

Supporting information

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Title: Effect of Space Linkers in Dinuclear Copper Cryptates on the Efficiency of Atmospheric CO₂ Uptake: a DFT Study

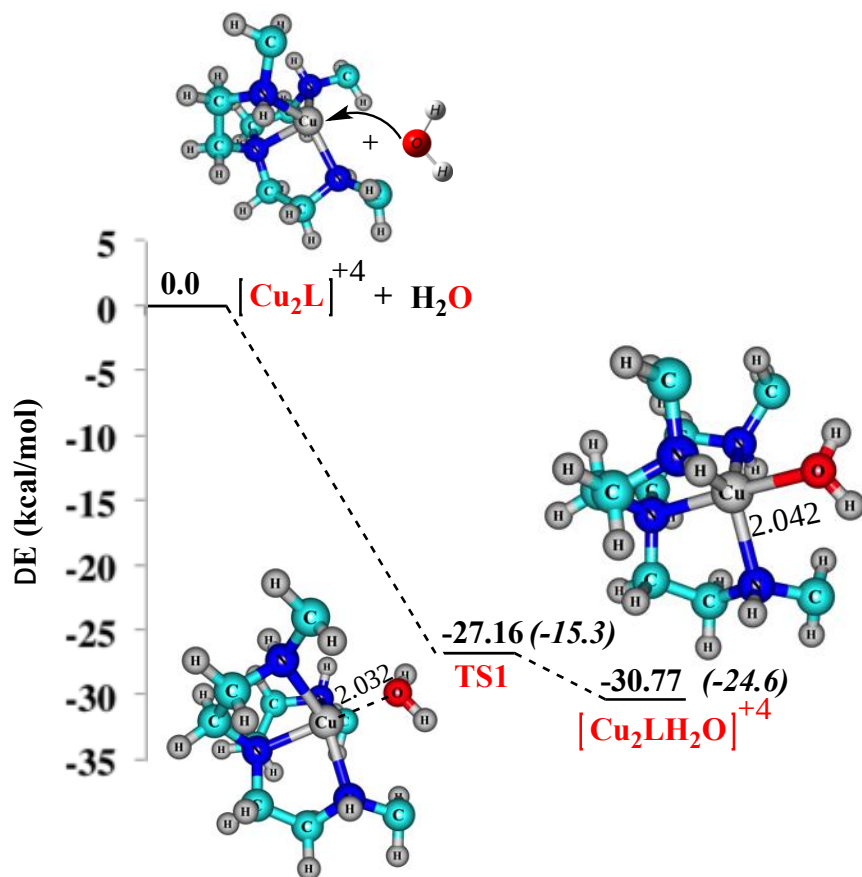


Figure S1: Reaction coordinate of interaction between the dinuclear copper cryptate linked to m-xylyl $[\text{Cu}_2\text{-m-ben}]^{4+}$ species and H_2O molecule at M06L/Gen (6-31G(d)+SDDAll) level of theory, The values refer to relative to total energies vis-à-vis the starting reactants and in aqueous solution solvent relative energies using SMD model.

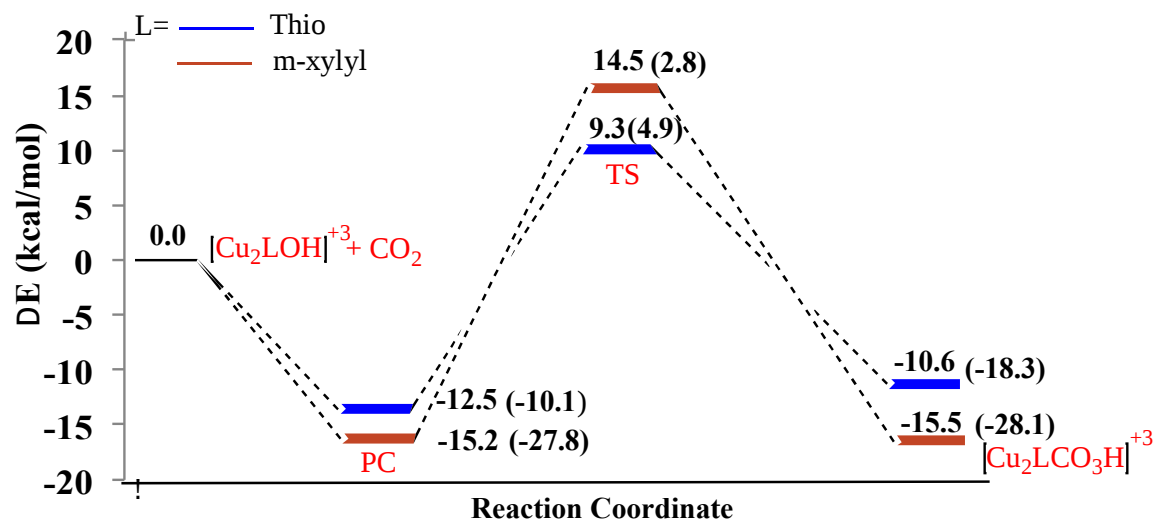


Figure S2: The computed relative energy (kcal/mol) profile for CO₂ fixation by dinuclear copper cryptate linked to m-xylyl and -Thio spacer in gas phase. The values refer to relative to total energies vis-à-vis the starting reactants and in aqueous solution solvent relative energies using SMD model.

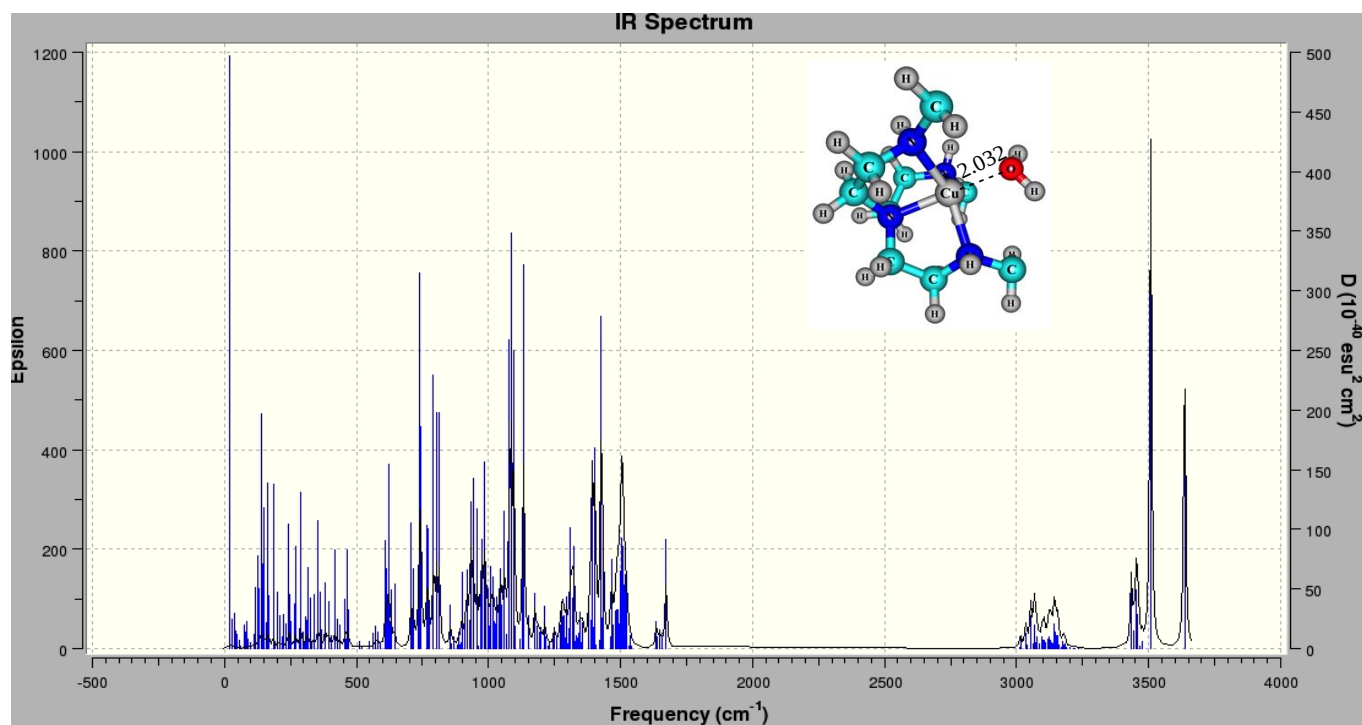
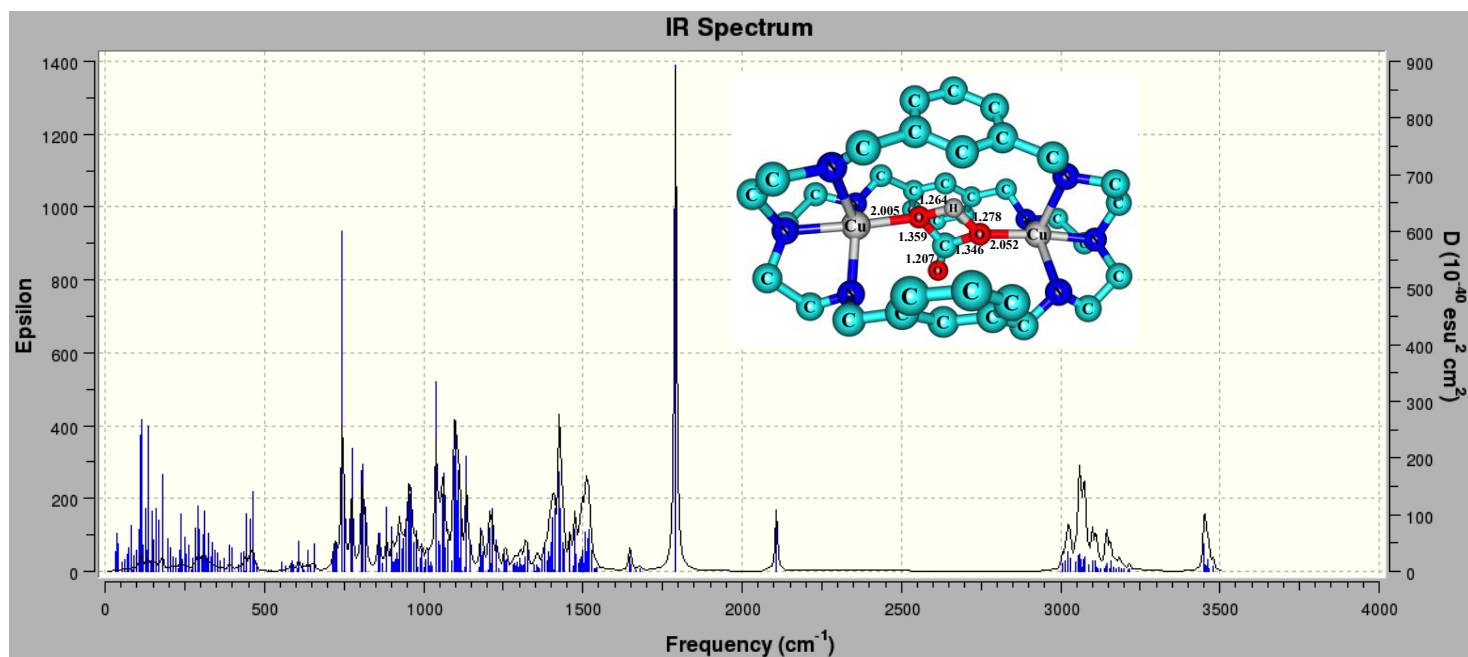


