Supplementary information
Optimised geometries and energies of stationary points.

^{2}1

energy = -2729.788865 au

Cu	-0.229252	0.387434	0.007255
N	1.341348	0.722179	1.192608
N	-1.069404	-0.954720	1.271129
N	-1.351854	1.979965	1.194918
C	1.132206	0.749052	2.644439
C	-0.951605	-0.754982	2.712429
C	-1.221506	1.826537	2.660047
C	-1.793328	0.474848	3.130713
C	0.257865	1.953176	3.063393
C	0.514179	-0.571901	3.138357
H	-1.845122	0.499611	4.230393
H	-2.824074	0.351106	2.766533
H	0.306933	2.043570	4.159684
H	0.686795	2.877766	2.648805
H	0.557026	-0.582574	4.238706
H	1.115377	-1.418226	2.778885
H	2.112616	0.868312	3.138007
H	-1.359928	-1.637634	3.237779
H	-1.783600	2.620381	3.185495
C	2.558602	0.907303	0.769532
C	3.006226	0.988004	-0.583483
C	4.396874	1.145651	-0.819515
C	4.905140	1.257149	-2.095611
C	4.007242	1.219004	-3.188044
C	2.649132	1.074012	-2.997913
C	2.086775	0.947780	-1.690098
H	5.067229	1.176950	0.042048
H	5.974266	1.374324	-2.262566
H	4.397153	1.307722	-4.203065
H	1.957444	1.046119	-3.838104
O	0.809380	0.817740	-1.558824
C	-1.755412	-1.970312	0.843561
C	-2.179463	-2.180169	-0.508776
C	-2.737748	-3.431743	-0.866219
C	-3.254615	-3.657220	-2.125843
C	-3.244108	-2.599271	-3.061958
C	-2.728083	-1.359243	-2.741192
C	-2.161164	-1.096131	-1.459077
H	-2.750349	-4.226930	-0.117877
H	-3.669797	-4.627415	-2.392640
H	-3.656106	-2.764020	-4.058572
H	-2.725632	-0.542873	-3.461343
O	-1.723761	0.091342	-1.177589
H	-1.090675	2.928601	0.918284
H	-2.317865	1.837737	0.893054
H	3.346179	1.029228	1.530145
H	-2.081646	-2.724399	1.579033

^{3}1^{+}

Energy: -2725.381139 au

Cu	-0.314559	0.512359	0.100069
N	1.305036	0.679751	1.241153

N	-1.161209	-0.850869	1.273841
N	-1.298394	2.123291	1.259424
C	1.126692	0.684086	2.701831
C	-1.058295	-0.671437	2.730796
C	-1.157556	1.927631	2.731177
C	-1.826359	0.602714	3.167815
C	0.334627	1.943290	3.139355
C	0.418534	-0.603364	3.175135
H	-1.881058	0.597544	4.263222
H	-2.854554	0.555627	2.789019
H	0.384354	2.002838	4.233393
H	0.826094	2.839030	2.740609
H	0.445559	-0.623456	4.271204
H	0.958885	-1.482242	2.807163
H	2.117246	0.725297	3.179007
H	-1.525892	-1.534777	3.227370
H	-1.657906	2.745675	3.269590
C	2.514391	0.764629	0.788349
C	2.896456	0.903280	-0.594857
C	4.258397	0.839262	-0.932398
C	4.686139	1.039735	-2.240215
C	3.742935	1.337506	-3.247470
C	2.399880	1.426773	-2.949112
C	1.920229	1.204559	-1.618360
H	4.985025	0.631173	-0.153815
H	5.738698	0.977375	-2.483997
H	4.081436	1.500536	-4.263547
H	1.662140	1.658748	-3.705997
O	0.655426	1.305990	-1.379488
C	-1.780764	-1.903178	0.845413
C	-2.099414	-2.201546	-0.528626
C	-2.650988	-3.455084	-0.840563
C	-3.043632	-3.766168	-2.137711
C	-2.911234	-2.801370	-3.159738
C	-2.391378	-1.554066	-2.886359
C	-1.955839	-1.205773	-1.567497
H	-2.772018	-4.188896	-0.050401
H	-3.458017	-4.740458	-2.361863
H	-3.225553	-3.045420	-4.167317
H	-2.286417	-0.799443	-3.654782
O	-1.482528	-0.024017	-1.351945
H	-0.906943	3.034579	1.004610
H	-2.293413	2.174785	1.022984
H	3.344235	0.757724	1.503835
H	-2.128598	-2.641380	1.576617

