

H2SO4

7

S	0.00000	0.00000	0.16525
O	0.00000	1.26281	0.82607
O	0.00000	-1.26281	0.82607
O	1.24736	-0.04726	-0.85164
O	-1.24736	0.04726	-0.85164
H	-1.45614	-0.86095	-1.11745
H	1.45614	0.86095	-1.11745

(H2SO4)2

14

S	-2.10168	0.06720	0.13003
O	-1.45833	0.95689	-0.99340
O	-1.11544	-0.22369	1.14212
O	-2.32502	-1.34478	-0.60091
O	-3.36039	0.64085	0.46002
H	-0.49720	0.73023	-1.10507
H	-3.11441	-1.28605	-1.16074
S	2.10163	-0.06727	-0.13003
O	2.32538	1.34506	0.60016
O	1.11520	0.22320	-1.14207
O	1.45846	-0.95624	0.99405
O	3.36017	-0.64130	-0.45997
H	3.11483	1.28648	1.15995
H	0.49733	-0.72959	1.10570

(H2SO4)3

21

S	0.23889	1.32218	-0.06775
O	-0.08527	-0.03025	-0.53661
O	1.34713	1.96195	-0.71510
H	3.05453	1.12985	-0.80430
O	0.44820	1.26739	1.48671
O	-0.99976	2.23484	-0.17148
O	3.78195	0.47267	-0.77271
S	3.35233	-0.77723	0.10392
O	4.49687	-1.59365	0.26065
O	2.33074	-1.55727	-0.83284
O	-2.51923	-1.11432	-1.06908
H	1.44138	-1.14862	-0.77305
H	-1.61065	-0.76685	-0.88555
O	2.60941	-0.29204	1.25382
O	-3.15323	0.82296	0.31113
H	1.25122	0.70524	1.64899

H	-1.84617	1.74077	0.04326
O	-4.85702	-0.80146	-0.54173
S	-3.55631	-0.51760	-0.04612
O	-3.28590	-1.35781	1.28940
H	-3.76006	-2.20211	1.23252

(H2SO4)4

28

S	2.01942	-0.43944	0.61625
O	3.21017	-1.09163	1.09475
O	0.82630	-0.47432	1.42211
O	2.30459	1.07549	0.34478
H	3.23141	1.20231	0.00507
O	1.73379	-1.06241	-0.79430
H	0.81211	-0.84564	-1.09416
S	6.05084	0.53497	-0.16122
O	7.30206	1.18357	0.02729
O	4.84514	1.27590	-0.44084
O	5.81750	-0.40339	1.07918
O	6.15437	-0.49269	-1.38799
H	7.04630	-0.87265	-1.40263
H	4.87794	-0.71799	1.10779
S	-2.01960	-0.46713	-0.59600
O	-3.21007	-1.14076	-1.04451
O	-0.82630	-0.53879	-1.39919
O	-1.73432	-1.02455	0.84179
O	-2.30497	1.05868	-0.39442
H	-0.81253	-0.79476	1.13143
H	-3.23113	1.20064	-0.05906
S	-6.05056	0.54193	0.13759
O	-5.81744	-0.44819	-1.06207
O	-6.15448	-0.43290	1.40667
O	-4.84476	1.29380	0.38575
O	-7.30162	1.18219	-0.07847
H	-7.04664	-0.81135	1.43735
H	-4.87865	-0.76575	-1.07600

H2SO4-NH3

11

S	-0.61420	-0.11657	0.09700
O	0.40159	-0.45210	-1.04242
O	0.07328	-0.07261	1.35642
O	-0.99057	1.43239	-0.20999
O	-1.79359	-0.89867	-0.10978
H	1.37076	-0.23941	-0.72673
H	-1.69153	1.43524	-0.87732
N	2.77605	0.04129	-0.05239
H	3.23015	0.91045	-0.31557

H	3.45311	-0.70953	-0.14648
H	2.50661	0.10720	0.92687

H2SO4-(NH3)2

15

N	3.13680	-0.84898	0.01388
H	3.07245	-0.04524	-0.60762
H	3.32696	-1.67127	-0.54994
H	3.92265	-0.70633	0.64016
N	-3.13686	-0.84896	-0.01383
H	-3.92265	-0.70685	-0.64031
H	-3.07274	-0.04481	0.60717
H	-3.32694	-1.67094	0.55046
S	0.00001	0.46827	-0.00002
O	-1.01449	1.17784	0.73433
O	1.01455	1.17770	-0.73445
O	0.70028	-0.50852	1.02133
O	-0.70028	-0.50868	-1.02122
H	-1.64070	-0.73399	-0.68265
H	1.64070	-0.73389	0.68279

H2SO4-(NH3)3

19

S	-0.285701000	1.162060000	-0.597054000
O	0.572781000	2.488916000	-1.013071000
O	0.671645000	0.036987000	-0.705990000
O	-1.373925000	1.060526000	-1.568565000
O	-0.691028000	1.449258000	0.769866000
H	0.787980000	2.399287000	-1.951168000
N	-0.553848000	-2.091184000	0.421171000
H	-0.149229000	-3.022437000	0.395768000
H	0.066083000	-1.384193000	-0.058481000
H	-1.476680000	-2.054719000	-0.098960000
H	-0.670226000	-1.742966000	1.415795000
N	-0.735382000	-0.659192000	2.843819000
H	-1.585833000	-0.606897000	3.396736000
H	0.042564000	-0.680193000	3.496758000
H	-0.665046000	0.213120000	2.307902000
N	-2.843842000	-1.513742000	-1.146572000
H	-2.476404000	-0.595425000	-1.423649000
H	-3.740747000	-1.351632000	-0.697480000
H	-3.030820000	-2.034794000	-1.998518000

H2SO4-(NH3)4

23

S	0.58830	-0.33140	0.27326
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O	1.90850	-1.11795	0.69514
O	-0.23274	-0.33906	1.50138
O	-0.04385	-1.06399	-0.82730
O	1.01557	1.02645	-0.12355
H	2.69473	-0.72660	0.20454
N	-2.69424	0.45115	0.80702
H	-3.40474	0.61338	1.51417
H	-1.78341	0.11327	1.23545
H	-2.98874	-0.29871	0.12122
H	-2.44181	1.34309	0.29912
N	-1.46836	2.64937	-0.51399
H	-1.63829	2.81031	-1.50257
H	-1.42256	3.56147	-0.06894
H	-0.53679	2.22155	-0.43341
N	-2.90125	-1.68199	-1.02818
H	-1.87431	-1.67018	-1.05957
H	-3.23800	-1.58356	-1.98118
H	-3.18750	-2.60109	-0.70411
N	3.82669	0.27147	-0.63063
H	3.12512	1.00371	-0.73398
H	4.14767	-0.00365	-1.55252
H	4.61601	0.64578	-0.11534

NH3

4

N	0.00000	0.00000	0.11611
H	0.00000	0.93930	-0.27093
H	0.81346	-0.46965	-0.27093
H	-0.81346	-0.46965	-0.27093

(H2SO4)2-NH3

18

S	1.82137	-0.35028	-0.04742
O	2.45017	0.85230	-0.62365
O	1.07612	0.00751	1.17781
O	3.02858	-1.32222	0.39100
O	1.06466	-1.16748	-0.97967
H	1.42724	2.09442	-0.31716
H	3.65576	-0.80945	0.92035
S	-2.12174	-0.12570	-0.01143
O	-1.50439	-0.49166	1.39086
O	-3.53339	-0.22814	0.08340
O	-1.61394	-1.26387	-0.96947
O	-1.52786	1.13490	-0.45078
H	-0.51089	-0.36289	1.37715
H	-0.61957	-1.24844	-1.04282
N	0.61482	2.72437	-0.04303
H	-0.26049	2.14961	-0.13693

