

Electronic Supporting Information for:

**Interaction of Oxalic Acid with Methylamine and Its Atmospheric
Implications**

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Table S1. $\text{H}_2\text{C}_2\text{O}_4\text{-CH}_3\text{NH}_2$

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I-a	E[DF-MP2-F12]	-473.6629682
C	-0.975404	0.813045 -0.031767
C	-1.113210	-0.748773 -0.006552
O	0.194342	1.335741 -0.215175
O	-2.021921	1.438305 0.131678
O	-0.210562	-1.549698 -0.143532
O	-2.383748	-1.089408 0.191935
H	1.068331	0.645684 -0.358266
H	-2.840943	-0.204720 0.260757
C	3.203963	0.004365 0.585565
H	4.045389	-0.696583 0.512729
H	3.593686	1.027248 0.591071
H	2.687114	-0.167607 1.534912
N	2.235639	-0.145700 -0.515518
H	1.800210	-1.072751 -0.512715
H	2.679768	-0.002727 -1.422593

Table S2. $\text{H}_2\text{C}_2\text{O}_4\text{-(CH}_3\text{NH}_2)_2$

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II-a	E[DF-MP2-F12]	-569.3872719
C	1.644113	0.704589 0.469208
C	1.541616	-0.479028 -0.562458
O	0.613734	1.417201 0.662131
O	2.768500	0.793480 0.998664
O	0.549634	-0.783336 -1.205920
O	2.700444	-1.124212 -0.633369
H	-0.580284	1.194418 -0.093896
H	3.246303	-0.590551 0.028444
C	-2.017107	-1.984161 1.255481
H	-1.224154	-1.381657 1.713233
H	-2.956513	-1.746124 1.767378
H	-1.785320	-3.044491 1.434792
N	-2.127307	-1.630117 -0.169966
H	-2.855759	-2.183159 -0.620675
H	-1.246067	-1.836788 -0.649966
C	-2.531281	2.142425 -0.195116
H	-2.700638	2.027391 0.879094
H	-2.114696	3.137519 -0.375436

H	-3.486320	2.044982	-0.721992
N	-1.571660	1.109097	-0.635004
H	-1.359667	1.180168	-1.632198
H	-1.926667	0.117412	-0.468730

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II-b E[DF-MP2-F12] -569.3857189

C	1.777033	0.126134	-0.714363
C	1.558968	-0.195334	0.818388
O	2.993145	-0.258629	-1.081649
O	0.974122	0.640246	-1.478564
O	2.552441	-0.741767	1.337411
O	0.452242	0.107012	1.356023
H	3.337181	-0.629728	-0.205614
H	-0.597961	0.732944	0.580042
C	-1.903390	2.464669	0.368115
H	-2.609018	2.887317	-0.354701
H	-2.412032	2.323949	1.326428
H	-1.074818	3.163987	0.512258
N	-1.377628	1.168950	-0.100128
H	-0.823327	1.243674	-0.967056
H	-2.129943	0.442038	-0.227181
C	-2.171153	-2.194735	-0.159409
H	-1.560393	-2.032815	0.735344
H	-2.614633	-3.199374	-0.107581
H	-1.500780	-2.157262	-1.025034
N	-3.166685	-1.107557	-0.272271
H	-3.818753	-1.150750	0.511755
H	-3.729685	-1.233023	-1.114023

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II-c E[DF-MP2-F12] -569.3857158

C	-1.776863	0.126302	-0.714358
C	-1.558936	-0.195094	0.818469
O	-2.992823	-0.258765	-1.081770
O	-0.973920	0.640436	-1.478558
O	-2.552440	-0.741657	1.337322
O	-0.452265	0.107201	1.356237
H	-3.336835	-0.629838	-0.205684
H	0.597961	0.733104	0.580432
C	1.903556	2.464711	0.367744
H	2.609031	2.887087	-0.355385
H	1.075007	3.164085	0.511762
H	2.412400	2.324404	1.326012

N	1.377702	1.168829	-0.099901
H	2.129958	0.441851	-0.226875
H	0.823210	1.243255	-0.966778
C	2.170584	-2.194837	-0.159610
H	1.559500	-2.032811	0.734908
H	1.500571	-2.157121	-1.025506
H	2.613728	-3.199621	-0.107659
N	3.166458	-1.107960	-0.271990
H	3.729677	-1.233365	-1.113590
H	3.818209	-1.151317	0.512276

Table S3.