Figure S1a: IR spectrum of $[\text{Cu}_2\text{-}m\text{-ben-H}_2\text{O}]^{4+}$, relative atoms are only shown for a clarity



FigureS2a: IR spectrum of TS2 (m-benz), hydrogens are omitted for a clarity

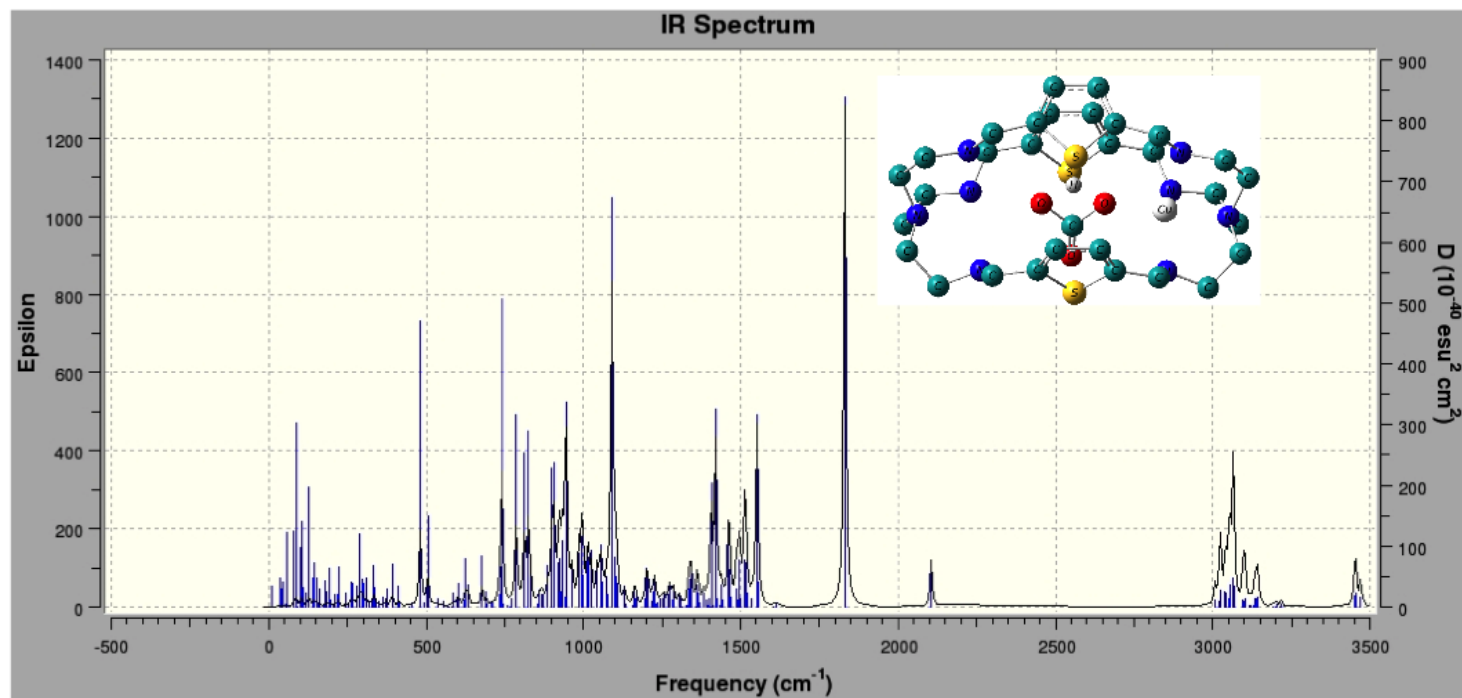


Figure S2b: IR spectrum of TS2 (-Thio), hydrogens are omitted for a clarity

Full optimized reaction coordinates are given at M06L level of theory(6-31G(d) + SDDAll basis set) for dinuclear copper cryptate linked to *m*-xylyl and –Thio spacer in gas phase.

Cryptands: (*m*-xylyl)

6	5.451731	1.616634	-0.160045	7	3.393255	-0.674921	-1.694616
6	4.350490	2.490390	0.426482	7	-5.119441	-0.115818	-0.032156
6	5.477562	-0.171268	1.516911	7	-3.267749	2.074637	0.362516
6	4.542308	-1.295639	1.945248	7	-3.083148	-1.565631	1.504860
6	5.691305	-0.719048	-0.863450	7	-2.753470	-0.802467	-1.591068
6	4.789174	-0.688426	-2.092135	1	5.422142	1.718977	-1.254052
6	-5.594338	1.257547	-0.057624	1	6.444620	1.994856	0.161250
6	-4.666352	2.160689	0.757665	1	4.489708	2.620216	1.515036
6	-5.499684	-0.891096	1.132304	1	4.456688	3.508105	-0.001758
6	-4.470988	-1.990909	1.439503	1	5.264997	0.707566	2.142317
6	-5.193963	-0.806541	-1.303551	1	6.531616	-0.452789	1.720778
6	-4.019254	-0.428495	-2.199516	1	4.883400	-2.263527	1.533495
6	1.972393	2.897369	0.075589	1	4.619316	-1.406470	3.044959
6	0.837780	2.501612	-0.831772	1	5.629265	-1.722805	-0.419760
6	1.083780	2.023885	-2.125646	1	6.749982	-0.573379	-1.163567
6	0.030657	1.801517	-3.004859	1	5.016633	0.190584	-2.721549
6	-1.282118	2.059810	-2.608480	1	5.032275	-1.567619	-2.720750
6	-1.552764	2.517268	-1.317444	1	-5.595367	1.593817	-1.104661
6	-0.482779	2.719325	-0.440404	1	-6.640902	1.350866	0.294692
6	-2.960918	2.797017	-0.865243	1	-4.994260	3.207604	0.686438
6	2.137905	-1.493092	2.418044	1	-4.739985	1.888517	1.823037
6	0.977810	-0.539957	2.529141	1	-6.510357	-1.342690	1.041216
6	1.210657	0.806977	2.832287	1	-5.554377	-0.197594	1.982559
6	0.147628	1.682162	3.013315	1	-4.741129	-2.468252	2.393890
6	-1.161672	1.223334	2.898142	1	-4.539945	-2.783817	0.678589
6	-1.418460	-0.117895	2.612854	1	-6.145708	-0.614579	-1.837394
6	-0.339543	-0.986599	2.420359	1	-5.168059	-1.888528	-1.116782
6	-2.840254	-0.607470	2.572015	1	-4.159945	-0.886448	-3.200709
6	2.482972	-1.397645	-2.569176	1	-4.016886	0.660792	-2.347947
6	1.378818	-2.076299	-1.805524	1	2.368461	3.869183	-0.292616
6	1.682658	-2.987309	-0.786606	1	1.572619	3.106820	1.081281
6	0.667471	-3.637754	-0.096476	1	2.108317	1.831289	-2.448048
6	-0.667728	-3.386180	-0.407665	1	0.232832	1.439568	-4.013092
6	-0.991860	-2.492759	-1.425754	1	-2.106583	1.909260	-3.309276
6	0.040970	-1.846050	-2.111453	1	-0.694863	3.062881	0.572688
6	-2.418146	-2.209451	-1.795062	1	-3.082575	3.871982	-0.651499
7	5.246345	0.218348	0.143423	1	-3.655516	2.585576	-1.706527
7	3.043026	1.920788	0.165141	1	2.557695	-1.645777	3.434143
7	3.183016	-1.020223	1.521367	1	1.771354	-2.482632	2.098445

1	2.236497	1.169710	2.920850
1	0.338640	2.730597	3.243724
1	-1.998039	1.914170	3.006430
1	-0.542406	-2.030231	2.176858
1	-3.086666	-1.113597	3.522350
1	-3.501611	0.281763	2.535609
1	3.036533	-2.165183	-3.149427
1	2.046262	-0.716183	-3.320019
1	2.726071	-3.177146	-0.529428
1	0.915550	-4.343830	0.695468
1	-1.466779	-3.866739	0.156693
1	-0.200980	-1.142273	-2.912481
1	-2.605344	-2.514072	-2.847425
1	-3.088562	-2.826964	-1.177654
1	3.074540	1.293951	-0.642372
1	3.068503	-0.028793	1.295956
1	3.295734	-0.979057	-0.721513
1	-3.058429	1.082687	0.211034
1	-2.846312	-1.126334	0.608687
1	-2.001003	-0.220926	-1.956297

[Cu₂-*m*-ben]⁴⁺ :