H	0.56318	3.54518	-0.64257
H	0.72725	3.00590	0.92895

(H₂SO₄)₂-(NH₃)₂

22

S	2.16488	-0.00019	-0.13611
O	2.19410	-1.22168	0.68654
O	3.55598	0.00549	-0.96778
O	1.15849	-0.00686	-1.18600
O	2.17378	1.22370	0.67936
H	0.76396	-2.03997	0.89762
H	4.28181	0.02771	-0.32823
S	-2.27092	0.04530	-0.20206
O	-2.06988	1.41016	-0.71658
O	-1.42086	-0.93735	-1.19106
O	-1.57039	-0.09193	1.12030
O	-3.60332	-0.47837	-0.22841
H	-0.90247	2.16925	0.13959
H	-0.53775	-0.53050	-1.34624
N	-0.25491	2.42734	0.94140
H	-0.24662	3.42857	1.11578
H	-0.64398	1.91486	1.73528
H	0.71438	2.05785	0.76909
N	-0.22813	-2.37626	1.02186
H	-0.29390	-3.08555	1.74671
H	-0.82320	-1.51583	1.23661
H	-0.57755	-2.73099	0.13081

(H₂SO₄)₂-(NH₃)₃

26

S	1.637549000	0.688279000	-0.688183000
O	0.254896000	1.046935000	-1.190036000
N	-1.066714000	-1.331867000	-1.532552000
H	-1.811628000	-1.439886000	-2.215406000
H	-0.674735000	-0.360005000	-1.555940000
O	2.502445000	0.213625000	-1.742431000
O	1.393976000	-0.635117000	0.214496000
N	1.344113000	-2.665069000	-2.072766000
H	1.552708000	-3.278099000	-2.855028000
H	-0.247688000	-1.982075000	-1.747316000
N	-0.453349000	2.831484000	0.693469000
H	-0.636849000	3.821942000	0.561417000
H	-1.235882000	2.343588000	1.191221000
S	-1.778472000	-0.106626000	1.937696000
O	-0.332688000	0.038173000	2.171873000
O	-2.111100000	-1.240325000	1.071907000
O	-2.423582000	1.155043000	1.575227000
H	0.835139000	-0.402649000	0.998881000

O	2.123098000	1.739206000	0.193567000
H	1.676774000	-3.120825000	-1.227435000
H	1.912206000	-1.819796000	-2.169235000
H	-1.443251000	-1.469216000	-0.574220000
H	-0.309031000	2.321745000	-0.218086000
H	0.438816000	2.685709000	1.177936000
O	-2.436797000	-0.432633000	3.385127000
H	-2.027396000	-1.244858000	3.714710000

(H2SO4)2-(NH3)4

30

S	-1.85784	0.31946	-0.58183
O	-1.33947	0.57265	0.79871
O	-3.22755	-0.14186	-0.60945
O	-1.02200	-0.96452	-1.10451
O	-1.51469	1.43971	-1.46381
H	-0.06784	-0.72442	-1.23942
N	-0.57115	-1.84506	1.78972
H	0.38849	-1.92500	1.39727
H	-0.55084	-2.02128	2.79022
H	-1.26940	-2.48032	1.30043
H	-0.88878	-0.86431	1.58548
N	-2.60373	-3.11986	0.30119
H	-3.29291	-3.79837	0.61073
H	-2.18793	-3.47166	-0.55693
H	-3.09646	-2.26602	0.02966
N	0.73556	2.71095	-0.45931
H	1.19517	3.39790	-1.05031
H	1.43284	2.02713	-0.09494
H	0.23267	3.16543	0.35466
H	-0.00416	2.20259	-0.99582
S	2.37992	-0.46002	-0.04669
O	1.58425	-0.38507	-1.28265
O	2.02779	-1.60885	0.79345
O	2.47169	0.81504	0.65700
O	3.91432	-0.71107	-0.52638
H	3.92592	-1.53381	-1.03475
N	-0.94374	3.43449	1.67147
H	-1.32541	2.48736	1.60538
H	-0.61075	3.57604	2.62001
H	-1.70688	4.08579	1.51435

(NH3)2

8

N	1.54381	-0.00000	-0.08119
N	-1.54382	-0.00001	0.08119
H	-2.12616	0.81510	-0.08516
H	-0.81675	0.00001	-0.63083

H	-2.12621	-0.81506	-0.08521
H	0.81680	0.00000	0.63089
H	2.12620	-0.81507	0.08515
H	2.12619	0.81508	0.08511

(H₂SO₄)₃-(NH₃)₁

25

N	-0.12815	0.45147	2.58768
H	-1.02102	0.22676	2.09870
H	0.53597	-0.30090	2.34936
H	-0.26920	0.51080	3.59306
S	1.15991	2.06506	-0.16914
O	0.05311	1.17452	-0.55407
O	1.08786	2.51127	1.21286
H	0.26898	1.33980	2.20484
O	2.45073	1.48146	-0.58063
S	-2.92638	-0.31834	-0.11935
O	-2.24906	-1.32155	-1.13732
O	-2.56670	1.10382	-0.68710
O	-4.33302	-0.47256	-0.22204
O	-2.26605	-0.49000	1.16727
H	-1.32207	-1.53143	-0.88287
H	-1.57997	1.24858	-0.65963
S	1.61244	-1.85650	-0.06169
O	2.45221	-3.21033	-0.01836
O	2.48419	-1.00566	-1.00717
O	0.33800	-2.16845	-0.66489
O	1.64445	-1.33354	1.28018
H	2.16329	-3.78099	-0.74633
H	2.45292	0.01523	-0.81193
O	1.01051	3.43170	-1.00579
H	1.28256	3.26308	-1.91968

(H₂SO₄)₃-(NH₃)₂

29

N	0.03694	-2.05892	0.29910
H	-0.84102	-2.22589	-0.23372
H	0.90220	-2.17490	-0.25204
H	0.06101	-2.66286	1.11764
N	-2.42210	1.99063	1.75362
H	-3.27761	2.52372	1.61018
H	-2.06907	2.15428	2.69418
H	-2.62740	0.96205	1.61849
S	-3.18923	-0.85606	-0.14188
O	-2.54650	-2.04767	-0.69408
O	-2.96716	0.36032	-0.93718
O	-2.92052	-0.64059	1.28659
H	-1.35318	0.64965	-1.42971

S	0.30608	1.56860	-0.41267
O	-0.37161	0.71659	-1.57453
O	1.60670	1.93930	-0.93127
O	-0.59623	2.67863	-0.09404
O	0.40765	0.64164	0.76568
H	0.04062	-1.05809	0.59408
H	-1.69494	2.29469	1.04117
O	-4.78207	-1.13521	-0.16612
H	-5.02859	-1.38441	-1.06883
S	3.58345	-0.73453	0.12582
O	3.90821	0.56379	-0.70173
O	2.88461	-0.17905	1.44333
O	4.81568	-1.32197	0.51669
O	2.59982	-1.51642	-0.60307
H	3.07381	1.06299	-0.90985
H	1.99675	0.21387	1.22689

(H2SO4)3-(NH3)3

33

S	2.814485000	-1.230928000	0.040528000
O	1.779295000	-2.263638000	-0.010616000
O	4.230395000	-2.011549000	0.218819000
O	3.013021000	-0.502739000	-1.213671000
H	4.119054000	-2.667548000	0.921393000
S	-2.993306000	-1.056250000	-0.022080000
O	-3.209010000	0.371743000	0.148853000
O	-4.415438000	-1.684376000	0.445704000
O	-2.796708000	-1.507941000	-1.408285000
H	-4.410579000	-2.620725000	0.203486000
S	-0.356528000	2.271409000	-0.028759000
O	0.164668000	0.936847000	-0.416429000
O	-0.586668000	2.330128000	1.419050000
O	-1.743117000	2.470138000	-0.769538000
O	0.502191000	3.340936000	-0.546029000
H	2.032846000	2.662715000	-0.550009000
O	2.678089000	-0.344710000	1.212449000
N	-0.061958000	-0.231931000	2.253209000
N	2.929161000	2.115931000	-0.412685000
N	-0.111521000	-1.317856000	-1.888717000
H	3.749256000	2.683847000	-0.609906000
H	2.961351000	1.761762000	0.548835000
H	2.927779000	1.241481000	-0.982859000
H	-2.361261000	1.754707000	-0.467407000
H	0.490513000	-1.889473000	-1.269610000
H	0.202319000	-1.398192000	-2.851876000
H	-1.123742000	-1.569362000	-1.788999000
H	-0.013044000	-0.336295000	-1.548710000
H	0.888807000	-0.403941000	1.885322000
H	-0.767518000	-0.805252000	1.731144000
H	-0.294042000	0.775643000	2.078869000