$\text{H}_2\text{C}_2\text{O}_4-(\text{CH}_3\text{NH}_2)_3$

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III-a E[DF-MP2-F12] -665.1125584

C	1.707335	-0.002628	-0.638926
C	1.798868	0.000526	0.937321
O	0.561781	-0.002075	-1.153562
O	2.844076	-0.005351	-1.168104
O	0.855793	0.003325	1.722273
O	3.064749	-0.000312	1.321792
H	-0.732147	0.002527	1.097922
H	3.514554	-0.002789	0.409118
C	-0.937668	-3.415299	-0.560096
H	-1.775631	-4.006886	-0.172822
H	-0.389528	-4.030448	-1.289860
H	-0.260896	-3.207564	0.277046
N	-1.433747	-2.142201	-1.105076
H	-2.051096	-2.312490	-1.898605
H	-0.646135	-1.572131	-1.444061
C	-2.730906	0.004607	1.798712
H	-3.736837	0.004361	1.367299
H	-2.610940	-0.883798	2.425932
H	-2.610055	0.895060	2.422852
N	-1.720368	0.002305	0.724035
H	-1.784967	0.855177	0.086412
H	-1.785837	-0.852444	0.089065
C	-0.931069	3.414060	-0.564489
H	-0.380524	4.027567	-1.293824
H	-1.767915	4.007944	-0.178314
H	-0.255747	3.204792	0.273447
N	-1.429850	2.142085	-1.109624
H	-0.643263	1.569851	-1.447340
H	-2.045838	2.313664	-1.903922

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III-b E[DF-MP2-F12] -665.1111002

C	1.864446	-1.295859	0.143684
C	0.509741	-2.071719	-0.046471
O	2.890932	-2.137749	0.064778
O	1.979035	-0.095403	0.329116
O	0.668506	-3.294149	-0.242672
O	-0.556857	-1.396032	0.011031
H	2.400675	-3.005498	-0.095824
H	-0.527444	0.159636	0.293447
C	-0.939438	1.587132	1.805752
H	0.060830	1.521810	2.243515
H	-1.311358	2.612659	1.896226
H	-1.606689	0.911848	2.349411
N	-0.871546	1.182113	0.387899
H	-0.202495	1.796767	-0.156819
H	-1.816561	1.126991	-0.063291
C	1.898264	3.768972	-0.430654
H	2.917345	3.949664	-0.805874
H	1.275214	4.628578	-0.704299
H	1.947295	3.728221	0.663504
N	1.285478	2.530280	-0.933540
H	1.843231	1.714938	-0.657027
H	1.263874	2.537565	-1.953389
C	-4.434599	-0.338122	-0.154436
H	-4.229773	-0.509636	0.908642
H	-5.114140	0.519162	-0.228019
H	-4.958098	-1.226199	-0.541584
N	-3.173273	-0.033667	-0.846913
H	-3.345821	0.091537	-1.844527
H	-2.524114	-0.824884	-0.761489

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III-c E[DF-MP2-F12] -665.1093834

C	-1.815878	0.584872	-0.472037
C	-2.347072	-0.391739	0.646857
O	-0.759512	0.262604	-1.096329
O	-2.518906	1.605315	-0.606717
O	-1.821981	-1.429626	1.013148
O	-3.473170	0.086852	1.168692
H	1.550499	-1.478945	-0.074010
H	-3.576459	0.940165	0.643797
C	3.203799	-0.353564	1.736051

H	3.958701	0.411382	1.974848
H	2.263346	-0.054875	2.214295
H	3.521090	-1.299107	2.191992
N	2.976656	-0.534699	0.293237
H	3.846036	-0.812581	-0.163271
H	2.681962	0.368621	-0.138120
C	0.709200	-2.928146	-1.394160
H	-0.287781	-3.250914	-1.707601
H	1.244315	-2.537855	-2.264761
H	1.257046	-3.786096	-0.991780
N	0.592658	-1.862417	-0.379948
H	0.031730	-2.157600	0.429397
H	0.012987	-1.006601	-0.736858
C	1.518845	3.044973	0.068882
H	0.839993	3.834851	-0.289157
H	1.089830	2.634810	0.990970
H	2.478918	3.507598	0.328819
N	1.733724	1.952388	-0.892846
H	2.113886	2.330999	-1.760673
H	0.827820	1.529715	-1.134891

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III-d E[DF-MP2-F12] -665.1068096