6	5.927108	0.944205	-1.015777
6	5.159325	2.115027	-0.439299
6	5.925028	-0.523330	0.989414
6	4.890082	-1.249223	1.832339
6	5.631116	-1.526508	-1.261206
6	4.439528	-1.711729	-2.175695
6	-5.650072	1.501257	-0.412349
6	-4.578603	2.358262	0.247749
6	-5.873602	-0.418063	1.133789
6	-4.800434	-1.260005	1.789553
6	-5.810565	-0.800795	-1.342383
6	-4.877436	-0.577650	-2.516070
6	2.861981	2.922460	0.063517
6	1.502197	3.069776	-0.553378
6	1.390616	3.670840	-1.814675
6	0.138553	3.918336	-2.375969
6	-1.009025	3.604093	-1.659033
6	-0.923939	2.998752	-0.396603
6	0.342291	2.708442	0.135519
6	-2.161692	2.804526	0.427372
6	2.550351	-1.277499	2.555907
6	1.274223	-0.511329	2.754795
6	1.252498	0.699895	3.459131

6	0.042685	1.312445	3.776385
6	-1.160590	0.700672	3.429361
6	-1.163035	-0.503406	2.714198
6	0.059193	-1.079694	2.360242
6	-2.428322	-1.275387	2.480177
6	1.984721	-1.912397	-2.225680
6	0.734318	-2.373619	-1.523875
6	0.761371	-3.370564	-0.539350
6	-0.419411	-3.891968	-0.018999
6	-1.647268	-3.445931	-0.501150
6	-1.704595	-2.476547	-1.511452
6	-0.506407	-1.928314	-1.992367
6	-3.026434	-2.192496	-2.174302
7	5.460052	-0.325211	-0.404606
7	3.697645	1.908373	-0.645871
7	3.607828	-0.504561	1.854417
7	3.186709	-1.774769	-1.360066
7	-5.423637	0.057767	-0.197851
7	-3.233198	2.046970	-0.278850
7	-3.500484	-0.516488	1.774701
7	-3.448978	-0.759122	-2.096449
1	5.767502	0.873695	-2.099246
1	7.008891	1.068980	-0.860159
1	5.320330	2.214370	0.640865
1	5.489868	3.057803	-0.893757
1	6.151285	0.456628	1.423946
1	6.870009	-1.085552	0.985343
1	4.680102	-2.248001	1.423760
1	5.291170	-1.406181	2.842977
1	5.743702	-2.397062	-0.603807
1	6.560304	-1.449935	-1.842749
1	4.333459	-0.868985	-2.872123
1	4.558735	-2.617551	-2.785004
1	-5.674561	1.699818	-1.488788
1	-6.638399	1.787592	-0.025265
1	-4.833681	3.416956	0.099234
1	-4.555672	2.201123	1.335856
1	-6.811177	-0.983080	1.046919
1	-6.095007	0.460097	1.752485
1	-5.082887	-1.528271	2.816494
1	-4.637190	-2.200884	1.245155
1	-6.851943	-0.607183	-1.641240
1	-5.770678	-1.842858	-1.001130
1	-5.122615	-1.267058	-3.333787
1	-4.977347	0.433400	-2.923622
1	3.389235	3.888560	0.028543

1	2.802216	2.630227	1.119209
1	2.283102	4.013603	-2.340505
1	0.062497	4.417022	-3.338964
1	-1.976542	3.904670	-2.064263
1	0.418351	2.270791	1.133806
1	-1.933910	2.282358	1.365497
1	-2.558217	3.796132	0.701996
1	2.931518	-1.619043	3.531805
1	2.361947	-2.181756	1.962177
1	2.176715	1.141696	3.834452
1	0.035930	2.229994	4.360113
1	-2.093761	1.140035	3.787248
1	0.063583	-2.031235	1.827387
1	-2.230472	-2.180250	1.892595
1	-2.839754	-1.610190	3.446780
1	2.221388	-2.628603	-3.030736
1	1.822331	-0.945341	-2.719430
1	1.704313	-3.800998	-0.199782
1	-0.381608	-4.685942	0.723736
1	-2.565768	-3.917025	-0.148919
1	-0.528880	-1.212920	-2.817401
1	-3.010062	-2.493258	-3.232291
1	-3.814313	-2.785679	-1.695493
1	3.508893	2.013472	-1.648799
1	3.764707	0.352389	2.390934
1	3.252144	-2.612434	-0.776662
1	-3.213629	2.329903	-1.261634
1	-3.636526	0.367255	2.276167
1	-2.862671	-0.225461	-2.740056
29	3.353432	-0.056167	-0.233029
29	-3.251814	-0.153548	-0.192035

[Cu₂-*m*-ben-OH₂]⁴⁺ :

6	5.686536	1.350352	-1.017051
6	4.818715	2.383432	-0.327824
6	5.915642	-0.238156	0.884105
6	4.973688	-1.116358	1.691629
6	5.718132	-1.113463	-1.424407
6	4.531064	-1.432964	-2.305758
6	-5.661505	1.300129	-0.793130
6	-4.874770	2.383051	-0.092371
6	-5.711452	-0.416815	0.987640
6	-4.734897	-1.318439	1.701104
6	-5.518037	-1.112224	-1.371840
6	-4.501616	-1.117810	-2.487013

6	2.499401	2.917253	0.368733
6	1.191999	3.273143	-0.279443
6	1.187486	3.982939	-1.485548
6	-0.009609	4.393437	-2.064742
6	-1.217986	4.100643	-1.440293
6	-1.244567	3.390730	-0.233289
6	-0.031395	2.979623	0.340254
6	-2.565921	3.112042	0.429078
6	2.644436	-1.373750	2.444570
6	1.337261	-0.674943	2.695829
6	1.290130	0.524269	3.415741
6	0.067978	1.101007	3.754620
6	-1.123459	0.474888	3.396821
6	-1.104797	-0.726218	2.677416
6	0.131874	-1.274918	2.309218
6	-2.371307	-1.480281	2.379351
6	2.152684	-2.085239	-2.265920
6	1.020698	-2.689503	-1.483876
6	1.238789	-3.712087	-0.549447
6	0.165077	-4.339159	0.073725
6	-1.140064	-3.958941	-0.237972
6	-1.385608	-2.953784	-1.181701
6	-0.294146	-2.327641	-1.792355
6	-2.807344	-2.695575	-1.605743
7	5.401721	-0.004536	-0.487147
7	3.369429	2.056078	-0.495850
7	3.629649	-0.497188	1.766812
7	3.334219	-1.695576	-1.448758
7	-5.193835	-0.052440	-0.366398
7	-3.431168	2.214060	-0.393303
7	-3.420583	-0.633128	1.764072
7	-3.140617	-1.278191	-1.905669
1	5.486947	1.336150	-2.096303
1	6.751197	1.599025	-0.892898
1	5.015732	2.415841	0.750371
1	5.035766	3.387528	-0.714777
1	6.045385	0.730462	1.379243
1	6.914040	-0.694871	0.835276
1	4.856428	-2.105558	1.225398
1	5.401641	-1.293396	2.688041
1	5.988802	-1.992714	-0.826954
1	6.599618	-0.863799	-2.030557
1	4.279346	-0.595131	-2.969261
1	4.753144	-2.296001	-2.947825
1	-5.533218	1.374053	-1.879784
1	-6.738417	1.394251	-0.592699

1	-5.236993	3.374906	-0.395080
1	-4.992712	2.331027	0.997501
1	-6.698186	-0.889149	0.885056
1	-5.864553	0.506167	1.558179
1	-5.109314	-1.577633	2.700929
1	-4.589090	-2.265386	1.163432
1	-6.536381	-0.954458	-1.753600
1	-5.523951	-2.074182	-0.846960
1	-4.729862	-1.915971	-3.206160
1	-4.515615	-0.174959	-3.046373
1	3.051564	3.842070	0.595225
1	2.345120	2.397839	1.324308
1	2.127868	4.276176	-1.955160
1	0.001498	4.978427	-2.981064
1	-2.144307	4.481627	-1.872308
1	-0.033079	2.479946	1.315121
1	-2.431248	2.644774	1.414848
1	-3.099857	4.060154	0.598935
1	3.056547	-1.740956	3.398630
1	2.492218	-2.256374	1.808881
1	2.205610	0.985208	3.789425
1	0.044964	2.009546	4.352462
1	-2.063275	0.898078	3.754690
1	0.156558	-2.229605	1.776802
1	-2.173680	-2.315875	1.692651
1	-2.763986	-1.926381	3.308184
1	2.490472	-2.810761	-3.025270
1	1.825329	-1.195795	-2.817903
1	2.246800	-4.075096	-0.342034
1	0.339176	-5.151007	0.776063
1	-1.975050	-4.490268	0.219417
1	-0.448635	-1.561731	-2.552862
1	-3.030978	-3.297890	-2.502962
1	-3.499127	-3.049037	-0.830114
1	3.123095	2.258908	-1.469298
1	3.722209	0.350242	2.332100
1	3.564677	-2.490784	-0.846218
1	-3.286148	2.467306	-1.374960
1	-3.536270	0.193218	2.356729
1	-2.462445	-0.934428	-2.586331
29	3.273172	0.012968	-0.306131
29	-3.138698	0.064395	-0.262041
8	-1.102086	0.196683	-0.370749
1	-0.789727	1.122843	-0.252583
1	-0.679101	-0.309152	0.356396