H	-0.103705000	-0.447341000	3.245745000
O	-1.973398000	-1.627353000	0.873826000

(H2SO4)3-(NH3)4

37

S	-0.000214000	-1.498379000	-3.321132000
O	0.506945000	-2.585223000	-2.474876000
O	0.421176000	-1.874768000	-4.846205000
O	-1.454056000	-1.428484000	-3.421069000
H	1.381266000	-1.990147000	-4.861410000
S	2.637894000	1.646732000	1.044753000
O	1.514673000	2.592080000	0.832361000
O	3.956864000	2.575237000	1.278163000
O	2.539642000	0.901675000	2.288918000
H	4.203697000	2.950691000	0.421712000
S	-1.831077000	-0.151548000	1.039421000
O	-2.367709000	0.639917000	-0.136106000
O	-2.340800000	-1.542676000	0.955023000
O	-2.211261000	0.504402000	2.317930000
O	-0.331185000	-0.127977000	0.941663000
H	0.752609000	1.054676000	3.105532000
O	0.651468000	-0.216688000	-3.022985000
N	-0.232018000	1.806636000	-1.320023000
N	-0.024097000	1.730080000	3.120106000
N	1.569066000	-1.634103000	-0.073885000
N	-3.369896000	-1.523678000	-1.463504000
H	2.231861000	-0.848935000	-0.204489000
H	0.714822000	-1.202757000	0.389340000
H	1.283961000	-2.039365000	-0.989184000
H	1.981506000	-2.344236000	0.524392000
H	0.240014000	2.386267000	2.372261000
H	-0.071635000	2.205419000	4.017062000
H	-0.952240000	1.237768000	2.863722000
H	-2.668854000	-1.667128000	-2.220645000
H	-3.453380000	-0.507600000	-1.308415000
H	-4.260554000	-1.961015000	-1.678362000
H	-2.979227000	-1.821711000	-0.518704000
H	0.158179000	1.077971000	-1.951919000
H	0.456169000	2.053878000	-0.585006000
H	-1.099950000	1.407165000	-0.856111000
H	-0.467082000	2.632430000	-1.864352000
O	2.915551000	0.852043000	-0.154389000

(NH3)3

12

N	1.78681	0.13950	0.00000
N	-1.01422	1.47768	0.00000
H	-1.23872	2.04058	0.81500

H	0.00000	1.32438	0.00000
H	-1.23872	2.04058	-0.81500
H	1.14694	-0.66219	0.00000
H	2.38655	0.05247	-0.81500
H	2.38655	0.05247	0.81500
N	-0.77260	-1.61717	0.00000
H	-1.14783	-2.09305	-0.81500
H	-1.14694	-0.66219	0.00000
H	-1.14783	-2.09305	0.81500

(H2SO4)4-(NH3)1

32

N	-1.84333	0.39447	2.54204
H	-2.43956	0.64495	3.32758
H	-2.41453	0.21779	1.70042
H	-1.31925	-0.47164	2.74629
S	0.26631	-2.10506	1.24036
O	0.17033	-0.86245	0.48841
O	-0.45469	-2.14226	2.48683
H	-1.17361	1.18012	2.32334
O	-0.20589	-3.27663	0.29681
S	3.07485	-0.15925	-0.92644
O	1.69104	-0.14696	-1.70268
O	2.84044	0.84769	0.25545
O	3.25270	-1.45281	-0.27982
O	4.06348	0.28180	-1.84553
H	0.97594	-0.42572	-1.08892
H	2.23918	1.60720	0.00593
S	-2.58581	-0.76023	-1.17776
O	-3.81671	-0.61154	-2.18342
O	-2.03488	-2.08361	-1.37194
O	-1.56313	0.27261	-1.68398
O	-3.12236	-0.39737	0.10687
H	-3.59486	-1.03959	-3.02480
H	-0.89916	-2.92928	-0.31986
O	1.73273	-2.48452	1.51525
H	2.35856	-2.09009	0.81012
S	-0.21258	2.82797	0.45712
O	-0.47829	4.41178	0.57864
O	-0.15904	2.39762	1.84856
O	1.02156	2.67255	-0.30672
H	-0.32541	4.81299	-0.28935
O	-1.40039	2.29113	-0.25081
H	-1.48317	1.14095	-1.09279

(H2SO4)4-(NH3)2

36

N	-1.97546	2.21625	0.25455
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H	-1.12999	2.55531	-0.24052
H	-2.80519	2.09626	-0.34784
H	-2.19715	2.83941	1.02794
N	1.41601	-1.19962	1.98551
H	2.37606	-1.51551	1.79435
H	1.14021	-1.44262	2.93399
H	1.38617	-0.16423	1.85208
S	1.61209	1.83353	-0.05026
O	0.61993	2.74450	-0.58240
O	1.69834	0.55719	-0.84209
O	1.48079	1.52166	1.37591
H	0.11613	-0.08362	-1.32101
S	-1.32263	-1.33704	-0.31971
O	-0.83123	-0.32674	-1.46015
O	-2.46630	-2.01475	-0.89388
O	-0.18325	-2.18389	0.03141
O	-1.70414	-0.46442	0.84140
H	-1.76642	1.25668	0.61028
H	0.76104	-1.64258	1.28812
O	2.99471	2.58705	-0.27379
H	3.73106	2.03474	0.06578
S	-5.09394	0.06571	0.02702
O	-5.05948	-1.29547	-0.76193
O	-4.34575	-0.26768	1.39190
O	-6.44758	0.34997	0.34672
O	-4.29099	1.03915	-0.69227
H	-4.12064	-1.56957	-0.93640
H	-3.38024	-0.43534	1.22683
S	4.65763	-0.73136	-0.00276
O	3.84240	-0.76621	-1.33194
O	6.00369	-1.41388	-0.48308
O	4.91468	0.64133	0.37383
O	4.10814	-1.62250	0.98070
H	6.49740	-0.79919	-1.04831
H	2.98572	-0.22230	-1.21713

(H2SO4)4-(NH3)3

40

S	-1.56338	-2.29988	0.46388
O	-1.49961	-1.82922	-0.94333
O	-3.08417	-2.71790	0.72511
O	-0.79146	-3.49699	0.70471
H	-3.65355	-1.94869	0.51948
S	3.04750	-1.15181	-0.45097
O	3.32701	-1.46815	0.95434
O	1.43177	-0.90905	-0.50484
O	3.66297	0.07938	-0.93100
H	1.21497	0.06319	-0.55871
S	1.58479	2.56840	0.39362
O	1.06051	3.92801	0.34866

O	0.77729	1.64724	-0.47332
O	1.75591	2.01701	1.73660
O	3.01467	2.66207	-0.28902
H	3.34428	1.74615	-0.48117
O	-1.27365	-1.19211	1.41003
N	-1.08039	3.49847	-1.24464
N	1.31610	-0.56430	2.53237
N	0.82572	-3.46370	-1.64223
H	1.40315	-0.71417	3.53415
H	0.41247	-0.92583	2.18797
H	1.38864	0.45561	2.30823
H	2.10388	-1.03089	2.01293
H	1.81797	-3.08093	-1.55859
H	0.49738	-3.82631	-0.73493
H	0.19057	-2.67965	-1.83575
H	0.75440	-4.17839	-2.36210
H	-1.06430	3.94915	-2.15643
H	-0.61411	2.56878	-1.28461
H	-2.05010	3.37728	-0.92105
H	-0.47251	4.00785	-0.56591
O	3.21495	-2.31067	-1.33924
S	-3.23208	1.01393	-0.27443
O	-2.24810	0.61632	-1.44494
O	-2.28491	1.20061	0.96968
O	-3.70372	2.33074	-0.59907
O	-4.14276	-0.07514	-0.02885
H	-1.89028	0.31314	1.22222
H	-1.93601	-0.33706	-1.32206