C	0.426019	-0.074783	0.755990
C	0.703518	-1.190194	-0.324357
O	1.433704	0.658459	1.172039
O	-0.714363	0.102273	1.182713
O	1.857921	-1.624809	-0.448399
O	-0.320811	-1.559214	-0.991233
H	2.396419	0.417826	0.794017
H	-1.615082	-1.141014	-0.726064
C	-2.311247	2.755317	-0.832274
H	-1.484015	2.281359	-1.373467
H	-3.098336	2.985770	-1.560068
H	-1.939578	3.703783	-0.414818
N	-2.823211	1.815785	0.176491
H	-3.576986	2.244086	0.712909
H	-2.075532	1.568525	0.835607
C	-3.269281	-1.776642	0.504012
H	-4.336135	-1.592614	0.670928
H	-3.111906	-2.834312	0.273389
H	-2.703011	-1.520978	1.403290
N	-2.747654	-0.943514	-0.601535
H	-2.884647	0.085588	-0.383243

H	-3.217688	-1.161838	-1.482117
C	4.429025	1.014546	-0.690985
H	4.642431	1.997467	-0.255276
H	5.354374	0.624881	-1.140955
H	3.695280	1.154694	-1.492341
N	3.852411	0.130567	0.328839
H	4.511356	-0.047617	1.085470
H	3.552426	-0.768612	-0.069114

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III-e E[DF-MP2-F12] -665.1053288

C	1.136904	-1.515046	-0.057830
C	2.280567	-0.452431	-0.250611
O	-0.038430	-1.180585	-0.392120
O	1.541663	-2.588227	0.430362
O	2.137270	0.681846	-0.677598
O	3.446672	-0.957853	0.138750
H	-0.328983	0.176623	-1.010430
H	3.159704	-1.880314	0.429411
C	-3.849198	-1.771763	0.468105
H	-4.836142	-1.371358	0.732268
H	-3.828629	-1.895750	-0.621903
H	-3.758244	-2.775881	0.916097
N	-2.804167	-0.821287	0.865776
H	-1.881785	-1.190515	0.611262
H	-2.802996	-0.715128	1.880179
C	-2.074487	1.189223	-1.759153
H	-2.630399	0.857858	-0.873061
H	-2.371626	2.203082	-2.046308
H	-2.282594	0.502539	-2.585043
N	-0.630081	1.147263	-1.429385
H	-0.349586	1.879049	-0.702803
H	-0.035007	1.309165	-2.244521
C	-0.015656	2.482313	1.915826
H	0.665132	2.814875	2.713402
H	-1.006649	2.909550	2.105367
H	-0.107171	1.392033	1.977145
N	0.428410	2.851231	0.560777
H	1.348740	2.445218	0.367776
H	0.520924	3.863280	0.477819

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III-f E[DF-MP2-F12] -665.1039141

C	-2.728735	-0.459824	-0.346029
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C	-1.957512	0.839611	0.109871
O	-3.976705	-0.148567	-0.681213
O	-2.279460	-1.593210	-0.399203
O	-2.657855	1.868343	0.052539
O	-0.748491	0.721365	0.473672
H	-3.971419	0.846277	-0.516693
H	-0.047014	-0.608225	0.451183
C	0.825018	-2.073822	1.747914
H	1.232346	-3.088555	1.696931
H	1.589863	-1.393934	2.133639
H	-0.034539	-2.063544	2.424068
N	0.404526	-1.610850	0.409672
H	-0.384196	-2.156347	0.034352
H	1.210876	-1.596150	-0.278284
C	3.798583	-0.850160	-0.601053
H	4.648805	-0.529744	-1.221522
H	3.474938	-0.007796	0.025255
H	4.140472	-1.661362	0.052348
N	2.635857	-1.318088	-1.384973
H	2.904089	-2.083508	-2.004296
H	2.309396	-0.564532	-1.992112
C	2.392224	2.882243	-0.232270
H	1.890721	3.859027	-0.125156
H	3.476097	3.055916	-0.217917
H	2.137111	2.493759	-1.226672
N	2.030147	1.887211	0.783816
H	1.018084	1.720499	0.756367
H	2.233275	2.258569	1.711946

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III-g E[DF-MP2-F12] -665.1033331

C	-0.544757	-0.398218	0.288580
C	-0.981782	0.919120	-0.451740
O	0.612114	-0.366497	0.837515
O	-1.319325	-1.366735	0.263954
O	-0.161378	1.609798	-1.055397
O	-2.255278	1.246394	-0.419047
H	1.561281	0.656353	0.481554
H	-2.897108	0.560270	0.067089
C	4.282544	-2.171662	-0.081356
H	4.404742	-1.849025	0.959107
H	4.116764	-3.260313	-0.078234
H	5.224895	-1.970551	-0.604145
N	3.197447	-1.398785	-0.703683