[Cu ₂ - <i>m</i> -ben-OH] ³⁺ :			
6	5.588638	1.227103	-1.249389
6	4.749664	2.317744	-0.613477
6	5.953089	-0.176788	0.757654
6	5.057786	-0.973132	1.690455
6	5.622131	-1.240047	-1.438648
6	4.411422	-1.604447	-2.273116
6	-5.643204	1.242248	-0.815833
6	-4.852096	2.365179	-0.186337
6	-5.624816	-0.348108	1.071664
6	-4.597898	-1.164774	1.818235
6	-5.542649	-1.190153	-1.238183
6	-4.551146	-1.299993	-2.372481
6	2.505545	2.917348	0.206864
6	1.181779	3.284899	-0.392564
6	1.146620	4.013471	-1.586932
6	-0.065468	4.415556	-2.136700
6	-1.254645	4.098066	-1.489020
6	-1.242473	3.364317	-0.298391
6	-0.018396	2.960535	0.242772
6	-2.540778	3.045935	0.382428
6	2.773705	-1.154966	2.578042
6	1.466448	-0.444749	2.781802
6	1.411280	0.773290	3.471379
6	0.185640	1.373889	3.741186
6	-0.998944	0.746683	3.355167
6	-0.965019	-0.466488	2.662331
6	0.275827	-1.031679	2.355371
6	-2.207303	-1.252485	2.361166
6	2.050032	-2.257013	-2.178964
6	0.937939	-2.827658	-1.346765
6	1.179612	-3.750883	-0.321555
6	0.120468	-4.328563	0.369177
6	-1.192050	-3.996947	0.035868
6	-1.455856	-3.091555	-0.994170
6	-0.381341	-2.515112	-1.673082
6	-2.882380	-2.852268	-1.407455
7	5.346568	-0.066903	-0.585177
7	3.296406	1.996565	-0.668967
7	3.718743	-0.352934	1.769755
7	3.227513	-1.807640	-1.393177
7	-5.153602	-0.075843	-0.319208
7	-3.409854	2.164266	-0.448998
7	-3.306389	-0.449773	1.789220
7	-3.195318	-1.455648	-1.798686

1	5.321325	1.114337	-2.308584
1	6.654192	1.503242	-1.219410
1	5.008031	2.438026	0.446167
1	4.952937	3.285954	-1.091756
1	6.100481	0.833225	1.157878
1	6.951537	-0.633493	0.700165
1	4.918809	-1.997272	1.313723
1	5.530040	-1.067332	2.679166
1	5.879962	-2.080710	-0.781470
1	6.497413	-1.068877	-2.081609
1	4.155441	-0.806120	-2.982603
1	4.620308	-2.505362	-2.867710
1	-5.520062	1.256162	-1.906134
1	-6.718802	1.346659	-0.613952
1	-5.199058	3.339114	-0.558953
1	-4.984948	2.387868	0.902600
1	-6.601640	-0.848761	1.042585
1	-5.780348	0.611231	1.577804
1	-4.937612	-1.371215	2.843552
1	-4.442053	-2.141343	1.337246
1	-6.567547	-1.036767	-1.602454
1	-5.549853	-2.114717	-0.649198
1	-4.812388	-2.139299	-3.032128
1	-4.551839	-0.393855	-2.990082
1	3.095151	3.832214	0.368999
1	2.377413	2.436685	1.186317
1	2.077530	4.313435	-2.071271
1	-0.081587	5.008138	-3.047873
1	-2.198256	4.464259	-1.896854
1	0.005165	2.410554	1.188638
1	-2.373692	2.546359	1.347644
1	-3.091983	3.975675	0.592885
1	3.224266	-1.405833	3.552716
1	2.612072	-2.104243	2.049128
1	2.323388	1.231922	3.856985
1	0.148557	2.304018	4.303927
1	-1.947708	1.190830	3.663065
1	0.307993	-1.975980	1.808681
1	-1.979406	-2.052933	1.644911
1	-2.562187	-1.740283	3.285605
1	2.387095	-3.015737	-2.905580
1	1.697811	-1.399248	-2.764224
1	2.195870	-4.065375	-0.077760
1	0.312264	-5.058466	1.152090
1	-2.017801	-4.476546	0.562161
1	-0.551122	-1.803016	-2.480049

1	-3.139668	-3.507447	-2.257409
1	-3.561150	-3.138031	-0.592977
1	2.982331	2.154109	-1.629398
1	3.826267	0.549567	2.238596
1	3.464821	-2.568207	-0.751235
1	-3.217119	2.378750	-1.430457
1	-3.404351	0.403352	2.344102
1	-2.495142	-1.141031	-2.470128
29	3.184430	-0.041605	-0.309271
29	-3.098576	0.051051	-0.342034
8	-1.275923	0.063170	-0.587968
1	-0.898995	0.827135	-0.118817

PC (*m*-benz)

6	5.519938	1.157212	-1.210751
6	4.748804	2.343933	-0.687073
6	5.705828	-0.068295	0.943964
6	4.850494	-0.913714	1.863765
6	5.595778	-1.298435	-1.181730
6	4.517665	-1.743671	-2.137303
6	-5.558788	1.333464	-0.839684
6	-4.766290	2.377244	-0.087548
6	-5.670653	-0.441139	0.863683
6	-4.708453	-1.337759	1.610251
6	-5.433645	-1.032018	-1.515134
6	-4.360293	-1.021512	-2.581910
6	2.547123	2.917488	0.302141
6	1.230384	3.369646	-0.248247
6	1.190508	4.155330	-1.405105
6	-0.027547	4.579002	-1.923889
6	-1.211363	4.218997	-1.287908
6	-1.190016	3.432542	-0.132137
6	0.038775	3.023355	0.384768
6	-2.477948	3.042872	0.531560
6	2.541167	-1.264446	2.613511
6	1.227233	-0.613061	2.953714
6	1.164885	0.596946	3.647466
6	-0.066640	1.151719	3.995984
6	-1.250675	0.500146	3.663087
6	-1.215874	-0.717466	2.969660
6	0.028641	-1.254475	2.621674
6	-2.478209	-1.454776	2.609296
6	2.123381	-2.320654	-2.210626
6	0.963589	-2.868594	-1.429113
6	1.120099	-3.726149	-0.335856

6	0.006517	-4.238535	0.323797
6	-1.276194	-3.887540	-0.092089
6	-1.452408	-3.051713	-1.197162
6	-0.326099	-2.566635	-1.863264
6	-2.824140	-2.737069	-1.714128
7	5.165721	-0.072515	-0.447648
7	3.298275	2.038414	-0.649640
7	3.480174	-0.376683	1.889269
7	3.265663	-1.902113	-1.367225
7	-5.123838	-0.034460	-0.457525
7	-3.326868	2.192775	-0.350070
7	-3.423410	-0.635588	1.806579
7	-3.045311	-1.284771	-1.949711
1	5.270081	0.969081	-2.262597
1	6.604644	1.333025	-1.162321
1	5.054220	2.593348	0.334792
1	4.954828	3.235679	-1.294195
1	5.726645	0.965876	1.303914
1	6.747436	-0.418241	0.930758
1	4.791455	-1.950711	1.502336
1	5.310486	-0.964002	2.861996
1	5.785972	-2.085266	-0.442220
1	6.547594	-1.111494	-1.696689
1	4.333822	-1.001321	-2.925229
1	4.806009	-2.677020	-2.641502
1	-5.400027	1.446979	-1.919296
1	-6.638387	1.447604	-0.663008
1	-5.108749	3.385744	-0.360977
1	-4.917734	2.286303	0.996483
1	-6.643431	-0.934528	0.728347
1	-5.861105	0.465720	1.449918
1	-5.158778	-1.653385	2.563343
1	-4.497261	-2.255973	1.042322
1	-6.426077	-0.832777	-1.943838
1	-5.489689	-2.017410	-1.038212
1	-4.589679	-1.763247	-3.359668
1	-4.304732	-0.044206	-3.076553
1	3.181972	3.786447	0.529163
1	2.407358	2.360817	1.239769
1	2.117288	4.467620	-1.889575
1	-0.053589	5.208350	-2.809619
1	-2.160277	4.584787	-1.683641
1	0.069861	2.410252	1.287956
1	-2.285702	2.485060	1.459667
1	-3.048008	3.943737	0.808944
1	3.016833	-1.633813	3.538421

1	2.364807	-2.144057	1.978182
1	2.077034	1.104896	3.964678
1	-0.100145	2.081233	4.559819
1	-2.200534	0.925337	3.990330
1	0.065267	-2.191495	2.062198
1	-2.237248	-2.347267	2.016977
1	-2.983542	-1.806694	3.524154
1	2.482796	-3.074994	-2.931130
1	1.805260	-1.446403	-2.792683
1	2.110456	-4.044967	-0.005753
1	0.137614	-4.928144	1.155095
1	-2.144464	-4.307736	0.416664
1	-0.436649	-1.938236	-2.746861
1	-3.007668	-3.274592	-2.659632
1	-3.585996	-3.090094	-1.008279
1	2.897076	2.173092	-1.581956
1	3.503652	0.521189	2.376264
1	3.421265	-2.623048	-0.658848
1	-3.137546	2.474488	-1.314713
1	-3.621377	0.209340	2.348801
1	-2.307107	-0.948587	-2.571202
29	3.099668	-0.041564	-0.346855
29	-3.015080	0.030005	-0.306537
8	-0.964070	0.224015	0.041904
6	0.202623	0.198405	-0.748392
8	0.104609	0.452017	-1.932939
8	1.209425	-0.113910	-0.017283
1	-0.700996	-0.037341	0.949984

TS2 (*m*-benz)

6	5.518462	1.200317	-1.149718
6	4.748323	2.377971	-0.610106
6	5.676937	-0.057427	0.984074
6	4.816604	-0.938331	1.863410
6	5.606756	-1.245773	-1.160712
6	4.539407	-1.684100	-2.129084
6	-5.499178	1.344200	-0.840534
6	-4.735244	2.381805	-0.057585
6	-5.663914	-0.458323	0.824988
6	-4.736540	-1.382732	1.577178
6	-5.341350	-0.998526	-1.558488
6	-4.239019	-0.946354	-2.590931
6	2.564300	3.005789	0.339381
6	1.237432	3.431713	-0.202439
6	1.180445	4.236793	-1.345691