$^{4}\mathbf{1}^{2+}$

Energy: -2726.436281 au

Cu	-0.237771	0.444426	0.086291
N	1.372098	0.722816	1.198510
N	-1.071325	-0.984473	1.238429
N	-1.284773	1.931419	1.098255
C	1.085610	0.713547	2.618629
C	-0.897267	-0.736800	2.653641
C	-1.157630	1.733509	2.543543
C	-1.724634	0.455971	3.053943
C	0.237104	1.877211	3.035557
C	0.515371	-0.579530	3.100700
H	-1.630642	0.535721	4.139552

H	-2.767024	0.326659	2.802555
H	0.145196	1.817431	4.122730
H	0.682512	2.826512	2.778287
H	0.456918	-0.483003	4.188296
H	1.131215	-1.428587	2.834174
H	2.011376	0.840280	3.188796
H	-1.318171	-1.561205	3.237397
H	-1.728222	2.524933	3.027402
C	2.580179	0.949629	0.810654
C	3.017161	1.071144	-0.540217
C	4.358716	1.251605	-0.820273
C	4.811562	1.344964	-2.126681
C	3.930693	1.242435	-3.203717
C	2.603990	1.049050	-2.971818
C	2.115811	0.941244	-1.644239
H	5.075469	1.336809	0.003210
H	5.872080	1.493883	-2.300636
H	4.304183	1.319018	-4.219555
H	1.809929	0.947719	-3.715811
O	0.859814	0.745981	-1.498090
C	-1.796440	-1.975590	0.856485
C	-2.294600	-2.164678	-0.470388
C	-2.896063	-3.355673	-0.819525
C	-3.371515	-3.572516	-2.106499
C	-3.229142	-2.605289	-3.103334
C	-2.624599	-1.424506	-2.809059
C	-2.109731	-1.181335	-1.504107
H	-3.032898	-4.129976	-0.057168
H	-3.848261	-4.521515	-2.330598
H	-3.608381	-2.795276	-4.102347
H	-2.441309	-0.585039	-3.485140
O	-1.550629	-0.051395	-1.307021
H	-0.911085	2.809138	0.827156
H	-2.213404	1.770848	0.785633
H	3.388749	1.075351	1.533926
H	-2.101821	-2.762505	1.549813

^{3}2

Energy: -2726.436281 au

Cu	-0.237771	0.444426	0.086291
N	1.372098	0.722816	1.198510
N	-1.071325	-0.984473	1.238429
N	-1.284773	1.931419	1.098255
C	1.085610	0.713547	2.618629
C	-0.897267	-0.736800	2.653641
C	-1.157630	1.733509	2.543543
C	-1.724634	0.455971	3.053943
C	0.237104	1.877211	3.035557
C	0.515371	-0.579530	3.100700
H	-1.630642	0.535721	4.139552
H	-2.767024	0.326659	2.802555
H	0.145196	1.817431	4.122730
H	0.682512	2.826512	2.778287
H	0.456918	-0.483003	4.188296
H	1.131215	-1.428587	2.834174
H	2.011376	0.840280	3.188796
H	-1.318171	-1.561205	3.237397
H	-1.728222	2.524933	3.027402
C	2.580179	0.949629	0.810654

C	3.017161	1.071144	-0.540217
C	4.358716	1.251605	-0.820273
C	4.811562	1.344964	-2.126681
C	3.930693	1.242435	-3.203717
C	2.603990	1.049050	-2.971818
C	2.115811	0.941244	-1.644239
H	5.075469	1.336809	0.003210
H	5.872080	1.493883	-2.300636
H	4.304183	1.319018	-4.219555
H	1.809929	0.947719	-3.715811
O	0.859814	0.745981	-1.498090
C	-1.796440	-1.975590	0.856485
C	-2.294600	-2.164678	-0.470388
C	-2.896063	-3.355673	-0.819525
C	-3.371515	-3.572516	-2.106499
C	-3.229142	-2.605289	-3.103334
C	-2.624599	-1.424506	-2.809059
C	-2.109731	-1.181335	-1.504107
H	-3.032898	-4.129976	-0.057168
H	-3.848261	-4.521515	-2.330598
H	-3.608381	-2.795276	-4.102347
H	-2.441309	-0.585039	-3.485140
O	-1.550629	-0.051395	-1.307021
H	-0.911085	2.809138	0.827156
H	-2.213404	1.770848	0.785633
H	3.388749	1.075351	1.533926
H	-2.101821	-2.762505	1.549813