(H2SO4)4-(NH3)4

44

S	3.79876	-1.35569	-0.57027
O	4.28274	-0.33948	0.36691
O	4.76061	-1.26108	-1.87597
O	3.92670	-2.72583	-0.05767
O	2.47349	-1.08276	-1.12290
H	5.67813	-1.30628	-1.57086
S	0.30438	3.82241	-0.03562
O	-1.16090	3.87286	-0.10222
O	0.83072	5.05031	-0.95722
O	0.85772	3.98208	1.29617
O	0.87818	2.65910	-0.75179
H	0.45865	5.86762	-0.59613
S	-0.72949	-1.29390	1.50522
O	-0.65853	-1.79713	0.05104
O	0.16473	-2.11863	2.32827
O	-2.13925	-1.33054	1.95045
O	-0.26665	0.13945	1.48059
N	-2.45324	1.76622	1.08626
H	-1.65419	1.17903	1.42832

H	-2.06527	2.66647	0.72414
H	-3.13293	1.91622	1.82739
H	-2.87990	1.24582	0.29904
N	0.11865	0.19760	-1.75216
H	1.06761	-0.16471	-1.92865
H	0.20592	1.17504	-1.40587
H	-0.28576	-0.42524	-1.01810
H	-0.46923	0.16987	-2.58171
N	2.23882	1.29416	1.30941
H	1.96251	1.85781	0.48489
H	1.39847	0.72397	1.55063
H	3.05148	0.68980	1.06847
H	2.44956	1.94128	2.06585
N	1.43067	-3.66101	0.51946
H	2.42535	-3.39221	0.31318
H	0.81075	-3.22288	-0.17308
H	1.30937	-4.67010	0.53104
H	1.09860	-3.22382	1.41437
S	-3.79702	-1.11423	-1.01964
O	-4.26885	-1.25252	0.47617
O	-4.92791	-1.27750	-1.86442
O	-2.82596	-2.33122	-1.22574
O	-2.99724	0.10776	-1.12203
H	-3.46252	-1.32646	1.08423
H	-1.97391	-2.17653	-0.69015

(NH3)4

16

N	-1.54344	1.54344	0.00041
N	1.54344	1.54344	-0.00041
H	1.90033	2.03690	0.81305
H	0.51953	1.65368	-0.00015
H	1.89983	2.03628	-0.81447
H	-1.65368	0.51953	0.00015
H	-2.03628	1.89983	0.81447
H	-2.03690	1.90033	-0.81305
N	-1.54344	-1.54344	-0.00041
H	-1.90033	-2.03690	0.81305
H	-0.51953	-1.65368	-0.00015
H	-1.89983	-2.03628	-0.81447
N	1.54344	-1.54344	0.00041
H	2.03690	-1.90033	-0.81305
H	2.03628	-1.89983	0.81447
H	1.65368	-0.51953	0.00015

(H2SO4)1-(DMA)1

17

H	1.20266	-0.11641	0.80551
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S	-1.28566	-0.15981	0.01278
O	-1.79996	1.40526	0.03811
O	-0.43906	-0.25916	-1.20271
O	-2.46902	-0.97911	-0.01043
O	-0.45644	-0.21585	1.23005
H	-2.60080	1.43854	-0.50189
N	1.88260	-0.02687	0.00787
H	1.15942	-0.13011	-0.76016
C	2.85648	-1.14047	-0.00738
H	3.50399	-1.07711	0.86762
H	3.45913	-1.08826	-0.91447
H	2.30579	-2.07980	0.01158
C	2.45983	1.33730	-0.01614
H	3.09396	1.48470	0.85839
H	1.63904	2.05286	-0.00015
H	3.04708	1.47061	-0.92491

(H₂SO₄)₁-(DMA)₂

27

S	-0.05346	-0.75313	-0.01507
O	0.73208	0.01994	1.14788
O	0.88284	-1.65436	-0.65637
O	-0.56009	0.31231	-0.93345
O	-1.18120	-1.38997	0.69573
H	1.66961	0.20981	0.80386
H	-2.58358	-0.45900	0.47578
C	-4.13767	0.05424	-0.85565
H	-4.97075	-0.29846	-0.24636
H	-3.82859	-0.73235	-1.54257
H	-4.44564	0.93346	-1.42262
N	-2.98942	0.39533	0.00965
C	-3.22689	1.45819	1.01174
H	-2.11461	0.61466	-0.56050
H	-4.03076	1.15945	1.68546
H	-2.30729	1.60118	1.57749
H	-3.49586	2.38639	0.50651
N	3.12663	0.29244	-0.05477
C	4.38939	0.17694	0.67421
C	3.09468	1.40216	-1.01168
H	2.92036	-0.57731	-0.54277
H	4.53487	1.06377	1.29730
H	4.35211	-0.69535	1.32939
H	5.26204	0.08103	0.01083
H	3.18358	2.34913	-0.47179
H	3.90691	1.35298	-1.75183
H	2.13646	1.39369	-1.53317

(H₂SO₄)₁-(DMA)₃

37

S	-0.61456	-0.50034	-0.65818
O	-1.99994	-1.01403	-1.23573
O	0.32375	-0.52546	-1.77486
O	-0.21752	-1.46783	0.40997
O	-0.84991	0.83925	-0.09118
H	-2.75580	-0.72502	-0.61465
H	2.40372	-0.07323	0.34505
C	3.03388	-1.80677	-0.67195
H	4.07039	-1.48154	-0.77715
H	2.45126	-1.54383	-1.55284
H	3.00198	-2.88681	-0.52234
N	2.40855	-1.13273	0.49184
C	3.02108	-1.45673	1.79725
H	1.36403	-1.37290	0.50645
H	4.06822	-1.14959	1.80745
H	2.47829	-0.93002	2.58171
H	2.95605	-2.53038	1.97736
N	-3.96719	-0.12202	0.35942
C	-4.19397	1.25523	-0.10096
C	-3.52623	-0.19225	1.75970
H	-4.81884	-0.66328	0.24529
H	-3.23683	1.77842	-0.09744
H	-4.56831	1.23616	-1.12635
H	-4.90950	1.80214	0.52995
H	-2.56088	0.30859	1.84058
H	-4.23765	0.28108	2.45203
H	-3.39041	-1.23687	2.04525
N	2.05784	1.66254	0.11567
C	2.39015	2.09651	-1.24861
C	2.52886	2.59882	1.13887
H	1.03804	1.58030	0.17156
H	3.47347	2.05423	-1.40187
H	1.89756	1.42782	-1.95451
H	2.06017	3.12587	-1.45000
H	3.62318	2.61980	1.15300
H	2.17700	3.62709	0.96874
H	2.17999	2.27868	2.12358

(H2SO4)1-(DMA)4

47

S	-0.00000	-0.94033	-0.00001
O	1.04696	-1.82415	-0.62905
O	0.64477	-0.09180	1.04189
O	-1.04696	-1.82416	0.62903
O	-0.64478	-0.09180	-1.04190
N	-3.38268	-1.03429	-0.05984
H	-3.28440	0.01259	0.03621
H	-2.39028	-1.40919	0.25933
C	-4.43766	-1.54423	0.83544

H	-5.41262	-1.14396	0.54825
H	-4.20826	-1.24415	1.85786
H	-4.46509	-2.63364	0.78495
C	-3.55411	-1.38473	-1.48728
H	-4.48621	-0.96688	-1.87487
H	-2.69469	-0.98402	-2.02272
H	-3.56853	-2.47059	-1.59093
C	4.43767	-1.54423	-0.83542
H	4.46509	-2.63364	-0.78493
H	4.20828	-1.24415	-1.85784
H	5.41263	-1.14396	-0.54822
C	3.55409	-1.38473	1.48729
H	3.56851	-2.47060	1.59094
H	4.48619	-0.96688	1.87490
H	2.69466	-0.98403	2.02272
N	-2.60721	1.71002	0.15458
H	-1.79126	1.35645	-0.35650
C	-2.18101	2.07288	1.50955
H	-1.57311	2.99091	1.52732
H	-1.57645	1.26440	1.92310
H	-3.05445	2.23850	2.14953
C	-3.22479	2.81868	-0.56846
H	-4.16913	3.10066	-0.09122
H	-3.44119	2.51616	-1.59590
H	-2.58851	3.71733	-0.60325
N	2.60721	1.71002	-0.15457
H	1.79126	1.35645	0.35650
C	2.18103	2.07287	-1.50955
H	3.05448	2.23848	-2.14953
H	1.57313	2.99090	-1.52734
H	1.57647	1.26439	-1.92310
C	3.22478	2.81868	0.56847
H	4.16914	3.10065	0.09123
H	3.44117	2.51617	1.59591
H	2.58851	3.71733	0.60323
N	3.38267	-1.03429	0.05985
H	3.28440	0.01259	-0.03619
H	2.39028	-1.40919	-0.25933