H	2.313014	-1.567228	-0.211103
H	3.051923	-1.709636	-1.664457
C	3.094486	2.213087	0.823177
H	2.388561	2.923509	1.263375
H	3.593489	1.668048	1.630171
H	3.844865	2.765075	0.247338
N	2.364133	1.261795	-0.029870
H	2.960742	0.504699	-0.442840
H	1.795440	1.710856	-0.762671
C	-5.054623	-0.769403	-0.252203
H	-4.659930	-0.943876	-1.259045
H	-5.629884	-1.657233	0.050172
H	-5.738025	0.085670	-0.305067
N	-3.936117	-0.456723	0.646521
H	-3.235547	-1.208131	0.663434
H	-4.257731	-0.293726	1.599594

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III-h	E[DF-MP2-F12]	-665.1030927	
C	2.367651	-0.424757	-0.587763
C	1.726381	0.644085	0.381664
O	3.508417	0.043344	-1.081333
O	1.911796	-1.521298	-0.872026
O	2.396842	1.692215	0.458657
O	0.635808	0.358796	0.962206
H	3.543063	0.950693	-0.640998
H	-0.088813	-0.934363	0.691145
C	-1.568592	3.340269	-0.014316
H	-0.840037	4.070305	0.376481
H	-1.187537	2.985088	-0.980318
H	-2.510415	3.868823	-0.209727
N	-1.816423	2.188097	0.861230
H	-2.167892	2.512230	1.762189
H	-0.929925	1.708084	1.052807
C	-0.583211	-2.819005	1.582891
H	0.416743	-2.923265	2.013165
H	-1.251673	-2.399292	2.340182
H	-0.952036	-3.804983	1.282895
N	-0.527050	-1.906718	0.423021
H	-1.482754	-1.765475	-0.017580
H	0.161755	-2.219166	-0.278765
C	-2.962080	-0.121797	-1.494954
H	-3.885303	0.187979	-2.006174
H	-2.648556	0.678245	-0.810527

H	-2.181472	-0.263426	-2.251580
N	-3.114332	-1.370427	-0.714437
H	-3.509689	-2.109336	-1.297164
H	-3.784610	-1.216037	0.040098

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III-i	E[DF-MP2-F12]	-665.1030557	
C	-2.720184	-0.498622	-0.190586
C	-1.918546	0.858755	-0.098673
O	-3.978946	-0.254719	-0.537943
O	-2.284035	-1.620711	0.012971
O	-2.614109	1.853066	-0.382440
O	-0.696280	0.815304	0.235245
H	-3.957052	0.750488	-0.622504
H	-0.407593	-2.069452	0.452228
C	3.664312	-0.966848	-0.921225
H	4.449440	-0.915199	-1.690270
H	3.327191	0.053026	-0.687996
H	4.100984	-1.410345	-0.018453
N	2.487689	-1.763164	-1.332101
H	2.771279	-2.699003	-1.624252
H	2.055837	-1.330813	-2.150507
C	0.917163	-1.683062	2.032828
H	1.738367	-0.985167	2.219711
H	0.108006	-1.475258	2.738691
H	1.272825	-2.707294	2.183268
N	0.427190	-1.497319	0.652365
H	1.182837	-1.675979	-0.071794
H	0.007574	-0.493895	0.494775
C	2.491092	2.823785	0.791246
H	1.955593	3.762174	1.015586
H	2.411074	2.181848	1.677945
H	3.553926	3.064717	0.659833
N	1.994719	2.094458	-0.381081
H	2.044448	2.695770	-1.203612
H	1.002008	1.868990	-0.251148

Table S4.

$\text{H}_2\text{C}_2\text{O}_4-(\text{CH}_3\text{NH}_2)_4$

36

IV-a	E[DF-MP2-F12]	-760.8345915	
C	-1.603488	1.541350	0.137303
C	-2.706470	0.421439	0.089980
O	-0.433300	1.193585	0.462374

