

Oxyanion thioacyl @MP2/6-311(2df,2p)

H	0.020162	0.182997	0.131637
C	-0.058074	-0.042362	1.211375
O	1.011141	-0.056960	1.915937
C	-0.971602	-1.233585	1.440388
H	-0.428789	-2.147645	1.187847
F	-2.112989	-1.208888	0.625476
H	-1.291233	-1.256936	2.479551
S	-1.346306	1.565598	1.707982
C	-0.195789	2.293850	2.887308
H	0.659089	1.600903	2.913917
H	-0.636298	2.370899	3.879933
H	0.139593	3.279817	2.568872

Oxyanion thioacyl @PM3

H	-0.587023	0.325556	-0.102980
C	-0.226651	0.128008	0.927595
O	1.026065	0.132667	1.108971
C	-1.030118	-1.008004	1.629266
H	-0.669399	-1.203107	2.651203
F	-0.918671	-2.188489	0.951323
H	-2.107495	-0.780174	1.674943
S	-1.146888	1.811830	1.824194
C	0.400770	2.456177	2.461594
H	1.188396	1.728734	2.131188
H	0.418463	2.521188	3.552272
H	0.645823	3.443380	2.062351

alpha-hydroxy sulfide @MP2/6-311(2df,2p)

H	-0.002543	0.002009	-0.001903
C	0.008751	-0.001011	1.091356
O	1.326445	-0.006202	1.604603
C	-0.586901	-1.300812	1.589762
H	0.037570	-2.127188	1.255111
F	-1.856383	-1.472157	1.078401
H	-0.638707	-1.307738	2.676186
S	-0.930015	1.478540	1.533055
C	-1.005196	1.280772	3.327995
H	-1.753602	0.548161	3.614930
H	-1.285962	2.247779	3.735486
H	-0.030165	1.004187	3.719023
H	1.710467	0.856986	1.418177

alpha-hydroxy sulfide @PM3

H	-0.288706	0.219627	-0.051305
C	-0.146166	0.042921	1.042355
O	1.218024	-0.078494	1.345701
C	-0.798737	-1.296196	1.457235
H	-0.576716	-1.553746	2.507345
F	-0.348454	-2.324773	0.694984

H	-1.892929	-1.249598	1.325053
S	-1.019213	1.494767	1.812734
C	-0.737906	1.327414	3.583711
H	-1.147552	0.397495	3.994565
H	-1.242762	2.165984	4.078922
H	0.323432	1.367796	3.852859
H	1.651329	0.690086	0.998022

Methythiolate-Nicotinamide @MP2/6-311(2df,2p)

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.383895
C	1.138410	0.000000	2.104681
C	2.475395	-0.136930	1.466330
C	2.387773	0.199566	0.014641
C	1.193219	0.204418	-0.629106
S	3.136513	-1.858609	1.767225
C	1.936077	-2.778098	0.786570
C	3.576846	0.500234	-0.819363
O	3.497523	1.016846	-1.928574
C	-1.247483	0.212183	-0.711329
N	4.779579	0.201368	-0.233494
H	2.189736	-3.830974	0.877908
H	-0.974792	0.029078	1.850414
H	1.072694	0.018102	3.182965
H	3.224604	0.475412	1.971941
H	1.162255	0.405570	-1.691796
H	4.798939	-0.558116	0.431557
H	5.578274	0.297273	-0.839829
H	0.932307	-2.615137	1.174608
H	1.985721	-2.483695	-0.259434
H	-2.019412	-0.426149	-0.288918
H	-1.110634	-0.056642	-1.754260
H	-1.572646	1.252094	-0.651959

Methythiolate-Nicotinamide @PM3

C	0.046590	-0.135411	-0.032626
C	0.094845	-0.049149	1.449517
C	1.492106	-0.077220	1.971433
C	2.532365	-0.436631	1.178518
N	2.346227	-0.847177	-0.163006
C	1.103067	-0.494751	-0.777328
S	-1.014970	-1.344981	2.195749
C	-0.263258	-2.926945	1.780388
C	1.792297	0.351132	3.364691
O	2.933916	0.526956	3.783999
N	0.732237	0.661031	4.252381
H	-0.889560	-3.714873	2.216025
H	1.059333	-0.575583	-1.870943
H	-0.913583	0.100344	-0.506211
H	-0.413649	0.894359	1.770752
H	3.567160	-0.455434	1.557711
H	-0.096365	0.122891	4.103043
H	0.995543	0.716351	5.211187
H	-0.208197	-3.099669	0.699715
H	0.749074	-3.037907	2.184688
C	3.539265	-0.837057	-1.037106