DMA

10

N	0.00000	0.56391	-0.14859
C	1.21545	-0.22252	0.02031
C	-1.21545	-0.22252	0.02031
H	0.00000	1.32911	0.51715
H	1.28278	-0.96583	-0.78047
H	2.08969	0.42794	-0.06116
H	1.27538	-0.76522	0.98130
H	-1.28278	-0.96583	-0.78046
H	-1.27538	-0.76522	0.98130

H	-2.08969	0.42794	-0.06117
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(H2SO4)2-(DMA)1

24

S	1.45139	-1.26063	-0.09244
O	2.27682	-0.26899	-0.77460
O	0.85594	-0.72110	1.15011
O	2.52756	-2.37895	0.35079
O	0.46354	-1.95225	-0.92292
H	1.70707	1.29076	-0.35818
H	2.04243	-3.17598	0.60814
S	-2.27733	0.02184	0.00577
O	-1.75798	-0.54126	1.38333
O	-3.66585	0.29057	0.12903
O	-2.10622	-1.18325	-0.99238
O	-1.37624	1.09090	-0.41108
H	-0.76152	-0.65560	1.35400
H	-1.15060	-1.46520	-1.04751
N	1.14345	2.12353	-0.06600
H	0.16818	1.76274	-0.04535
C	1.23521	3.18616	-1.10060
H	2.26749	3.52547	-1.18068
H	0.58868	4.01804	-0.82317
H	0.90698	2.76976	-2.05139
C	1.55504	2.53434	1.30300
H	2.58939	2.87620	1.27881
H	1.46580	1.66453	1.95071
H	0.90496	3.33676	1.65072

(H2SO4)2-(DMA)2

34

H	0.58654	1.56536	0.54566
S	-2.55649	-0.01115	-0.37052
O	-4.03888	0.07490	0.32066
O	-2.28611	1.33009	-0.91214
O	-2.61493	-1.06896	-1.36015
O	-1.70511	-0.30561	0.79728
H	-4.68176	0.12168	-0.40054
N	-0.08982	2.34883	0.38897
H	-0.87207	1.95946	-0.18775
C	0.59352	3.43694	-0.35804
H	1.37495	3.86519	0.26933
H	-0.13527	4.20219	-0.62474
H	1.04897	3.00515	-1.24660
C	-0.66018	2.75018	1.70052
H	0.14267	3.09123	2.35393
H	-1.15373	1.87923	2.12708
H	-1.38594	3.54892	1.54923

H	-0.58652	-1.56535	0.54567
S	2.55648	0.01114	-0.37053
O	4.03884	-0.07496	0.32070
O	1.70506	0.30557	0.79725
O	2.28610	-1.33008	-0.91222
O	2.61497	1.06898	-1.36013
H	4.68175	-0.12180	-0.40049
N	0.08984	-2.34881	0.38896
H	0.87205	-1.95944	-0.18780
C	-0.59354	-3.43693	-0.35799
H	-1.37494	-3.86517	0.26943
H	0.13524	-4.20219	-0.62470
H	-1.04902	-3.00516	-1.24654
C	0.66026	-2.75012	1.70050
H	-0.14256	-3.09116	2.35395
H	1.15382	-1.87916	2.12702
H	1.38601	-3.54887	1.54920

(H2SO4)2-(DMA)3

44

S	1.35153	-0.29524	-1.08858
O	2.73756	-0.04037	-1.56028
C	-1.84545	-3.37696	0.16606
H	-2.92677	-3.51688	0.16674
H	-1.35040	-4.29962	-0.13909
H	-1.51818	-3.08386	1.16213
N	3.73412	0.00077	0.87957
H	3.69533	-0.01980	-0.17980
H	2.74229	0.32351	1.02081
C	4.72721	0.96348	1.39940
C	3.85719	-1.39207	1.38192
H	4.83598	-1.78928	1.11236
H	3.07138	-1.98190	0.91065
H	3.73679	-1.40122	2.46553
H	5.73194	0.63270	1.13482
H	4.53718	1.93894	0.95339
H	4.64025	1.03444	2.48406
O	1.14524	-1.75481	-0.85087
O	0.32580	0.23183	-2.02389
N	-1.48660	-2.28524	-0.76878
C	-1.88310	-2.50141	-2.17938
H	-1.92726	-1.39288	-0.41536
H	-0.44183	-2.11818	-0.74595
H	-1.43083	-3.42235	-2.54890
H	-1.51348	-1.65814	-2.76072
H	-2.96943	-2.56619	-2.25087
C	0.03590	3.46147	-0.95727
H	0.89982	3.11169	-0.39558
H	-0.38085	4.35334	-0.48840
H	0.32999	3.68044	-1.98406

N	-0.97150	2.37700	-0.94821
C	-2.22348	2.67333	-1.68354
H	-1.22377	2.14509	0.05123
H	-0.52250	1.51392	-1.34753
H	-2.89396	1.82776	-1.54279
H	-2.68088	3.57303	-1.27097
H	-2.00320	2.81874	-2.74175
S	-2.15816	0.34471	1.55571
O	-3.05354	-0.05572	2.60498
O	-0.81247	-0.53429	1.79463
O	-1.72237	1.75686	1.56725
O	-2.60071	-0.02706	0.17852
O	1.18038	0.42858	0.25538
H	-0.07229	-0.14967	1.24912

(H2SO4)2-(DMA)4

54

S	-1.459802000	0.387864000	0.861331000
O	-2.874254000	0.715762000	1.487191000
O	-0.943310000	-0.818060000	1.532826000
O	-0.628815000	1.569592000	1.127096000
O	-1.690887000	0.148363000	-0.587436000
H	0.752369000	-0.632588000	2.134773000
N	0.005189000	-2.029255000	-1.400906000
H	0.965743000	-1.840023000	-0.905133000
H	-0.573849000	-1.192418000	-1.215265000
O	2.926790000	0.632069000	0.402772000
O	2.029812000	0.215938000	-1.821935000
S	2.947730000	-0.352320000	-0.750711000
O	2.278243000	-1.623117000	-0.248309000
O	4.284091000	-0.597550000	-1.245910000
H	2.202890000	0.054220000	1.617582000
N	1.693746000	-0.366486000	2.477652000
H	0.464666000	2.182867000	-0.156905000
N	0.947721000	2.436157000	-1.037036000
H	1.409670000	1.507455000	-1.376320000
C	2.021346000	3.423503000	-0.776755000
C	-0.073241000	2.867551000	-2.017363000
C	-0.641183000	-3.202120000	-0.770631000
C	1.537272000	0.674496000	3.519609000
H	0.033424000	-4.056638000	-0.830848000
H	-0.845143000	-2.955370000	0.269675000
H	-1.575279000	-3.437044000	-1.284940000
H	-0.839268000	2.095241000	-2.067187000
H	-0.524345000	3.808402000	-1.697339000
H	0.395991000	2.997029000	-2.993199000
H	2.732366000	2.959482000	-0.096111000
H	2.522529000	3.656960000	-1.716619000
H	1.598240000	4.333507000	-0.347340000
H	0.924268000	1.474032000	3.107834000