O	-2.037898	2.671389	-0.171557
O	-2.534998	-0.761610	0.329994
O	-3.876966	0.946406	-0.264606
H	0.006562	-0.319065	0.817505
H	-3.615117	1.914253	-0.377588
C	0.131979	-1.625739	2.458574
H	-0.954565	-1.715155	2.546140
H	0.600979	-2.579707	2.720267
H	0.482192	-0.852311	3.148715
N	0.477577	-1.247760	1.073034
H	1.527605	-1.100453	0.953640
H	0.117211	-1.973316	0.393900
C	2.561008	2.816713	-1.201818
H	3.631360	3.008808	-1.348785
H	2.258258	2.061624	-1.937559
H	2.010858	3.743129	-1.433503
N	2.323929	2.294677	0.151163
H	1.317613	2.115293	0.279579
H	2.579036	3.002404	0.840380
C	3.830009	-1.121913	-0.539197
H	4.034023	-2.189479	-0.389878
H	3.129893	-1.034553	-1.379244
H	4.771204	-0.633765	-0.838296
N	3.213493	-0.547437	0.665280
H	3.025748	0.468683	0.520304
H	3.857961	-0.619815	1.453167
C	-0.508989	-2.711356	-2.200758
H	0.421226	-3.236561	-2.448360
H	-1.278870	-3.014255	-2.927112
H	-0.330352	-1.637380	-2.330857
N	-0.868089	-2.971818	-0.798783
H	-1.058703	-3.963439	-0.658285
H	-1.721493	-2.459686	-0.553131

36

IV-b E[DF-MP2-F12] -760.8341884

C	2.585786	-0.913496	0.376223
C	1.326789	-1.765000	-0.026937
O	3.685409	-1.659817	0.305751
O	2.579805	0.261311	0.702473
O	1.608598	-2.942972	-0.333246
O	0.202576	-1.188750	-0.006837
H	3.289940	-2.538601	0.006787
H	-0.026991	0.352489	0.408554

C	-0.356412	1.495754	2.137734
H	-1.020385	0.755473	2.593969
H	0.660773	1.335743	2.506483
H	-0.693844	2.499937	2.413771
N	-0.369502	1.335230	0.668705
H	-1.352660	1.431873	0.268981
H	0.295746	2.024518	0.221726
C	-4.163100	1.438105	0.463270
H	-4.021942	0.838974	1.370957
H	-4.234007	2.489170	0.769571
H	-5.129153	1.147227	0.020293
N	-3.011486	1.243133	-0.429571
H	-3.144205	1.782735	-1.285853
H	-2.947053	0.241660	-0.715197
C	-3.305316	-2.657157	-0.227693
H	-4.363097	-2.650239	-0.519675
H	-2.935329	-3.692563	-0.303785
H	-3.253852	-2.365907	0.828600
N	-2.553849	-1.685633	-1.033913
H	-2.577856	-1.964389	-2.015087
H	-1.562163	-1.698254	-0.754912
C	1.838722	2.910203	-1.929174
H	1.513965	1.935578	-2.312023
H	1.152416	3.668619	-2.324075
H	2.843211	3.112222	-2.332046
N	1.771546	2.896435	-0.460233
H	2.087019	3.789129	-0.081947
H	2.392589	2.171825	-0.085671

36

IV-c E[DF-MP2-F12] -760.8329922

C	-0.334203	1.499434	-0.663009
C	-1.533132	2.247016	0.014093
O	-0.582387	0.395483	-1.204793
O	0.769833	2.105936	-0.549329
O	-2.642868	1.787413	0.176005
O	-1.162179	3.465391	0.436027
H	0.590497	-0.697692	-1.150267
H	-0.194140	3.477802	0.198331
C	1.563615	-2.435676	-1.902014
H	0.633443	-2.967967	-2.124366
H	1.917991	-1.950611	-2.816844
H	2.315438	-3.158040	-1.567766
N	1.322811	-1.425415	-0.855916

H	0.912966	-1.860311	0.037169
H	2.191706	-0.851688	-0.638912
C	0.304906	-1.507489	2.609772
H	0.334440	-0.447827	2.328372
H	-0.392626	-1.606226	3.456002
H	1.306316	-1.788477	2.959252
N	-0.069529	-2.307623	1.432919
H	-1.028046	-2.029389	1.120109
H	-0.115600	-3.294938	1.687191
C	-3.104316	-2.047215	-0.819101
H	-3.214710	-3.124198	-0.635569
H	-4.033107	-1.685003	-1.289217
H	-2.294069	-1.904318	-1.543213
N	-2.749425	-1.355705	0.427643
H	-3.530237	-1.404471	1.082952
H	-2.612802	-0.357592	0.226000
C	3.911086	0.740224	0.945769
H	3.159492	0.546292	1.720159
H	4.722992	0.015642	1.082190
H	4.317848	1.748490	1.120498
N	3.296403	0.564722	-0.377965
H	3.979997	0.758110	-1.109990
H	2.523468	1.239014	-0.505197