6	-0.046241	4.654047	-1.849490	1	-5.862002	0.437815	1.424957
6	-1.220543	4.270205	-1.209542	1	-5.201472	-1.701448	2.521655
6	-1.180141	3.459932	-0.071161	1	-4.528709	-2.296796	1.002121
6	0.055591	3.051088	0.428095	1	-6.324701	-0.784962	-2.000360
6	-2.456272	3.044625	0.596985	1	-5.406646	-1.997727	-1.112909
6	2.520618	-1.338841	2.607855	1	-4.442661	-1.652623	-3.407798
6	1.199915	-0.702301	2.937971	1	-4.161014	0.051216	-3.039681
6	1.133215	0.504712	3.642091	1	3.199554	3.886785	0.511662
6	-0.099376	1.051465	3.989394	1	2.450336	2.496786	1.306456
6	-1.278183	0.396018	3.642272	1	2.100926	4.571853	-1.826685
6	-1.235492	-0.807071	2.932687	1	-0.086046	5.298987	-2.723453
6	0.008075	-1.341255	2.586728	1	-2.176939	4.634612	-1.588201
6	-2.491490	-1.539529	2.555660	1	0.094716	2.423323	1.320757
6	2.188524	-2.351970	-2.248084	1	-2.250074	2.479505	1.517190
6	1.021702	-2.918875	-1.492415	1	-3.038960	3.933645	0.886131
6	1.176195	-3.794708	-0.413883	1	3.007455	-1.687234	3.534526
6	0.061676	-4.305425	0.246326	1	2.367758	-2.227169	1.979272
6	-1.219094	-3.927431	-0.150003	1	2.043912	1.006096	3.974160
6	-1.391325	-3.066847	-1.237171	1	-0.140052	1.973683	4.564652
6	-0.265869	-2.590563	-1.909133	1	-2.230716	0.814279	3.971687
6	-2.759340	-2.708729	-1.728777	1	0.049197	-2.275356	2.021833
7	5.165051	-0.038825	-0.411976	1	-2.251167	-2.408240	1.929562
7	3.294716	2.084977	-0.588681	1	-2.994403	-1.926651	3.457848
7	3.433566	-0.426922	1.877329	1	2.587573	-3.104145	-2.950088
7	3.288398	-1.890440	-1.372387	1	1.868288	-1.494312	-2.852854
7	-5.057315	-0.027274	-0.465578	1	2.166627	-4.128091	-0.098850
7	-3.294614	2.196152	-0.292336	1	0.190773	-5.011735	1.063778
7	-3.446303	-0.696338	1.793721	1	-2.089450	-4.342761	0.359132
7	-2.952124	-1.246205	-1.922092	1	-0.376911	-1.945058	-2.781084
1	5.272923	1.030694	-2.205784	1	-2.961992	-3.211271	-2.689682
1	6.602997	1.378896	-1.095564	1	-3.522110	-3.069005	-1.027568
1	5.047368	2.608062	0.418239	1	2.914134	2.235142	-1.527097
1	4.962981	3.280382	-1.198316	1	3.443362	0.461541	2.382503
1	5.674283	0.966974	1.371813	1	3.464985	-2.621874	-0.679926
1	6.723950	-0.392524	0.989079	1	-3.081097	2.458571	-1.257569
1	4.783206	-1.967895	1.479910	1	-3.629990	0.138230	2.356788
1	5.250769	-1.000521	2.872018	1	-2.183005	-0.886594	-2.493752
1	5.802027	-2.044664	-0.435665	29	3.043436	-0.001712	-0.293656
1	6.559003	-1.042607	-1.669730	29	-2.963939	0.011626	-0.216967
1	4.346266	-0.922813	-2.896815	8	-0.993379	0.273207	0.045383
1	4.850839	-2.595494	-2.659893	6	-0.074576	0.275519	-0.956297
1	-5.317294	1.474979	-1.914172	8	-0.214876	0.567334	-2.119444
1	-6.584050	1.436239	-0.687310	8	0.998962	-0.185716	-0.286954
1	-5.073138	3.392849	-0.328714	1	0.060815	-0.176611	0.580395
1	-4.911825	2.278788	1.021681				
1	-6.637216	-0.932228	0.636790				

[Cu₂-*m*-ben-CO₃H]³⁺

6	5.592279	1.245627	-1.117086	1	5.382091	1.111582	-2.186207
6	4.770842	2.385369	-0.557194	1	6.668291	1.458431	-1.025337
6	5.724742	-0.094656	0.966335	1	5.025447	2.574300	0.491946
6	4.816091	-0.954030	1.823547	1	4.993184	3.316467	-1.095964
6	5.676930	-1.215446	-1.222799	1	5.758869	0.922177	1.372363
6	4.581641	-1.649686	-2.169371	1	6.755806	-0.475247	0.996905
6	-5.551409	1.278526	-0.918622	1	4.746219	-1.975613	1.420817
6	-4.792879	2.358247	-0.186128	1	5.250330	-1.052408	2.829912
6	-5.690755	-0.442027	0.842907	1	5.896979	-2.025600	-0.516665
6	-4.751208	-1.320350	1.636987	1	6.610907	-1.005759	-1.762001
6	-5.375834	-1.106347	-1.512656	1	4.371209	-0.883918	-2.927884
6	-4.286053	-1.098024	-2.560943	1	4.877872	-2.560559	-2.708996
6	2.520915	2.910847	0.332287	1	-5.370667	1.356193	-1.997496
6	1.206666	3.339411	-0.247116	1	-6.636356	1.370039	-0.768234
6	1.178762	4.128878	-1.400727	1	-5.126703	3.353780	-0.512200
6	-0.032265	4.555372	-1.935073	1	-4.975512	2.311189	0.895576
6	-1.223952	4.197930	-1.314061	1	-6.660762	-0.931640	0.681126
6	-1.214811	3.404920	-0.162366	1	-5.893689	0.482093	1.396786
6	0.005296	2.985012	0.365525	1	-5.220032	-1.616535	2.587157
6	-2.509166	3.020512	0.488737	1	-4.523760	-2.249829	1.094246
6	2.545317	-1.255277	2.665057	1	-6.369339	-0.935250	-1.949574
6	1.225229	-0.598287	2.971665	1	-5.413331	-2.078840	-1.008280
6	1.161016	0.625473	3.653136	1	-4.487154	-1.857110	-3.329735
6	-0.072078	1.183776	3.975113	1	-4.232404	-0.130265	-3.074107
6	-1.255443	0.534143	3.621307	1	3.120511	3.795596	0.593020
6	-1.218839	-0.674641	2.926556	1	2.367423	2.340930	1.260639
6	0.028512	-1.226729	2.613666	1	2.111007	4.448350	-1.869971
6	-2.469415	-1.423836	2.547098	1	-0.045477	5.188331	-2.818508
6	2.219677	-2.344165	-2.228492	1	-2.167825	4.570465	-1.715477
6	1.065997	-2.879687	-1.427972	1	0.015849	2.362920	1.263240
6	1.243703	-3.704058	-0.311557	1	-2.329904	2.468620	1.422018
6	0.143303	-4.216888	0.369884	1	-3.087293	3.921580	0.747511
6	-1.147100	-3.887987	-0.038763	1	3.043932	-1.542728	3.605953
6	-1.344868	-3.074936	-1.156875	1	2.381702	-2.184036	2.100146
6	-0.231631	-2.602484	-1.855148	1	2.072668	1.123564	3.986441
6	-2.728697	-2.776530	-1.651812	1	-0.113634	2.114918	4.535723
7	5.253028	-0.028006	-0.438695	1	-2.205906	0.971878	3.930497
7	3.323607	2.064766	-0.606235	1	0.067266	-2.170840	2.066721
7	3.449865	-0.398392	1.856736	1	-2.211417	-2.262756	1.887176
7	3.340683	-1.860961	-1.386609	1	-2.932961	-1.859599	3.448789
7	-5.093922	-0.070179	-0.475254	1	2.600402	-3.121089	-2.912720
7	-3.346207	2.164800	-0.398323	1	1.889840	-1.504333	-2.852591
7	-3.476938	-0.602972	1.832221	1	2.241820	-4.002388	0.014410
7	-2.987245	-1.331654	-1.889320	1	0.291114	-4.886508	1.214627
				1	-2.004742	-4.303533	0.491136
				1	-0.362524	-1.998478	-2.752622

1	-2.913359	-3.313169	-2.598029
1	-3.476387	-3.148154	-0.939443
1	2.978787	2.249844	-1.551543
1	3.505127	0.508687	2.326120
1	3.541279	-2.584949	-0.692827
1	-3.114349	2.400840	-1.366467
1	-3.665447	0.227863	2.397645
1	-2.223986	-0.943372	-2.451164
29	3.120561	-0.020404	-0.396052
29	-3.049645	0.024781	-0.259040
8	-1.189057	0.059718	0.140281
6	-0.260641	0.199363	-0.742211
8	-0.327496	0.409368	-1.938704
8	0.990837	0.061988	-0.132608
1	0.808805	-0.127476	0.812639

Cryptands: (-Thio)

7	5.250898	0.362323	0.009956
7	3.208662	2.083616	-1.179105
7	2.920768	-0.070831	1.829358
7	3.530773	-1.420708	-1.118446
7	-5.251246	0.363741	0.010480
7	-3.206823	2.083386	-1.178742
7	-2.920050	-0.069996	1.829348
7	-3.532676	-1.420796	-1.117071
6	5.505411	1.753069	-0.294625
6	4.632548	2.262694	-1.442239
6	2.704988	3.079610	-0.226789
6	1.254652	2.929115	0.071514
6	0.706979	2.306473	1.158669
6	-0.708350	2.307915	1.157590
6	-1.252930	2.931763	0.069574
6	-2.702343	3.084586	-0.232314
6	-4.630510	2.261912	-1.443325
6	-5.504040	1.754515	-0.295238
6	5.406810	-0.028391	1.399854
6	4.219375	0.429420	2.246178
6	2.691331	-1.482106	2.128770
6	1.253126	-1.852046	1.960124
6	0.709592	-2.990960	1.428927
6	-0.710449	-2.990878	1.429256
6	-1.253584	-1.851888	1.960694
6	-2.691614	-1.481249	2.129431
6	-5.406330	-0.025637	1.400803
6	-4.218000	0.431926	2.246007