H	2.520814000	1.054774000	3.797102000
H	1.044199000	0.251335000	4.396197000
C	0.261512000	-2.169546000	-2.853703000
H	0.797317000	-1.280202000	-3.178834000
H	-0.680346000	-2.287492000	-3.393435000
H	0.891583000	-3.044273000	-3.016836000
C	2.441277000	-1.571344000	2.910131000
H	1.908450000	-2.070359000	3.721527000
H	3.432401000	-1.269197000	3.249623000
H	2.542231000	-2.221612000	2.043599000
N	-4.703758000	-0.059450000	-0.253834000
H	-4.002814000	-0.198102000	-0.978187000
H	-3.627557000	0.391018000	0.863262000
C	-5.387882000	-1.323359000	0.033739000
C	-5.610655000	1.025585000	-0.640754000
H	-6.233394000	0.771285000	-1.509796000
H	-6.271796000	1.261382000	0.196661000
H	-5.026796000	1.917392000	-0.873795000
H	-6.041264000	-1.192496000	0.899659000
H	-5.999383000	-1.678986000	-0.807436000
H	-4.649087000	-2.087619000	0.280972000

(DMA)2

20

N	1.56055	-0.00021	-0.09102
H	0.83910	-0.00048	0.62417
H	-0.83916	-0.00050	-0.62430
N	-1.56054	-0.00022	0.09096
C	-2.35844	1.21547	-0.00745
C	-2.35938	-1.21529	-0.00739
C	2.35846	1.21546	0.00747
C	2.35936	-1.21530	0.00742
H	1.70383	-2.08933	-0.00001
H	2.98973	-1.26478	0.91297
H	3.02309	-1.29140	-0.85996
H	3.02212	1.29211	-0.85991
H	2.98880	1.26536	0.91302
H	1.70227	2.08899	0.00011
H	-3.02305	-1.29136	0.86003
H	-2.98980	-1.26478	-0.91291
H	-1.70386	-2.08933	0.00001
H	-2.98889	1.26536	-0.91292
H	-3.02200	1.29214	0.86001
H	-1.70224	2.08899	-0.00018

(H2SO4)3-(DMA)1

31

S	-0.89127	1.75857	-1.02002
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O	-1.55904	1.63499	0.29377
O	0.56027	1.90303	-0.87236
O	-1.45764	3.16998	-1.54745
O	-1.29413	0.74741	-1.99074
H	-0.26951	1.32196	1.54058
H	-1.19804	3.27631	-2.47492
S	-2.01073	-1.76168	0.23155
O	-2.94901	-0.60519	0.75339
O	-0.63992	-1.37502	0.57071
O	-2.15824	-1.71274	-1.33339
O	-2.53566	-2.99793	0.68502
H	-2.53170	0.28037	0.56959
H	-1.82127	-0.84379	-1.68020
N	0.55527	1.16109	2.14643
H	1.21289	0.59165	1.57559
C	0.15774	0.37651	3.34769
H	-0.56188	0.94946	3.93170
H	1.04432	0.16917	3.94535
H	-0.28753	-0.55608	3.00819
C	1.20143	2.47125	2.43385
H	0.51308	3.09556	3.00245
H	1.43769	2.94362	1.48265
H	2.11340	2.30011	3.00392
S	2.73875	-0.90759	-0.48354
O	4.01573	-1.46592	-0.74756
O	2.42698	0.12751	-1.62978
O	2.47035	-0.26479	0.79653
H	1.71237	0.76636	-1.36912
O	1.66862	-2.04887	-0.68731
H	0.81988	-1.83737	-0.22442

(H2SO4)3-(DMA)2

41

S	1.32581	-2.05234	-0.51314
O	2.69667	-2.10538	-0.93603
O	0.87840	-3.56537	-0.26802
O	1.12518	-1.34479	0.78770
O	0.38247	-1.49061	-1.51869
H	-1.81343	1.33280	0.43687
N	3.19616	0.64048	0.91958
H	2.47174	-0.10430	0.94521
H	2.87868	1.29337	0.16508
O	0.41240	1.62027	0.62960
O	2.08840	2.36299	-0.96841
S	0.65587	2.26455	-0.67242
O	-0.13459	3.47963	-0.85582
O	-0.00765	1.28296	-1.78676
H	0.34796	0.37021	-1.71771
H	-0.01468	-3.56284	0.13705
H	-1.70483	2.84459	-0.17123

N	-2.39342	2.15370	0.20111
C	-3.00664	2.65719	1.45824
C	-3.36349	1.79072	-0.87145
C	4.51785	0.05570	0.56378
C	3.16921	1.37924	2.21054
H	2.16165	1.76496	2.34608
H	3.88344	2.20086	2.16517
H	3.43383	0.69926	3.01997
H	4.83175	-0.62545	1.35422
H	5.24338	0.86128	0.45412
H	4.40822	-0.49801	-0.36535
H	-4.00872	0.99153	-0.51084
H	-3.94915	2.67239	-1.12970
H	-2.79448	1.44877	-1.73284
H	-3.58424	3.55538	1.24314
H	-3.65213	1.88322	1.87106
H	-2.20586	2.88649	2.15894
S	-2.31776	-1.69739	0.45607
O	-3.66061	-1.40270	0.83341
O	-2.20954	-1.42229	-1.09424
O	-1.70652	-2.96987	0.75799
H	-1.25185	-1.53466	-1.37799
O	-1.41366	-0.54486	1.08614
H	-0.43228	-0.77316	1.03404

(H2SO4)3-(DMA)3

51

S	-0.74477	-2.01125	-0.51203
O	0.39370	-2.92446	-0.47233
O	-1.92527	-2.58020	-1.17255
O	-1.09006	-1.40491	0.78495
O	-0.23918	-0.79630	-1.45370
H	0.48999	2.50711	-0.27133
N	2.79352	-2.61906	0.81862
H	1.86774	-2.63975	0.33452
H	3.34429	-1.84299	0.36550
O	1.98014	0.34472	0.46497
O	4.08247	-0.54614	-0.39562
S	3.03609	0.47767	-0.54768
O	3.54840	1.84096	-0.69141
O	2.31493	0.18926	-1.96979
H	1.49378	-0.32199	-1.80788
H	-3.31613	-1.79155	-0.63059
H	2.11976	2.83920	-0.40542
N	1.20973	3.23337	-0.07720
C	1.29556	3.43188	1.39759
C	0.84305	4.45371	-0.84071
C	3.47768	-3.91435	0.58658
C	2.56709	-2.27541	2.24669
H	2.08557	-1.30067	2.27317

H	3.52650	-2.23429	2.76241
H	1.92649	-3.03045	2.70217
H	2.87647	-4.72314	1.00134
H	4.45910	-3.89678	1.06016
H	3.59159	-4.05876	-0.48670
H	-0.14568	4.77733	-0.51950
H	1.58245	5.23261	-0.65534
H	0.82449	4.20717	-1.90131
H	2.06208	4.17764	1.60831
H	0.32285	3.75423	1.76344
H	1.56768	2.47550	1.83712
S	-2.00942	1.89524	0.43506
O	-2.00154	3.28760	0.80888
O	-1.01804	1.58024	-0.64128
O	-3.32692	1.32464	0.11977
H	-0.61943	0.07687	-1.13893
O	-1.45791	1.11630	1.73311
H	-1.20598	0.20333	1.45480
N	-4.10711	-1.23537	-0.22104
C	-4.42591	-1.78316	1.12260
C	-5.24741	-1.20217	-1.16904
H	-3.74075	-0.25725	-0.09892
H	-4.79530	-2.80358	1.02012
H	-3.50873	-1.77866	1.70786
H	-5.17884	-1.15569	1.59883
H	-5.62141	-2.21375	-1.32720
H	-6.03719	-0.57078	-0.76280
H	-4.90099	-0.78699	-2.11422

(H2SO4)3-(DMA)4

61

S	-0.83631	2.06238	0.42711
O	-2.28313	2.04710	0.79641
O	-0.31011	3.42846	0.24038
O	-0.05897	1.35927	1.51681
O	-0.66673	1.28323	-0.85461
H	-0.53475	-0.21911	-0.62653
N	-3.63721	0.88947	-1.25143
H	-3.12761	1.31809	-0.42969
H	-1.87771	-1.11127	1.88719
C	-3.52419	1.82725	-2.39534
H	-4.01710	2.76639	-2.14343
H	-3.98738	1.38517	-3.27786
H	-2.46427	2.00186	-2.56806
C	-5.02297	0.54248	-0.85799
H	-4.97502	-0.19510	-0.05831
H	-5.54777	0.11252	-1.71125
H	-5.54154	1.43772	-0.51405
S	-1.73955	-2.08688	-0.64816
O	-0.42899	-1.21064	-0.39486