36

IV-d E[DF-MP2-F12] -760.8323118

C	-0.316598	1.877211	0.141894
C	-0.962074	1.727302	-1.286534
O	-0.167361	0.829000	0.817838
O	-0.020219	3.068278	0.401988
O	-1.308771	0.678760	-1.817303
O	-1.077667	2.912434	-1.867735
H	-0.947003	-0.798237	-0.976273
H	-0.677741	3.497081	-1.141263
C	2.635926	-1.803634	-1.609792
H	3.732584	-1.738585	-1.535032
H	2.391480	-2.543284	-2.382196
H	2.265904	-0.830791	-1.955166
N	1.972486	-2.150516	-0.342435
H	2.245474	-1.462621	0.393664
H	2.296660	-3.063890	-0.021976
C	-3.335274	-0.831465	2.052779
H	-3.940189	-1.742543	2.133643
H	-3.606889	-0.163690	2.885019

H	-3.612527	-0.328673	1.118636
N	-1.907833	-1.179672	2.005322
H	-1.622665	-1.633493	2.872652
H	-1.337892	-0.328902	1.899601
C	-1.465797	-2.790487	-1.395808
H	-1.325876	-3.777505	-0.943601
H	-2.536855	-2.585358	-1.483519
H	-1.024980	-2.789711	-2.397171
N	-0.819388	-1.757819	-0.562179
H	0.237414	-1.938705	-0.459420
H	-1.243308	-1.707412	0.411716
C	3.572566	1.028388	1.219913
H	4.579689	0.607775	1.332775
H	3.430226	1.263839	0.158458
H	3.530184	1.978564	1.775942
N	2.566495	0.039945	1.634808
H	1.623204	0.440235	1.525114
H	2.680439	-0.169325	2.626778

36

IV-e E[DF-MP2-F12] -760.8305626

C	-0.967686	2.159033	0.301117
C	0.538104	2.142915	-0.146159
O	-1.604773	1.076039	0.195231
O	-1.338047	3.275415	0.724536
O	1.133292	1.176824	-0.596550
O	1.091084	3.337092	0.047297
H	-0.831324	-0.277095	-0.343234
H	0.296548	3.840317	0.418835
C	4.347998	-0.889357	-1.097702
H	3.684723	-1.296295	-1.870995
H	4.922228	-0.065050	-1.551552
H	5.053568	-1.682433	-0.820977
N	3.548289	-0.503064	0.071539
H	4.154429	-0.115145	0.794279
H	2.887669	0.239734	-0.183881
C	-0.457921	-1.467677	-2.045469
H	-1.258075	-1.010877	-2.635600
H	0.482801	-0.960565	-2.276048
H	-0.379695	-2.528486	-2.304617
N	-0.746182	-1.310865	-0.606459
H	0.019460	-1.763074	-0.007592
H	-1.695216	-1.673484	-0.342772
C	-4.650880	-1.329193	-0.548787

H	-4.940894	-2.368725	-0.742990
H	-5.529003	-0.796104	-0.151479
H	-4.391740	-0.871201	-1.510437
N	-3.475516	-1.295983	0.333993
H	-3.714693	-1.682766	1.247038
H	-3.182121	-0.324462	0.494669
C	1.022375	-2.022042	2.406517
H	0.158682	-2.606151	2.747414
H	1.853052	-2.201636	3.106733
H	0.750935	-0.961623	2.471998
N	1.338779	-2.352226	1.007601
H	1.586116	-3.339284	0.930936
H	2.170570	-1.805660	0.702333

36

IV-f E[DF-MP2-F12] -760.8301225

C	0.357805	1.760471	-0.732791
C	1.633242	1.503193	0.158923
O	-0.454421	0.811128	-0.897393
O	0.317950	2.930591	-1.174128
O	1.913830	0.462227	0.736929
O	2.378211	2.599948	0.207787
H	-0.311569	-0.673704	-0.269171
H	1.814795	3.216225	-0.369595
C	-1.427650	-2.482145	-0.285109
H	-2.352539	-1.920841	-0.106119
H	-1.339583	-2.690460	-1.356041
H	-1.440775	-3.430220	0.262324
N	-0.278582	-1.658435	0.151934
H	-0.257090	-1.512920	1.198794
H	0.655364	-2.064739	-0.125438
C	-1.017352	0.097063	3.313776
H	-1.871260	-0.486855	3.675417
H	-0.714378	0.796306	4.108017
H	-1.359931	0.684100	2.454069
N	0.052039	-0.815519	2.876902
H	0.376986	-1.384073	3.658372
H	0.857464	-0.280545	2.539085
C	-4.285306	0.219138	-1.562700
H	-5.253809	-0.216180	-1.285274
H	-4.477313	1.179839	-2.070766
H	-3.824664	-0.453868	-2.296949
N	-3.421950	0.306742	-0.379949
H	-3.838181	0.939042	0.303593