^{3}3

Energy: -2844.827622 au

C	2.687603	-1.349955	0.473506
C	3.369105	-0.601734	-0.552613
C	4.560069	-1.106467	-1.120717
C	5.094286	-2.323510	-0.737366
C	4.438178	-3.058370	0.268178
C	3.279881	-2.584738	0.859721
C	2.940598	0.723708	-0.932973
N	1.789630	1.225776	-0.646640
C	1.553830	2.645417	-0.794162
C	1.631110	3.273321	0.620383
C	0.443403	2.896046	1.526803
C	-0.865171	3.320462	0.847462
C	-1.051735	2.666413	-0.538050
C	0.178951	2.901512	-1.443471
N	-1.412235	1.244250	-0.343892
C	-2.652244	0.975473	-0.582224
C	-3.460139	-0.213399	-0.340441
C	-4.715849	-0.224004	-0.990058
C	-5.609629	-1.274808	-0.848502
C	-5.269941	-2.346316	-0.013319
C	-4.057259	-2.345521	0.666632
C	-3.141728	-1.290187	0.524430
N	0.399109	1.439752	1.819644
Cu	0.198097	0.068754	0.204898
O	1.615838	-0.934528	1.096247
O	-1.984837	-1.325508	1.222383
H	1.639262	4.371060	0.533020
H	2.582498	2.981959	1.088383
H	-0.850634	4.414039	0.723493

H	-1.730981	3.081024	1.482393
H	0.141521	3.957604	-1.753268
H	0.087072	2.295675	-2.355180
H	-1.903196	3.170471	-1.026681
H	2.334909	3.114342	-1.424547
H	0.547839	3.462661	2.468217
H	-4.974026	0.618135	-1.633746
H	-6.562505	-1.261523	-1.374736
H	-5.960347	-3.179846	0.114909
H	-3.789560	-3.161122	1.336303
H	5.061351	-0.507050	-1.883681
H	6.007110	-2.700483	-1.195313
H	4.849752	-4.015808	0.590673
H	2.779977	-3.149133	1.645778
H	-0.317922	1.248131	2.523608
H	1.287867	1.097598	2.193517
H	-3.251931	1.784755	-1.030869
H	3.687291	1.346071	-1.460913
O	-0.303314	-1.338842	-1.002669
C	-0.324063	-2.564088	-0.496048
H	-0.759927	-3.339578	-1.137560
H	0.495446	-2.885213	0.155545
H	-1.378229	-2.030581	0.764119

^{1}4

Energy: -2844.864803 au

C	-2.819673	0.079086	-0.927859
C	-2.899112	-0.853195	0.140226
C	-4.051737	-0.832654	0.955481
C	-5.071166	0.091987	0.767162
C	-4.958913	1.031871	-0.262283
C	-3.846424	1.016596	-1.100728
C	-1.857455	-1.805306	0.522438
N	-0.628595	-1.837270	0.122590
Cu	0.536687	-0.641547	-0.836799
O	-0.444534	0.565023	3.225634
C	-0.728356	1.372364	2.367240
O	-1.802384	0.024294	-1.826958
C	0.238899	-2.847758	0.759488
C	0.975816	-3.691321	-0.305082
C	2.153474	-2.988906	-1.006690
C	3.109548	-2.348126	0.021327
C	2.426587	-1.445308	1.077136
C	1.249600	-2.197543	1.742094
N	1.942626	-0.227816	0.443135
C	2.371490	0.931695	0.811009
C	1.925473	2.202021	0.271309
C	0.907534	2.340201	-0.748044
C	0.571307	3.669095	-1.136406
C	1.184520	4.778741	-0.582929
C	2.177910	4.639042	0.404118
C	2.525946	3.363896	0.812145
O	0.300444	1.334008	-1.309659
N	1.653688	-1.981634	-1.983100
H	3.617735	-3.169038	0.550543
H	3.893289	-1.776384	-0.499020
H	1.381191	-4.582559	0.198542
H	0.253204	-4.054248	-1.051760
H	1.673125	-3.008316	2.356377

H	0.714493	-1.515720	2.416768
H	-0.389845	-3.536145	1.354086
H	3.170543	-1.206430	1.862097
H	2.728012	-3.765901	-1.543032
H	-4.123110	-1.555708	1.769372
H	-5.943778	0.085655	1.418745
H	-5.747268	1.767002	-0.423168
H	-3.762978	1.717230	-1.930718
H	3.290401	3.231594	1.581041
H	2.659044	5.513676	0.838581
H	0.892804	5.774891	-0.919280
H	-0.193487	3.779476	-1.904978
H	1.122885	-2.460573	-2.714424
H	2.450625	-1.544514	-2.452517
H	-2.174756	-2.523943	1.296023
H	3.127415	0.994529	1.614438
H	-0.693088	1.131488	1.290713
H	-1.040282	2.406480	2.623277
H	-1.183953	0.803889	-1.741970