O	-2.54876	-1.98107	0.58449
O	-1.18347	-3.41843	-0.88780
O	-2.43952	-1.50102	-1.80405
H	-3.13023	0.00021	-1.48487
N	1.64216	-3.06844	-1.08797
H	1.84394	-2.04116	-0.94983
H	0.61067	-3.18882	-1.05525
C	2.25807	-3.81690	0.04025
H	2.12216	-4.88700	-0.11733
H	3.31232	-3.55445	0.10766
H	1.76351	-3.51014	0.95929
C	2.15159	-3.45723	-2.42503
H	3.22269	-3.26326	-2.46695
H	1.95133	-4.51409	-2.60166
H	1.64293	-2.85642	-3.17742
S	3.20644	-0.22111	0.45021
O	4.19067	-1.19842	0.85123
O	2.54999	-0.51694	-0.84694
O	3.63986	1.18814	0.50235
O	2.03935	-0.36328	1.56915
H	1.35479	0.33701	1.42762
N	2.24426	3.14664	-0.70189
H	1.27852	3.28062	-0.30339
H	2.70309	2.34860	-0.18591
C	3.04788	4.36931	-0.46860
H	2.59270	5.21249	-0.98873
H	3.07256	4.56969	0.60159
H	4.06345	4.20970	-0.83052
C	2.11702	2.74750	-2.12754
H	1.65070	3.55793	-2.68859
H	3.10721	2.52849	-2.52625
H	1.49367	1.85728	-2.16670
N	-1.50385	-0.56136	2.69589
H	-0.95116	0.23471	2.26592
C	-0.58214	-1.42245	3.47867
H	-1.10966	-2.31771	3.80842
H	-0.21457	-0.86560	4.34057
H	0.26036	-1.68776	2.84225
C	-2.63851	0.00405	3.46581
H	-3.29599	-0.80021	3.79731
H	-3.16968	0.69693	2.81608
H	-2.25102	0.54706	4.32797

(DMA)3

30

O			
N	-1.36556	-1.21324	-0.00346
H	-0.34523	-1.28702	0.00719
H	-0.93603	0.93727	-0.02038
N	-0.36701	1.78745	-0.01101

C	-0.61643	2.56416	-1.21951
C	-0.63007	2.54440	1.20714
C	-1.89447	-1.83872	-1.20981
C	-1.91685	-1.79080	1.21680
H	-1.43457	-1.34139	2.08828
H	-1.79322	-2.88599	1.28371
H	-2.98895	-1.57616	1.28117
H	-2.96475	-1.62531	-1.30370
H	-1.77193	-2.93593	-1.22952
H	-1.39430	-1.42569	-2.08941
H	0.08331	3.37057	1.29585
H	-1.64503	2.97694	1.24943
H	-0.50058	1.89796	2.07854
H	-1.63105	2.99708	-1.26631
H	0.09745	3.39192	-1.28623
H	-0.47650	1.93234	-2.09995
N	1.73533	-0.57825	0.00657
H	1.28229	0.33899	-0.00126
C	2.52408	-0.75018	-1.20790
C	2.53198	-0.72559	1.21911
H	1.89966	-0.55849	-2.08398
H	3.40414	-0.08551	-1.26263
H	2.88627	-1.78144	-1.27586
H	2.89427	-1.75544	1.30576
H	3.41264	-0.06025	1.25437
H	1.91339	-0.51568	2.09527

(H2SO4)4-(DMA)1

38

S	3.927880000	3.741355000	-0.922424000
O	3.419066000	5.185340000	-1.314448000
O	4.212757000	3.856388000	0.637499000
O	5.168811000	3.532932000	-1.573852000
O	2.830615000	2.805365000	-1.098956000
H	2.567911000	5.392794000	-0.861339000
H	3.352015000	3.899701000	1.116887000
S	-2.157272000	6.723738000	-0.537587000
O	-2.344255000	6.865009000	1.030490000
O	-0.801006000	7.493587000	-0.823126000
O	-3.200828000	7.448262000	-1.160736000
O	-1.945962000	5.316315000	-0.838917000
H	-1.718515000	6.266522000	1.497618000
H	-0.037796000	6.951050000	-0.521284000
S	-0.158401000	2.079685000	3.991940000
O	-1.089545000	3.351618000	4.104776000
O	1.308454000	2.677083000	4.129941000
O	-0.285209000	1.536488000	2.650242000
O	-0.402754000	1.267882000	5.127269000
H	-0.935867000	3.967642000	3.349976000
H	1.534799000	3.162375000	3.301727000

S	0.603412000	4.636127000	1.052841000
O	-0.135558000	3.603185000	0.088941000
O	-0.391514000	5.098993000	2.029738000
O	1.126268000	5.716000000	0.204987000
O	1.670396000	3.823768000	1.665767000
H	-0.872461000	4.104487000	-0.354835000
N	1.262177000	0.984537000	0.365942000
C	0.347486000	0.335731000	-0.614447000
C	2.304869000	0.080675000	0.927975000
H	0.700337000	1.362602000	1.148112000
H	1.733609000	1.782441000	-0.093845000
H	2.927999000	-0.293034000	0.117193000
H	1.819917000	-0.743223000	1.448864000
H	2.914513000	0.649628000	1.627642000
H	0.932297000	-0.034457000	-1.455132000
H	-0.366970000	1.080343000	-0.957292000
H	-0.175121000	-0.484252000	-0.124236000

(H2SO4)4-(DMA)2

48			
S	1.576219000	-1.790938000	0.127088000
O	2.049519000	-0.797192000	-0.832378000
O	0.700096000	-1.154987000	1.141990000
O	2.895851000	-2.264608000	0.889566000
H	0.919839000	0.486168000	-0.761807000
H	2.692748000	-3.065784000	1.420343000
S	-2.629784000	-1.028567000	0.653118000
O	-1.717665000	-1.617124000	1.770496000
O	-3.982171000	-1.332619000	1.042680000
O	-2.229672000	-1.817991000	-0.642119000
H	-0.727370000	-1.507135000	1.543642000
N	0.221839000	1.252913000	-0.601723000
C	-0.042713000	1.970768000	-1.875593000
H	0.880945000	2.427420000	-2.229346000
H	-0.799829000	2.736130000	-1.708696000
H	-0.402854000	1.252241000	-2.610207000
C	0.725612000	2.107175000	0.508953000
H	1.660979000	2.574291000	0.203104000
H	0.895219000	1.461898000	1.368203000
H	-0.018501000	2.866841000	0.745467000
H	-2.427829000	-2.797955000	-0.505526000
H	-0.653896000	0.798551000	-0.281620000
O	0.968477000	-2.976224000	-0.481149000
O	-2.275249000	0.347275000	0.370226000
S	-3.447304000	-4.898093000	1.060262000
O	-3.904968000	-6.268583000	0.849501000
O	-2.601000000	-4.815770000	2.276422000
O	-4.781277000	-4.078891000	1.371042000
H	-2.787369000	-7.260962000	1.682763000
H	-4.584836000	-3.116978000	1.339538000
S	0.738651000	-5.177661000	2.033891000

O	-0.195639000	-4.054951000	2.575666000
O	2.083538000	-4.692925000	2.205546000
O	0.376183000	-5.295139000	0.512138000
H	-1.180977000	-4.284333000	2.431666000
N	-2.099450000	-7.784894000	2.276894000
C	-1.809736000	-9.108954000	1.667813000
H	-2.728090000	-9.693399000	1.624618000
H	-1.062874000	-9.627327000	2.268100000
H	-1.426321000	-8.951075000	0.660982000
C	-2.636614000	-7.834771000	3.664741000
H	-3.567915000	-8.399863000	3.666258000
H	-2.821940000	-6.810776000	3.981836000
H	-1.904392000	-8.308010000	4.317911000
H	0.578610000	-4.417984000	0.056207000
H	-1.228206000	-7.222311000	2.292944000
O	-2.815791000	-4.285453000	-0.110236000
O	0.380357000	-6.462909000	2.598185000