6	5.808828	-0.570937	-0.945293
6	4.927479	-1.802775	-1.109014
6	2.683359	-2.351620	-1.823206
6	1.250935	-1.938917	-1.746000
6	0.710573	-0.779514	-1.264265
6	-0.712704	-0.779595	-1.263935
6	-1.253185	-1.939048	-1.745454
6	-2.685611	-2.351920	-1.821940
6	-4.929537	-1.802306	-1.107083
6	-5.810334	-0.569957	-0.943613
1	-6.848676	-0.873276	-0.697784
1	6.568292	1.955069	-0.544140
1	5.299116	2.342116	0.608374
1	4.903499	3.320651	-1.639049
1	4.872206	1.707839	-2.360112
1	2.694321	2.194660	-2.050908
1	3.240609	2.931154	0.721457
1	2.943499	4.112393	-0.554702
1	1.322345	1.821903	1.915068
1	-1.325610	1.824116	1.912984
1	-3.240574	2.944416	0.715699
1	-2.937081	4.115735	-0.567845
1	-2.691952	2.188589	-2.050943
1	-4.869593	1.705014	-2.360111
1	-4.901272	3.319409	-1.642785
1	-5.296800	2.344089	0.607207
1	-6.566689	1.957673	-0.544805
1	5.460252	-1.125774	1.429181
1	6.357950	0.339760	1.839110
1	4.385295	0.142759	3.294844
1	4.173131	1.531672	2.240789
1	2.852479	0.048056	0.813752
1	3.007065	-1.639513	3.174190
1	3.295395	-2.173653	1.508504
1	1.315206	-3.797573	1.018166
1	-1.316346	-3.797428	1.018793
1	-3.296140	-2.172698	1.509517
1	-3.007330	-1.637960	3.174962
1	-2.851479	0.048562	0.813745
1	-5.460623	-1.122959	1.431086
1	-6.356866	0.343586	1.840505
1	-4.383832	0.146656	3.295074
1	-4.170591	1.534131	2.239286
1	6.847248	-0.874822	-0.700482
1	5.865037	-0.057935	-1.915513
1	5.238799	-2.330087	-2.034117

1	5.093657	-2.522665	-0.287721
1	3.422198	-0.465339	-1.459156
1	2.993210	-2.508341	-2.881523
1	2.810629	-3.338341	-1.344931
1	1.311908	0.047911	-0.885534
1	-1.313922	0.047720	-0.884768
1	-2.812602	-3.338502	-1.343305
1	-2.995915	-2.508975	-2.880077
1	-3.423843	-0.465471	-1.457766
1	-5.095779	-2.521751	-0.285420
1	-5.241306	-2.329891	-2.031871
1	-5.867142	-0.057671	-1.914181
16	-0.001171	-3.047276	-2.220514
16	0.002344	3.530596	-0.984581
16	-0.000067	-0.757675	2.461248

[Cu₂-Thio]⁴⁺ :

N	-5.34133500	0.10436200	-0.42614600
N	-3.11492400	-1.14515900	-1.82691000
N	-3.56019400	-0.35944500	1.80427500
N	-3.53506900	2.28081600	-0.76451000
N	5.34146200	0.10668300	-0.42579200
N	3.11763700	-1.14807500	-1.82553100
N	3.56080500	-0.35376000	1.80562800
N	3.53138200	2.27995400	-0.76889500
Cu	-3.26337900	0.24597900	-0.20670000
Cu	3.26336000	0.24469600	-0.20686400
C	-5.53934400	-1.07652300	-1.30225500
C	-4.49633200	-1.10687300	-2.40042300
C	-2.69330500	-2.54208200	-1.55434300
C	-1.25104300	-2.73871900	-1.22850400
C	-0.70459200	-3.86072800	-0.64426900
C	0.70441000	-3.86153300	-0.64356100
C	1.25267200	-2.74013900	-1.22729300
C	2.69566600	-2.54439200	-1.55051900
C	4.49967300	-1.11074500	-2.39765400
C	5.54157000	-1.07629800	-1.29855700
C	-5.87049000	-0.07534600	0.95150800
C	-4.94313700	-0.92393600	1.78987100
C	-2.66480200	-1.31044400	2.54056100
C	-1.24990700	-0.88007200	2.73544800
C	-0.70828800	-0.06548800	3.70803100
C	0.70605500	-0.06378700	3.70903200
C	1.25104300	-0.87709500	2.73725600
C	2.66722300	-1.30427400	2.54491500

C	5.87086900	-0.06824300	0.95238500
C	4.94480400	-0.91580900	1.79320600
C	-5.79461000	1.37524400	-1.04835600
C	-4.98169800	2.54482400	-0.54074800
C	-2.67934600	3.29497500	-0.11287400
C	-1.24359900	2.88703300	-0.12026600
C	-0.70424900	1.68944400	0.31663800
C	0.70180300	1.68940600	0.31461500
C	1.23992900	2.88683200	-0.12375700
C	2.67548000	3.29544400	-0.11963600
C	4.97781400	2.54632500	-0.54658000
C	5.79235100	1.37668800	-1.05144400
H	6.86137200	1.53282000	-0.84527900
H	-6.55205700	-1.06189500	-1.73169900
H	-5.47779800	-1.97675900	-0.67959600
H	-4.67458900	-1.96643000	-3.05987300
H	-4.56404200	-0.21345200	-3.03116600
H	-2.49461000	-0.78604300	-2.55523000
H	-3.31164600	-2.94318200	-0.73979100
H	-2.93385400	-3.15533500	-2.44068800
H	-1.30715300	-4.67556300	-0.25001500
H	1.30565900	-4.67694500	-0.24851300
H	3.31242700	-2.94349600	-0.73377900
H	2.93800500	-3.15975300	-2.43491000
H	2.49808900	-0.79044600	-2.55523600
H	4.56747300	-0.21936500	-3.03123700
H	4.67910900	-1.97229100	-3.05416500
H	5.48031800	-1.97490200	-0.67350300
H	6.55468200	-1.06179100	-1.72708400
H	-5.98888100	0.91901900	1.39760200
H	-6.87426700	-0.52337300	0.91176200
H	-5.34443500	-1.02052400	2.80744100
H	-4.86528900	-1.94284000	1.38935200
H	-3.58871100	0.50291100	2.35741800
H	-2.70260600	-2.25750300	1.98852200
H	-3.11261100	-1.50985700	3.52623600
H	-1.30522900	0.46231900	4.44870400
H	1.30071300	0.46541800	4.45053500
H	3.11486200	-1.49879400	3.53162200
H	2.70795600	-2.25322400	1.99636500
H	3.58761100	0.51039000	2.35605600
H	5.98780300	0.92756800	1.39561100
H	6.87530200	-0.51490900	0.91395200
H	5.34606200	-1.00850800	2.81115100
H	4.86882100	-1.93609300	1.39587100
H	-6.86381400	1.52904700	-0.84141500

H	-5.69838400	1.28261400	-2.13573500	6	0.923536	-0.298438	2.782971
H	-5.30579200	3.47445400	-1.02664200	6	2.291178	-0.860267	2.557536
H	-5.12008300	2.68866000	0.53832200	6	5.573484	0.144953	0.988682
H	-3.35403700	2.33652700	-1.76980900	6	4.627536	-0.534702	1.949746
H	-2.82163900	4.28190200	-0.57617800	6	-5.403166	1.093444	-1.800543
H	-3.02479400	3.40029700	0.92613200	6	-4.615713	2.340350	-1.469144
H	-1.29704500	0.88299200	0.76324100	6	-2.521473	3.221585	-0.622817
H	1.29594300	0.88262500	0.75878500	6	-1.083198	3.051741	-0.273786
H	3.02203700	3.40447900	0.91862700	6	-0.582686	2.731563	0.968013
H	2.81651200	4.28101900	-0.58623900	6	0.829232	2.806635	1.034317
H	3.34981500	2.33293700	-1.77423900	6	1.406829	3.182846	-0.159433
H	5.11650300	2.69318100	0.53204200	6	2.865847	3.350223	-0.410110
H	5.30051300	3.47511900	-1.03500500	6	4.987563	2.330265	-1.088778
H	5.69592100	1.28112600	-2.13853500	6	5.654261	1.001852	-1.345410
S	-0.00248100	4.00713200	-0.55427500	1	6.745488	1.080518	-1.231882
S	0.00213300	-1.63747800	1.81086700	1	-6.407972	-1.372541	-1.813705
S	0.00174300	-1.66674800	-1.79070700	1	-5.516791	-2.004408	-0.430315
[Cu ₂ -Thio-OH ₂] ⁴⁺ :				1	-4.515252	-2.762188	-2.596098
7	-5.201506	0.040117	-0.775601	1	-4.257864	-1.098314	-3.086444
7	-2.995384	-1.695218	-1.511472	1	-2.302875	-1.530902	-2.243868
7	-3.767488	0.236655	1.710997	1	-3.272561	-3.159339	0.001762
7	-3.169599	2.033949	-1.261735	1	-2.953537	-3.808130	-1.603052
7	5.136685	-0.055736	-0.424319	1	-1.278324	-4.366285	1.272700
7	3.143375	-1.766997	-1.534137	1	1.334989	-4.343959	1.295899
7	3.242298	-0.026213	1.761959	1	3.342177	-3.164357	0.041185
7	3.509048	2.167928	-1.065840	1	3.009341	-3.869974	-1.534761
29	-3.155650	0.085420	-0.309611	1	2.543798	-1.647459	-2.354243
29	3.104954	0.115162	-0.428224	1	4.626057	-1.162280	-2.894819
6	-5.440913	-1.328586	-1.290555	1	4.801632	-2.836777	-2.391629
6	-4.319228	-1.753457	-2.211483	1	5.430277	-2.116974	-0.083269
6	-2.657165	-3.016229	-0.895092	1	6.534715	-1.423942	-1.264161
6	-1.221644	-3.186398	-0.540406	1	-6.012875	1.407505	0.599298
6	-0.677612	-3.870683	0.514013	1	-6.938380	-0.081121	0.447452
6	0.738605	-3.844392	0.535165	1	-5.707212	-0.011363	2.609000
6	1.294014	-3.141078	-0.507980	1	-5.128155	-1.351342	1.625462
6	2.736663	-3.035632	-0.865627	1	-3.797916	1.241838	1.905022
6	4.549676	-1.830979	-2.031021	1	-3.196044	-1.477618	2.752374
6	5.489256	-1.419100	-0.925261	1	-3.515617	-0.100030	3.796367
6	-5.916102	0.321379	0.495891	1	-1.425694	1.101081	4.737595
6	-5.175178	-0.256119	1.679708	1	1.169841	0.866519	4.595700
6	-3.038909	-0.395428	2.851146	1	2.739292	-1.057032	3.543550
6	-1.583038	-0.091981	2.936567	1	2.228209	-1.831903	2.048023
6	-0.916145	0.588310	3.925025	1	3.205129	0.923172	2.142480
6	0.494708	0.465703	3.841887	1	5.606459	1.221504	1.186243
				1	6.599309	-0.231739	1.110227
				1	4.976710	-0.393106	2.981697