H	-2.516808	0.714689	-0.638902
C	2.637636	-2.041358	-2.069514
H	2.352346	-2.951757	-2.609261
H	1.986170	-1.230598	-2.415953
H	3.672118	-1.786756	-2.346484
N	2.432573	-2.239366	-0.625292
H	2.683041	-1.385670	-0.117436
H	3.036240	-2.984287	-0.278526

36

IV-g E[DF-MP2-F12] -760.8296169

C	1.194166	-0.787932	0.290439
C	1.076868	0.790066	0.251839
O	2.391152	-1.330494	0.337007
O	0.180688	-1.483787	0.268001
O	2.084884	1.455508	-0.040371
O	-0.087061	1.229818	0.512472
H	3.214284	-0.671980	0.346300
H	-1.338283	0.304282	0.649155
C	-2.933288	-3.479280	-0.914842
H	-3.995682	-3.442524	-1.184255
H	-2.466172	-4.306040	-1.472896
H	-2.869414	-3.720528	0.152503
N	-2.312610	-2.168547	-1.151089
H	-1.324298	-2.180117	-0.871574
H	-2.335332	-1.941572	-2.145194
C	5.431647	-0.070485	-0.836055
H	5.954143	-1.021473	-0.680169
H	4.834765	-0.164311	-1.750033
H	6.183827	0.716557	-0.998691
N	4.531029	0.194945	0.290980
H	3.956350	1.033812	0.138427
H	5.044679	0.302875	1.164173
C	-2.839933	3.215901	-1.425773
H	-3.915984	3.350609	-1.589019
H	-2.328078	4.144942	-1.723265
H	-2.499252	2.419914	-2.098546
N	-2.593238	2.809639	-0.035258
H	-2.881599	3.551586	0.602191
H	-1.586351	2.662858	0.115707
C	-2.751899	-0.434697	2.052004
H	-2.541075	0.356073	2.778233
H	-3.813874	-0.696578	2.102191
H	-2.147282	-1.311626	2.300901

N	-2.390622	0.027512	0.698931
H	-2.860116	0.926686	0.438669
H	-2.549843	-0.728093	-0.022287

36

IV-h	E[DF-MP2-F12]	-760.8294411
C	0.044347	2.064232
C	1.598020	1.967284
O	-0.616443	0.987640
O	-0.351911	3.227244
O	2.221552	0.945001
O	2.154474	3.172594
H	0.075722	-0.483068
H	1.340573	3.736706
C	-3.061044	-1.872229
H	-3.132397	-2.950822
H	-3.329556	-1.686993
H	-3.800984	-1.366416
N	-1.674872	-1.426156
H	-1.591434	-0.424758
H	-1.412237	-1.549001
C	-2.989530	0.635755
H	-1.994303	0.406050
H	-3.150924	1.720442
H	-3.722054	0.111928
N	-3.078299	0.149899
H	-2.394293	0.645167
H	-3.997787	0.374199
C	-0.412044	-2.100161
H	-0.404268	-3.194089
H	0.191051	-1.767561
H	-1.439153	-1.733798
N	0.156335	-1.546537
H	-0.422734	-1.815942
H	1.174213	-1.810545
C	3.761994	-2.473340
H	4.840040	-2.253103
H	3.370192	-2.063344
H	3.635725	-3.561980
N	2.996894	-1.916100
H	3.374133	-2.255699
H	3.078242	-0.894189