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S	-1.099369000	-1.910367000	0.694052000
O	0.170584000	-2.638321000	0.673455000
O	-2.278150000	-2.772499000	0.775373000
O	-1.075047000	-0.846426000	1.728904000
O	-1.235401000	-1.166012000	-0.713366000
H	-0.421397000	2.658543000	-0.786859000
N	1.495507000	-0.623350000	2.905032000
H	0.635180000	-0.770642000	2.345259000
H	2.015556000	0.170892000	2.457043000
O	1.612843000	0.845270000	-0.129192000
O	2.979273000	1.361891000	1.820358000
S	2.769426000	1.619957000	0.391271000
O	2.686379000	3.033166000	0.039391000
O	4.058509000	1.091561000	-0.390752000
H	4.049884000	0.105533000	-0.375773000
H	-3.583268000	-2.178141000	-0.156304000
H	1.129063000	3.293706000	-0.672582000
N	0.203773000	3.418568000	-1.137779000
C	-0.366309000	4.741513000	-0.765561000
C	0.381315000	3.212876000	-2.599383000
C	2.363001000	-1.833230000	2.847637000
C	1.088272000	-0.221309000	4.275790000
H	0.456626000	0.663003000	4.206868000
H	1.977930000	0.007765000	4.861267000
H	0.531204000	-1.033856000	4.741013000
H	1.810429000	-2.691689000	3.225857000
H	3.251132000	-1.652974000	3.452866000
H	2.648399000	-2.004928000	1.812257000
H	-0.586455000	3.294976000	-3.092482000
H	1.068821000	3.963090000	-2.988574000

H	0.793914000	2.218246000	-2.758021000
H	0.269813000	5.529821000	-1.167616000
H	-1.379650000	4.817051000	-1.153835000
H	-0.401665000	4.809312000	0.319890000
S	-2.839523000	1.813725000	0.196750000
O	-3.085006000	3.228876000	0.129670000
O	-1.596572000	1.402903000	-0.543574000
O	-3.964744000	0.946280000	-0.179372000
H	-1.260718000	-0.162244000	-0.616994000
O	-2.507909000	1.505663000	1.737823000
H	-2.058582000	0.629096000	1.791444000
N	-4.309145000	-1.676939000	-0.718192000
C	-5.655070000	-1.949781000	-0.153139000
C	-4.146739000	-2.034470000	-2.151547000
H	-4.098076000	-0.657757000	-0.583250000
H	-5.873111000	-3.015000000	-0.226719000
H	-5.659650000	-1.641957000	0.891064000
H	-6.400066000	-1.375809000	-0.703154000
H	-4.350399000	-3.096755000	-2.284675000
H	-4.838948000	-1.443559000	-2.750841000
H	-3.119622000	-1.817376000	-2.437634000
S	2.777915000	-2.025634000	-1.702967000
O	3.491488000	-1.619965000	-0.495243000
O	1.788976000	-3.190453000	-1.342210000
O	3.506149000	-2.445763000	-2.850404000
H	1.170685000	-2.950058000	-0.596440000
O	1.829440000	-0.830963000	-2.104991000
H	1.723546000	-0.194426000	-1.331969000

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S	-2.44882	-2.02497	0.93130
O	-0.96823	-1.90648	0.81478
O	-2.88234	-0.74119	1.83113
O	-3.08705	-1.79653	-0.38612
O	-2.91889	-3.17021	1.65681
H	-4.20083	-0.57904	-0.50552
N	0.57952	-0.16170	2.40452
H	-0.08714	-0.66805	1.78656
H	1.13216	0.47251	1.79998
O	-3.57513	2.49257	-0.00616
O	-1.97775	1.60274	-1.62841
S	-2.17585	2.16669	-0.28228
O	-1.56592	1.30469	0.75463
O	-1.41497	3.55789	-0.20907
H	-0.44343	3.38353	-0.29608
H	-2.44768	0.06592	1.44450
H	-4.51371	1.05340	-0.25267
N	-4.95116	0.15884	-0.56947
C	-6.05412	-0.22723	0.34782

C	-5.33963	0.32643	-1.99349
C	1.48346	-1.16740	3.02729
C	-0.15148	0.67104	3.40141
H	-0.73350	1.41237	2.86171
H	0.57793	1.15785	4.04779
H	-0.80878	0.02818	3.98505
H	2.24030	-0.64609	3.61260
H	1.93813	-1.76316	2.24116
H	0.89363	-1.81608	3.67393
H	-5.68374	-0.62874	-2.38930
H	-6.13200	1.07099	-2.06802
H	-4.46261	0.66980	-2.53964
H	-6.82006	0.54811	0.34508
H	-6.47821	-1.17552	0.01905
H	-5.63689	-0.34378	1.34660
S	2.16765	-2.67989	-0.63814
O	1.94147	-1.19595	-0.42856
O	1.32344	-3.37918	0.54310
O	1.62042	-3.10763	-1.91067
O	3.54572	-3.02873	-0.34582
H	0.53370	-0.66302	-1.43816
N	4.45732	-0.07629	-0.30718
H	3.50154	-0.51210	-0.34059
H	4.28441	0.94570	-0.39992
O	1.18311	2.88139	-0.56502
O	3.59377	2.53481	-0.60831
S	2.40242	2.71758	0.23010
O	2.31316	1.74942	1.32170
O	2.61739	4.11800	1.03444
H	2.69351	4.82455	0.37751
H	0.40034	-3.03098	0.53706
H	-0.72559	0.40709	-1.80446
N	-0.05193	-0.27720	-2.20630
C	-0.83191	-1.37346	-2.85045
C	0.85072	0.45597	-3.13253
C	5.25475	-0.57025	-1.46033
C	5.05717	-0.37469	1.01902
H	4.43746	0.09813	1.77856
H	6.06675	0.03448	1.06147
H	5.07271	-1.45503	1.15235
H	5.30945	-1.65523	-1.40308
H	6.24850	-0.12312	-1.43023
H	4.75063	-0.27681	-2.38012
H	1.57675	-0.24535	-3.54179
H	0.25599	0.89359	-3.93363
H	1.34903	1.24752	-2.57497
H	-1.40406	-0.94837	-3.67556
H	-0.14025	-2.13612	-3.19909
H	-1.50650	-1.79050	-2.10491

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N	2.17446	0.08725	0.33009
H	1.56582	-0.70732	0.10407
H	0.70796	1.56344	-0.09782
N	-0.08713	2.17044	-0.32644
C	-0.06807	3.34725	0.53541
C	-0.03363	2.51700	-1.74258
C	2.53100	0.03121	1.74362
C	3.34518	0.06979	-0.54004
H	3.02790	0.04029	-1.58519
H	4.01532	-0.78906	-0.36098
H	3.93452	0.98159	-0.39566
H	3.06525	0.94217	2.03430
H	3.17548	-0.82686	2.00292
H	1.62388	-0.03141	2.34976
H	-0.94500	3.04944	-2.03533
H	0.82414	3.15934	-2.00811
H	0.02759	1.60560	-2.34242
H	0.79012	4.01640	0.34964
H	-0.98042	3.93527	0.38904
H	-0.03602	3.03730	1.58269
N	-2.17406	-0.08716	0.33123
H	-1.56533	0.70745	0.10558
C	-2.53248	-0.03058	1.74426
C	-3.34363	-0.07037	-0.54043
H	-1.62621	0.03266	2.35158
H	-3.17763	0.82738	2.00227
H	-3.06679	-0.94160	2.03466
H	-3.93304	-0.98217	-0.39628
H	-4.01412	0.78849	-0.36277
H	-3.02500	-0.04145	-1.58519
N	0.08728	-2.17042	-0.32638
H	-0.70750	-1.56347	-0.09652
C	0.03122	-2.51739	-1.74232
C	0.07001	-3.34697	0.53584
H	-0.78849	-4.01625	0.35197
H	0.98211	-3.93497	0.38781
H	0.04004	-3.03674	1.58309
H	-0.82693	-3.15994	-2.00608
H	0.94213	-3.04976	-2.03660
H	-0.03125	-1.60617	-2.34230