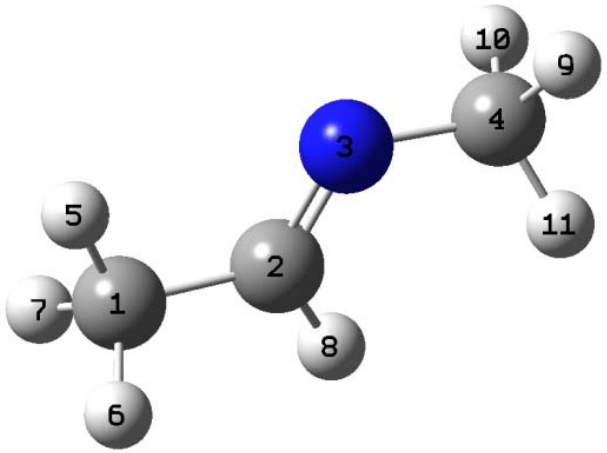
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	0.0272	0.3430	0.2915
2	N	-0.1727	-0.4363	-0.4578
3	C	-0.0343	0.1354	0.1323
4	C	-0.2424	-0.1905	-0.2204
5	C	-0.0337	0.1404	0.1339
6	N	-0.1741	-0.4447	-0.4593
7	C	-0.1599	-0.1634	-0.1017
8	H	0.1643	0.1210	0.1470
9	H	0.1544	0.1210	0.1366
10	H	0.1643	0.1210	0.1470
11	H	0.1038	0.0804	0.0850
12	H	0.1017	0.0862	0.0831
13	H	0.1013	0.0864	0.0828

E-acetaldimine



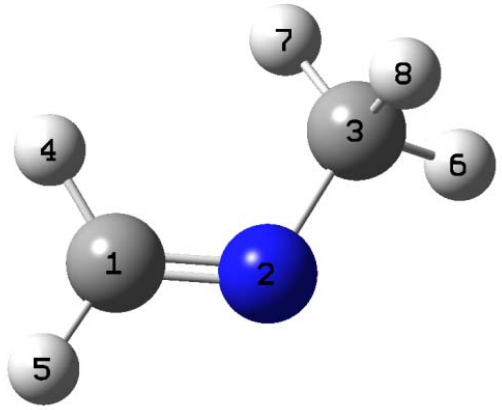
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1982	-0.1933	-0.1409
2	C	-0.064	0.0956	0.1549
3	N	-0.2353	-0.5590	-0.6244
4	H	0.0883	0.0791	0.0697
5	H	0.0885	0.0794	0.0699
6	H	0.1021	0.0881	0.0832
7	H	0.0807	0.0985	0.0637
8	H	0.138	0.3115	0.3239

N-methylacetaldimine



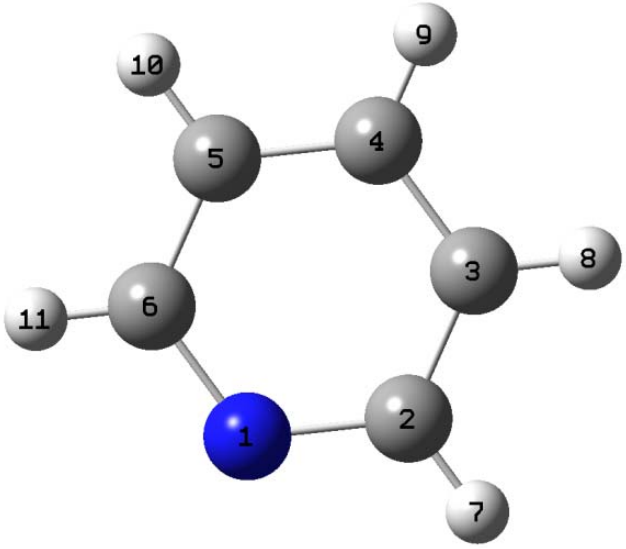
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1922	-0.1877	-0.135
2	C	-0.0747	0.0762	0.1377
3	N	-0.1902	-0.4130	-0.4820
4	C	-0.1521	-0.0588	-0.0020
5	H	0.1001	0.0869	0.0812
6	H	0.087	0.0773	0.0684
7	H	0.0873	0.0776	0.0687
8	H	0.0886	0.0984	0.0716
9	H	0.0968	0.0869	0.0785
10	H	0.0967	0.0870	0.0784
11	H	0.0528	0.0691	0.0343