1 4.597444 -1.619462 1.782448
1 -6.474377 1.330812 -1.884724
1 -5.094637 0.691783 -2.770836
1 -4.759546 3.092327 -2.255815
1 -4.980903 2.798279 -0.541788
1 -2.745338 1.924719 -2.186220
1 -2.673179 4.104790 -1.259377
1 -3.074767 3.417350 0.303831
1 -1.213362 2.511591 1.826849
1 1.397938 2.651990 1.949019
1 3.365531 3.488236 0.556471
1 3.082000 4.251390 -1.001652
1 3.172074 2.137543 -2.032339
1 5.285852 2.748573 -0.121729
1 5.302168 3.061966 -1.844269
1 5.466254 0.666160 -2.371290
16 0.199047 3.469250 -1.367441
16 -0.450310 -0.881741 1.879800
16 0.039168 -2.572721 -1.582364
8 1.128680 0.316023 -0.757670
1 0.747077 0.900646 -0.065085
1 0.624398 -0.525073 -0.706899

[Cu₂-Thio-OH]³⁺ :

7 -5.122181 0.076080 -0.888242
7 -2.922788 -1.694130 -1.522889
7 -3.752440 0.234695 1.646740
7 -3.062441 2.070655 -1.205747
7 5.049787 -0.084175 -0.493191
7 3.077204 -1.872867 -1.392231
7 3.185065 0.080079 1.698599
7 3.458068 2.104002 -1.147180
29 -3.034735 0.067258 -0.355934
29 3.021648 0.073754 -0.513928
6 -5.362996 -1.264091 -1.457071
6 -4.187362 -1.693420 -2.311017
6 -2.686714 -3.019464 -0.871363
6 -1.277855 -3.208612 -0.431546
6 -0.793328 -3.785337 0.712965
6 0.620591 -3.752452 0.792657
6 1.212960 -3.144509 -0.290554
6 2.669089 -3.060327 -0.595638
6 4.456934 -1.993525 -1.922454
6 5.421377 -1.478091 -0.878989
6 -5.869757 0.318499 0.363648

6 -5.146905 -0.270053 1.558016
6 -3.057714 -0.395422 2.800054
6 -1.607716 -0.077236 2.919508
6 -0.965038 0.506389 3.984121
6 0.445037 0.414737 3.895640
6 0.884936 -0.220937 2.757588
6 2.258722 -0.752840 2.517141
6 5.504332 0.245553 0.886867
6 4.580505 -0.368510 1.913438
6 -5.281830 1.159040 -1.879092
6 -4.491592 2.385517 -1.476962
6 -2.465523 3.218247 -0.463830
6 -1.025114 3.077435 -0.126751
6 -0.498589 2.818970 1.114721
6 0.913894 2.872400 1.138731
6 1.464221 3.167144 -0.085229
6 2.910862 3.272900 -0.398551
6 4.923079 2.242557 -1.341994
6 5.558659 0.882043 -1.510553
1 6.654993 0.948034 -1.450768
1 -6.293110 -1.284352 -2.045552
1 -5.502125 -1.964393 -0.623855
1 -4.380403 -2.684077 -2.744205
1 -4.048682 -1.006221 -3.152957
1 -2.163360 -1.559715 -2.191630
1 -3.358677 -3.116593 -0.009350
1 -2.974954 -3.809131 -1.585351
1 -1.432672 -4.196253 1.490012
1 1.187841 -4.172214 1.620610
1 3.242838 -3.068528 0.341797
1 2.987880 -3.957360 -1.154083
1 2.422436 -1.768583 -2.169282
1 4.514879 -1.408130 -2.846437
1 4.698181 -3.031151 -2.190465
1 5.377535 -2.102915 0.019889
1 6.460575 -1.505014 -1.234720
1 -5.981588 1.401313 0.492647
1 -6.888513 -0.091376 0.297358
1 -5.712799 -0.058977 2.476739
1 -5.081151 -1.363549 1.475724
1 -3.797053 1.237786 1.842824
1 -3.194294 -1.479707 2.679581
1 -3.559029 -0.123105 3.740670
1 -1.490876 0.920957 4.840716
1 1.116518 0.738018 4.688473
1 2.720427 -0.924585 3.502072

1	2.203216	-1.731533	2.020636	6	2.702447	-3.081962	-0.447110
1	3.100451	1.046217	2.021239	6	4.467540	-1.953655	-1.740628
1	5.504136	1.336081	0.992056	6	5.408489	-1.457967	-0.667542
1	6.541283	-0.089105	1.032784	6	-5.895183	0.263900	0.433187
1	4.935983	-0.136369	2.927588	6	-5.195890	-0.301846	1.652531
1	4.578348	-1.464293	1.835711	6	-3.154172	-0.339367	2.982399
1	-6.343268	1.421539	-2.008971	6	-1.699288	-0.041482	3.103015
1	-4.932626	0.787818	-2.849103	6	-1.041100	0.564312	4.145758
1	-4.593800	3.165759	-2.243243	6	0.367586	0.453071	4.047764
1	-4.897770	2.815955	-0.552792	6	0.792367	-0.216677	2.922822
1	-2.580416	2.007591	-2.105000	6	2.158124	-0.770916	2.675751
1	-2.648145	4.150002	-1.021640	6	5.447472	0.238020	1.129407
1	-3.026240	3.310610	0.474680	6	4.506011	-0.388116	2.133483
1	-1.111242	2.629098	1.993539	6	-5.263229	1.116480	-1.791455
1	1.504442	2.744098	2.042996	6	-4.492465	2.348718	-1.374396
1	3.469007	3.336013	0.544266	6	-2.485501	3.197993	-0.347322
1	3.142495	4.192039	-0.958682	6	-1.052029	3.061715	0.017064
1	2.990351	2.067683	-2.055864	6	-0.545751	2.847156	1.274755
1	5.322936	2.760763	-0.463852	6	0.866305	2.915218	1.323177
1	5.161429	2.880019	-2.202904	6	1.435002	3.177591	0.101038
1	5.318002	0.470198	-2.497169	6	2.883427	3.287235	-0.195927
16	0.231541	3.411681	-1.276840	6	4.907668	2.259655	-1.091000
16	-0.467071	-0.699022	1.772299	6	5.544986	0.902741	-1.260563
16	0.021447	-2.668876	-1.447373	1	6.640058	0.965853	-1.179142
8	1.227843	0.150227	-0.884912	1	-6.220018	-1.335956	-1.998435
1	0.803752	0.757919	-0.252853	1	-5.461504	-2.014872	-0.557407
PC (-Thio)				1	-4.259169	-2.683859	-2.663368
7	-5.108339	0.035064	-0.797453	1	-3.925261	-0.991284	-3.012910
7	-2.870120	-1.710121	-1.353415	1	-2.081011	-1.538902	-1.978028
7	-3.818126	0.238078	1.782835	1	-3.316654	-3.144399	0.148324
7	-3.070380	2.038481	-1.073777	1	-2.945926	-3.823557	-1.437154
7	5.017773	-0.074861	-0.263823	1	-1.399139	-4.187915	1.659401
7	3.082803	-1.871193	-1.221499	1	1.222813	-4.170706	1.790785
7	3.116749	0.074677	1.906224	1	3.273442	-3.095273	0.491740
7	3.439690	2.117577	-0.932928	1	3.038932	-3.963151	-1.020273
29	-3.033665	0.052104	-0.204568	1	2.439098	-1.772624	-2.008542
29	2.984814	0.065908	-0.285150	1	4.523345	-1.336036	-2.643903
6	-5.309262	-1.305789	-1.380998	1	4.728195	-2.977947	-2.040247
6	-4.096012	-1.702989	-2.196740	1	5.351481	-2.102130	0.216997
6	-2.648595	-3.043414	-0.716427	1	6.454988	-1.468768	-1.001974
6	-1.241555	-3.246788	-0.282337	1	-6.035832	1.344504	0.553326
6	-0.757497	-3.800352	0.872418	1	-6.901770	-0.169791	0.338982
6	0.656786	-3.771111	0.952182	1	-5.797520	-0.100058	2.550534
6	1.250288	-3.192270	-0.144697	1	-5.100812	-1.393817	1.578026
				1	-3.893858	1.245144	1.946423
				1	-3.306935	-1.426308	2.917777