H	3.331941	-1.417812	-1.945865
H	4.385527	-1.306475	-0.517562
H	3.839407	0.177321	-1.337764

Thioacyl backbone(proton on amide) @MP2/6-311(2df,2p)

C	-0.000142	-0.000581	0.000108
C	-0.000504	-0.001234	1.513958
N	1.217065	0.003618	2.063311
C	1.390171	0.016967	3.493619
C	2.860409	-0.179559	3.827542
S	3.938396	1.153180	3.231512
C	4.463629	0.340507	1.503012
C	5.452879	1.369019	0.956098
O	-1.061566	-0.011040	2.158952
O	3.466253	0.052321	0.705226
H	5.020198	-0.533005	1.903037
H	5.873343	0.974925	0.030062
H	6.260429	1.582045	1.658324
H	4.918964	2.289078	0.722701
H	2.090021	0.032210	1.462821
H	1.008792	0.019497	-0.405405
H	-0.555302	0.868433	-0.347921
H	-0.524027	-0.887812	-0.351021
H	0.787123	-0.778254	3.942115
H	1.037233	0.961755	3.915580
H	3.215446	-1.116723	3.391312
H	2.977926	-0.248107	4.909554

Thioacyl backbone(proton on amide) @PM3

C	2.596831	1.835795	-0.159853
C	2.409491	0.342027	-0.281537
O	3.212145	-0.379981	-0.877664
N	1.313228	-0.208770	0.402323
C	0.870298	-1.586120	0.073783
C	-0.490850	-1.888829	0.686545
S	-1.904770	-1.088888	-0.125940
C	-1.982862	0.889555	0.612724
O	-0.867103	1.493076	0.715635
C	-2.983894	1.443099	-0.405100
H	-2.452525	0.605091	1.579943
H	-3.449740	2.359915	-0.019007
H	-3.789882	0.727796	-0.615993
H	-2.505968	1.697643	-1.359164
H	0.539309	0.442400	0.581339
H	1.715206	2.373676	-0.535896
H	3.470746	2.184548	-0.724178
H	2.738213	2.129438	0.888614
H	1.634801	-2.283900	0.472974
H	0.845219	-1.744004	-1.024724
H	-0.491561	-1.633754	1.763203
H	-0.660100	-2.979980	0.633787

Thioacyl backbone(proton on thioacyl) @MP2/6-311(2df,2p)

C	0.011558	-0.011811	-0.002258
C	0.001268	-0.013447	1.518746
O	1.102640	-0.069491	2.121585
N	-1.212989	0.052488	2.062461
C	-1.232109	0.047291	3.506329
C	-2.513451	0.674613	4.030795
S	-4.053109	-0.221306	3.663613
C	-4.317593	0.250034	1.892844
O	-3.504128	-0.405953	0.998232
C	-5.767167	-0.053440	1.564800
H	-4.146070	1.336441	1.886762
H	-5.948478	0.199722	0.521255
H	-6.448649	0.508893	2.200141
H	-5.954036	-1.118698	1.692736
H	-2.523865	-0.239901	1.340838
H	-0.992807	0.023128	-0.418264
H	0.522734	-0.906824	-0.355599
H	0.583231	0.847208	-0.353238
H	-0.378852	0.610848	3.902434
H	-1.144491	-0.970882	3.907208
H	-2.481579	0.740024	5.120512
H	-2.617653	1.688240	3.637505

Thioacyl backbone(proton on thioacyl) @PM3

C	3.035479	1.169693	0.613780
C	2.429788	-0.120462	0.087904
O	3.162367	-0.992315	-0.431424
N	1.078506	-0.215854	0.224297
C	0.388867	-1.411061	-0.264318
C	-0.881293	-1.646683	0.548917
S	-2.346002	-0.622106	0.142393
C	-1.798717	1.188411	0.182356
O	-0.795195	1.515429	1.076610
C	-1.481464	1.637911	-1.241838
H	-2.698028	1.710736	0.575761
H	-1.264683	2.714012	-1.275159
H	-2.325709	1.446301	-1.915659
H	-0.603676	1.113136	-1.645907
H	0.005217	0.992897	0.830272
H	2.377182	1.692866	1.319866
H	3.240146	1.858190	-0.216434
H	3.988164	0.982395	1.125492
H	1.022740	-2.320711	-0.191546
H	0.141954	-1.289290	-1.340043
H	-1.243392	-2.680109	0.392466
H	-0.668428	-1.543665	1.628361