36

IV-i E[DF-MP2-F12] -760.8286288

C	0.036797	1.961141	-0.867953
C	1.196276	1.798009	0.185620
O	0.161842	3.118602	-1.505606
O	-0.850695	1.151638	-1.094209
O	1.978412	2.774748	0.189210
O	1.222925	0.742289	0.873674
H	0.993335	3.478401	-1.051405
H	0.319222	-0.613258	0.603799
C	-2.657091	-2.143465	-1.896419
H	-3.286182	-1.806288	-2.734618
H	-2.706097	-3.237858	-1.851084
H	-3.084675	-1.749651	-0.966910
N	-1.251945	-1.714440	-1.992975
H	-0.833518	-2.058862	-2.856821
H	-1.197801	-0.691009	-2.020616
C	-0.683757	-2.193527	1.609266
H	-0.180903	-2.005313	2.562786
H	-1.653613	-1.681573	1.597467
H	-0.824036	-3.272072	1.484817
N	0.144834	-1.661813	0.503372
H	-0.313261	-1.821432	-0.440679
H	1.127709	-2.036363	0.526702
C	3.863513	-1.808402	-0.411892
H	4.070437	-2.858542	-0.649529
H	3.337764	-1.370617	-1.268674
H	4.825094	-1.282627	-0.306182
N	3.000279	-1.728242	0.776018
H	2.790797	-0.745210	0.990493
H	3.484733	-2.110938	1.587741
C	-2.674095	1.083180	2.298772
H	-2.887450	2.162648	2.220381
H	-3.264791	0.681996	3.131844
H	-1.614952	0.975474	2.562466
N	-2.949485	0.311483	1.079056
H	-2.375800	0.671365	0.311401
H	-3.921516	0.442969	0.799396

36

IV-j E[DF-MP2-F12] -760.8286281

C	0.036445	1.961150	-0.868012
C	1.196010	1.798113	0.185408
O	0.161334	3.118580	-1.505742
O	-0.851049	1.151593	-1.094067

O	1.978140	2.774876	0.188856
O	1.222802	0.742471	0.873559
H	0.992866	3.478516	-1.051600
H	0.319351	-0.613143	0.603333
C	-0.683146	-2.193521	1.609019
H	-0.179989	-2.005270	2.562371
H	-1.653033	-1.681619	1.597548
H	-0.823386	-3.272073	1.484615
N	0.145069	-1.661723	0.502864
H	1.127999	-2.036120	0.526037
H	-0.313220	-1.821444	-0.441089
C	-2.657339	-2.143756	-1.896127
H	-2.706156	-3.238152	-1.850642
H	-3.084780	-1.749915	-0.966565
H	-3.286696	-1.806797	-2.734214
N	-1.252300	-1.714504	-1.993067
H	-1.198261	-0.691066	-2.020525
H	-0.834045	-2.058751	-2.857062
C	3.864047	-1.808116	-0.411772
H	4.070972	-2.858248	-0.649444
H	3.338536	-1.370236	-1.268650
H	4.825635	-1.282408	-0.305790
N	3.000528	-1.728001	0.775928
H	2.790960	-0.744994	0.990410
H	3.484739	-2.110764	1.587762
C	-2.673650	1.082863	2.299318
H	-3.264112	0.681609	3.132518
H	-1.614431	0.975159	2.562686
H	-2.887063	2.162323	2.221030
N	-2.949366	0.311218	1.079609
H	-2.375927	0.671221	0.311821
H	-3.921491	0.442690	0.800256

36

IV-k E[DF-MP2-F12] -760.8264762

C	0.296011	-1.463311	0.672555
C	-0.273288	-1.410683	-0.770420
O	-0.378621	-0.789035	1.546397
O	1.374159	-2.046304	0.894672
O	-1.346106	-1.985099	-1.035461
O	0.393989	-0.665028	-1.590384
H	-1.732805	-0.452101	1.069770
H	1.747276	-0.352208	-1.091335
C	1.566778	2.459983	1.935403

H	0.845211	2.639312	1.129178
H	1.071600	2.703572	2.889065
H	2.399576	3.159991	1.796098
N	2.051658	1.076435	1.846747
H	2.714063	0.885885	2.599013
H	1.269184	0.419491	1.983057
C	-1.627728	2.561795	-1.791299
H	-2.478682	3.229979	-1.611349
H	-0.905810	2.719697	-0.980880
H	-1.146138	2.868158	-2.733722
N	-2.073315	1.162445	-1.772157
H	-1.274951	0.535189	-1.950287
H	-2.737442	0.993342	-2.528067
C	-3.826646	0.013606	1.516152
H	-3.618702	0.986846	1.971719
H	-4.788522	0.064800	0.994526
H	-3.889881	-0.736430	2.310395
N	-2.739963	-0.333136	0.586623
H	-2.619168	0.351632	-0.217859
H	-2.843762	-1.249420	0.124650
C	3.845644	0.131030	-1.495911
H	3.645594	1.129932	-1.896091
H	4.803976	0.146855	-0.965589
H	3.910849	-0.572539	-2.331415
N	2.750885	-0.263967	-0.595613
H	2.625367	0.371961	0.246412
H	2.846321	-1.207181	-0.187173