1	-3.665908	-0.009592	3.898367	6	-5.363283	-1.434305	-1.007026
1	-1.553995	1.013101	4.992892	6	-4.354199	-1.980360	-1.992487
1	1.048572	0.792553	4.825837	6	-2.675102	-3.172304	-0.649602
1	2.605532	-0.994761	3.656816	6	-1.238480	-3.319682	-0.297418
1	2.085980	-1.724461	2.134828	6	-0.685251	-3.768426	0.873731
1	3.029464	1.036569	2.240528	6	0.731612	-3.761662	0.859706
1	5.445225	1.327246	1.247847	6	1.257457	-3.309128	-0.322789
1	6.481723	-0.098439	1.289495	6	2.684829	-3.152806	-0.706245
1	4.847842	-0.175858	3.156587	6	4.336482	-1.925396	-2.050803
1	4.496973	-1.482276	2.035485	6	5.358500	-1.415488	-1.059386
1	-6.325557	1.365257	-1.938543	6	-5.603574	0.344945	0.681649
1	-4.892514	0.750247	-2.755193	6	-4.831324	-0.225830	1.850424
1	-4.582410	3.127808	-2.143599	6	-2.689730	-0.405632	2.974435
1	-4.920372	2.777269	-0.458853	6	-1.254207	-0.017570	3.114948
1	-2.570274	1.941844	-1.960656	6	-0.694421	1.081949	3.722251
1	-2.654863	4.119398	-0.926466	6	0.724636	1.065308	3.717910
1	-3.061254	3.312310	0.579746	6	1.254769	-0.046478	3.106607
1	-1.173988	2.683118	2.147772	6	2.680083	-0.467168	2.954175
1	1.442559	2.821323	2.240871	6	5.612072	0.300397	0.691096
1	3.428804	3.353414	0.754117	6	4.828318	-0.295086	1.839610
1	3.118715	4.207404	-0.753234	6	-5.360498	0.907121	-1.710036
1	3.001350	2.085886	-1.856592	6	-4.667379	2.237284	-1.534925
1	5.286612	2.766721	-0.197106	6	-2.693351	3.294995	-0.607301
1	5.167619	2.907389	-1.938011	6	-1.253894	3.268239	-0.250900
1	5.321326	0.502423	-2.255718	6	-0.729211	3.231157	1.016139
16	0.222999	3.369481	-1.120557	6	0.682835	3.233346	1.032651
16	-0.576911	-0.708762	1.966812	6	1.236364	3.272397	-0.222098
16	0.062068	-2.746971	-1.316073	6	2.683518	3.306953	-0.546012
8	1.162151	0.113976	-0.526845	6	4.676008	2.273017	-1.459940
1	0.780382	0.747808	0.106450	6	5.369414	0.949617	-1.678181
6	0.366682	0.184091	-3.066732	1	6.461075	1.083928	-1.710135
8	-0.777387	0.297452	-2.845864	1	-6.381828	-1.461451	-1.420664
8	1.495166	0.062667	-3.346801	1	-5.373056	-2.045424	-0.096940
TS2 (-Thio)				1	-4.622449	-3.007095	-2.275701
7	-5.002985	-0.043859	-0.621995	1	-4.343156	-1.396756	-2.918803
7	-2.995855	-1.920257	-1.396635	1	-2.318363	-1.831597	-2.157014
7	-3.411197	0.192501	1.808741	1	-3.278248	-3.198734	0.267104
7	-3.220481	2.054178	-1.253926	1	-3.007820	-4.025432	-1.264903
7	5.006695	-0.037302	-0.624588	1	-1.278377	-4.069964	1.734002
7	2.987196	-1.884683	-1.434081	1	1.344570	-4.060383	1.707094
7	3.416397	0.151057	1.809066	1	3.309467	-3.197682	0.195063
7	3.225330	2.081091	-1.208037	1	3.003850	-3.992165	-1.347172
29	-2.956019	0.029674	-0.401143	1	2.297194	-1.783898	-2.181698
29	2.957006	0.039413	-0.400590	1	4.313170	-1.307501	-2.954565
				1	4.599219	-2.941551	-2.374801
				1	5.376805	-2.056390	-0.170091

1	6.372342	-1.431593	-1.484807
1	-5.602647	1.439375	0.739694
1	-6.656044	0.028253	0.721250
1	-5.321636	0.072840	2.789056
1	-4.842910	-1.324037	1.836006
1	-3.379980	1.207050	1.939891
1	-2.782511	-1.493810	2.868539
1	-3.226541	-0.140057	3.898785
1	-1.282527	1.864137	4.198568
1	1.333601	1.833417	4.190964
1	3.223237	-0.246420	3.886686
1	2.744069	-1.553361	2.812319
1	3.405730	1.161640	1.970503
1	5.629296	1.392242	0.784521
1	6.659134	-0.034525	0.721285
1	5.321878	-0.036942	2.788498
1	4.819919	-1.392325	1.788026
1	-6.451958	1.040767	-1.751212
1	-5.062257	0.450196	-2.659432
1	-4.834804	2.864952	-2.420038
1	-5.091511	2.792034	-0.690416
1	-2.727154	1.938583	-2.143625
1	-2.928159	4.153638	-1.256545
1	-3.272309	3.440318	0.313393
1	-1.348159	3.225611	1.909876
1	1.281034	3.229222	1.940263
1	3.242189	3.433088	0.389822
1	2.931200	4.179520	-1.171669
1	2.749485	1.983738	-2.109334
1	5.087656	2.792275	-0.586970
1	4.857315	2.935813	-2.316373
1	5.075099	0.525478	-2.644108
16	0.005014	3.354496	-1.440613
16	-0.013672	-1.093898	2.572706
16	-0.003812	-2.986588	-1.470670
8	1.014922	0.133183	-0.252007
8	-0.001840	0.121573	-2.348638
8	-1.015806	0.131247	-0.251517
6	-0.000760	0.131580	-1.146990
1	-0.000524	0.130283	0.491617

[Cu₂-Thio-CO₃H]³⁺ :

7	5.136060	0.053672	-0.889944
7	2.819281	1.749816	-1.319282
7	3.977103	-0.356651	1.705442

7	3.059122	-1.955498	-1.229626
7	-5.055505	0.069746	-0.175999
7	-3.195295	1.936510	-1.175081
7	-3.012225	-0.145969	1.868621
7	-3.495680	-2.086678	-1.021558
29	3.119803	0.012386	-0.165950
29	-3.051289	-0.049859	-0.325109
6	5.272056	1.418524	-1.439223
6	4.018141	1.798204	-2.202123
6	2.572980	3.070421	-0.652676
6	1.157850	3.278124	-0.249071
6	0.666728	3.740638	0.946422
6	-0.744988	3.737645	1.002640
6	-1.331771	3.271937	-0.152853
6	-2.781167	3.170466	-0.458406
6	-4.609258	2.003096	-1.615293
6	-5.479478	1.465037	-0.504220
6	5.996351	-0.208126	0.286754
6	5.332357	0.242908	1.571811
6	3.313553	0.103093	2.957451
6	1.850161	-0.168846	3.026167
6	1.153860	-0.812732	4.018196
6	-0.249798	-0.656223	3.899425
6	-0.640820	0.082722	2.807607
6	-1.994214	0.682903	2.575816
6	-5.383781	-0.301657	1.232231
6	-4.384298	0.298555	2.199400
6	5.249570	-0.996487	-1.924306
6	4.485384	-2.240387	-1.528386
6	2.464746	-3.181853	-0.617196
6	1.032177	-3.070214	-0.233161
6	0.542222	-2.859933	1.033598
6	-0.865126	-2.940056	1.104729
6	-1.450641	-3.206737	-0.106123
6	-2.905635	-3.300886	-0.379866
6	-4.969596	-2.230403	-1.107143
6	-5.627648	-0.875735	-1.181940
1	-6.715131	-0.953373	-1.036804
1	6.158435	1.495992	-2.087183
1	5.430575	2.106421	-0.598662
1	4.137044	2.794296	-2.648471
1	3.840063	1.105296	-3.031754
1	2.010543	1.545239	-1.911332
1	3.217827	3.153741	0.231621
1	2.890333	3.864233	-1.348974
1	1.305136	4.039291	1.773705

1	-1.318192	4.067620	1.866214	1	0.857225	-0.591431	-1.004900
1	-3.353054	3.245620	0.476435				
1	-3.095731	4.029128	-1.076999				
1	-2.596846	1.786304	-1.994815				
1	-4.702216	1.408225	-2.530144				
1	-4.903887	3.028558	-1.875029				
1	-5.370057	2.076258	0.398577				
1	-6.545618	1.473707	-0.769441				
1	6.195993	-1.285293	0.328334				
1	6.973160	0.283264	0.171010				
1	5.971195	-0.005125	2.431120				
1	5.196178	1.332969	1.582123				
1	4.085827	-1.371237	1.779721				
1	3.494439	1.185830	3.014770				
1	3.807040	-0.339741	3.833961				
1	1.635846	-1.323151	4.848270				
1	-0.953209	-1.017995	4.647141				
1	-2.398166	0.957382	3.563107				
1	-1.898812	1.616848	2.005462				
1	-2.893154	-1.119206	2.154890				
1	-5.363013	-1.394715	1.305797				
1	-6.408696	0.016567	1.470291				
1	-4.666114	0.049241	3.232568				
1	-4.389688	1.395338	2.137319				
1	6.306200	-1.245256	-2.105680				
1	4.859221	-0.598724	-2.866952				
1	4.589702	-3.003697	-2.312073				
1	4.915288	-2.680651	-0.618358				
1	2.578689	-1.797505	-2.119989				
1	2.628904	-4.040740	-1.285490				
1	3.045097	-3.387250	0.291222				
1	1.184451	-2.690170	1.895854				
1	-1.427195	-2.842941	2.030718				
1	-3.427973	-3.434437	0.576079				
1	-3.154558	-4.179362	-0.994994				
1	-3.106243	-1.994104	-1.964985				
1	-5.297654	-2.779871	-0.218119				
1	-5.270531	-2.841631	-1.967795				
1	-5.467011	-0.430159	-2.169396				
16	-0.260262	-3.404174	-1.345560				
16	0.764192	0.591189	1.907228				
16	-0.134169	2.920974	-1.352702				
8	-1.171094	-0.184043	-0.480557				
8	-1.539555	0.065149	-2.691539				
8	0.534825	-0.297265	-1.883471				
6	-0.809614	-0.126678	-1.727628				