N-methylformaldimine



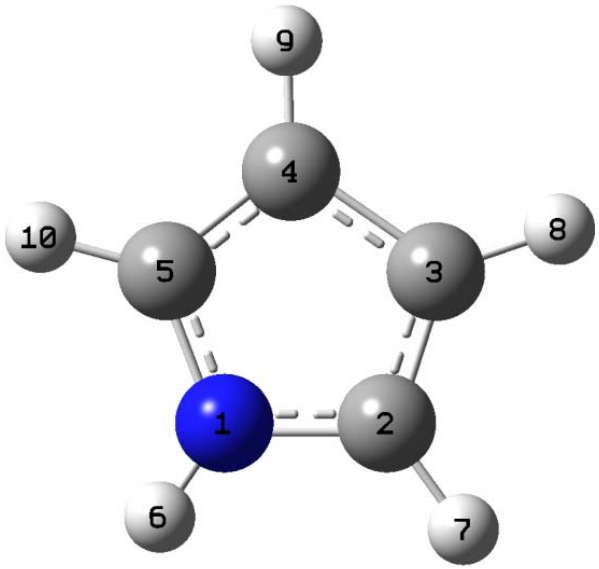
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.1274	0.0118	0.1078
2	N	-0.1821	-0.4008	-0.4775
3	C	-0.16	-0.0644	-0.0102
4	H	0.0858	0.0994	0.0686
5	H	0.1322	0.1039	0.1147
6	H	0.0985	0.0888	0.0802
7	H	0.0544	0.0727	0.0359
8	H	0.0986	0.0887	0.0803

pyridine



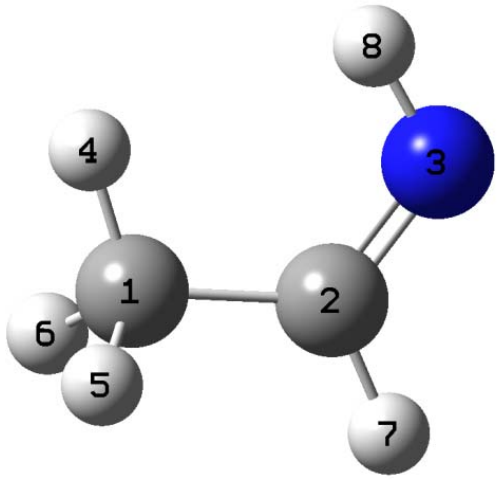
ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.1386	-0.4184	-0.4296
2	C	-0.0725	0.0984	0.0845
3	C	-0.1814	-0.1390	-0.1616
4	C	-0.0932	-0.0545	-0.0671
5	C	-0.1814	-0.1390	-0.1616
6	C	-0.0725	0.0984	0.0845
7	H	0.1584	0.1145	0.1410
8	H	0.1427	0.1102	0.1248
9	H	0.1374	0.1046	0.1194
10	H	0.1427	0.1102	0.1248
11	H	0.1584	0.1145	0.1410

pyrrole



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	N	-0.1808	-0.1135	-0.5844
2	C	-0.1456	-0.1135	-0.0153
3	C	-0.1964	-0.1776	-0.1718
4	C	-0.1964	-0.1777	-0.1718
5	C	-0.1455	-0.1135	-0.0153
6	H	0.2409	0.2336	0.4053
7	H	0.1619	0.1187	0.1445
8	H	0.1500	0.1124	0.1322
9	H	0.1500	0.1124	0.1322
10	H	0.1619	0.1187	0.1445

Z-acetaldimine



ATOM NO.	TYPE	MULLIKEN	DPPC	CM2
1	C	-0.246	-0.2336	-0.1863
2	C	-0.067	0.1410	0.1526
3	N	-0.2311	-0.6006	-0.6222
4	H	0.0825	0.0813	0.0635
5	H	0.0953	0.0897	0.0767
6	H	0.0954	0.0898	0.0768
7	H	0.139	0.1023	0.1217
8	H	0.1321	0.3301	0.3172