^{3}5

Energy: -2880.687857 au

C	2.539470	2.137918	3.250390
C	2.002579	1.446914	2.138565
C	1.528325	2.200128	0.995489
C	1.635389	3.617171	1.083620
C	2.158407	4.254168	2.193976
C	2.621926	3.517072	3.299525
C	2.008959	-0.000540	2.218625
N	1.460812	-0.787318	1.360842
C	1.629526	-2.226914	1.386250
C	2.687231	-2.598917	0.318845
C	2.183867	-2.414584	-1.125476
C	0.934943	-3.282811	-1.349951
C	-0.212462	-2.949030	-0.371610
C	0.280454	-2.941811	1.103461
N	-0.805845	-1.665488	-0.767316
Cu	0.232788	-0.112905	-0.115091
N	1.861973	-0.994630	-1.406274
O	1.061611	1.673749	-0.106332
C	-1.971532	-1.649190	-1.304189
C	-2.702219	-0.475737	-1.788977
C	-2.139296	0.799467	-2.042580
C	-2.964468	1.874456	-2.380174
C	-4.341509	1.700461	-2.498515
C	-4.911787	0.439217	-2.303403
C	-4.092563	-0.628308	-1.957695
O	-0.781519	0.937654	-2.039483
H	2.972337	-3.655513	0.440073
H	3.595141	-2.001263	0.488174
H	1.220453	-4.336867	-1.213028
H	0.573613	-3.181674	-2.384485
H	0.394675	-3.995417	1.401329
H	-0.500587	-2.497477	1.733981
H	-0.980968	-3.737755	-0.461243
H	1.997868	-2.563152	2.374879
H	2.976625	-2.775663	-1.805235
H	-4.531067	-1.610497	-1.778307
H	-5.985197	0.294968	-2.411293
H	-4.968845	2.550964	-2.762777

H	-2.509907	2.847078	-2.566484
H	2.896105	1.544859	4.095344
H	3.034935	4.020363	4.171936
H	2.213403	5.343670	2.209533
H	1.282267	4.189065	0.226089
H	1.622155	-0.873861	-2.392561
H	2.663437	-0.390405	-1.215609
H	-2.530298	-2.596498	-1.384180
H	2.545417	-0.430329	3.084933
H	-0.481673	1.762668	-1.612803
O	-1.294479	0.612516	0.870031
O	-1.834388	-0.247966	1.680220

^{3}6

Energy: -2880.712785 au

C	-4.301338	-0.997218	0.956646
C	-3.079155	-0.509768	0.430538
C	-2.445717	-1.188276	-0.666718
C	-3.111875	-2.333435	-1.188209
C	-4.294843	-2.789563	-0.640984
C	-4.906070	-2.126731	0.445780
C	-2.569582	0.733818	0.919719
N	-1.415766	1.259404	0.634949
C	-1.215646	2.669965	0.959856
C	-1.349592	3.512275	-0.332195
C	-0.183929	3.337383	-1.324114
C	1.155514	3.580173	-0.610085
C	1.340307	2.740410	0.674658
C	0.145703	2.913725	1.628149
N	1.556397	1.322667	0.351017
Cu	0.015211	0.264896	-0.363052
O	-0.398149	-2.275239	1.825194
O	-0.187120	-3.058960	0.769481
N	-0.185874	1.985415	-1.923537
O	-1.343943	-0.779294	-1.223885
C	2.761901	0.872026	0.517860
C	3.263606	-0.438298	0.223005
C	2.439287	-1.468401	-0.328029
C	3.045050	-2.729582	-0.572204
C	4.380182	-2.952545	-0.288773
C	5.192617	-1.934594	0.250619
C	4.628556	-0.699149	0.498646
O	1.172679	-1.296622	-0.609188
H	-1.391194	4.576480	-0.051909
H	-2.305788	3.275336	-0.822111
H	1.209681	4.644172	-0.332057
H	1.994649	3.388637	-1.295902
H	0.161563	3.946658	2.009043
H	0.261738	2.244449	2.491482
H	2.239950	3.120105	1.188896
H	-2.007778	2.996438	1.657438
H	-0.297496	4.112366	-2.104513
H	5.235248	0.105162	0.919093
H	6.242385	-2.121469	0.468891
H	4.810364	-3.934564	-0.488172
H	2.421516	-3.516942	-0.992802
H	-4.761947	-0.454898	1.784752
H	-5.839027	-2.498009	0.865994
H	-4.766525	-3.680354	-1.057988
H	-2.640931	-2.845995	-2.025294

H	0.507294	1.935886	-2.673246
H	-1.091449	1.768800	-2.344872
H	3.511985	1.569016	0.923471
H	-3.255279	1.315589	1.557058
H	0.263796	-2.449686	0.100703

CH_3OH

Energy: -115.721860 au

O	0.021736	0.000000	-0.024311
C	-0.018167	0.000000	1.392036
H	1.018453	0.000000	1.739429
H	-0.513404	0.891919	1.805788
H	-0.513404	-0.891919	1.805788
H	-0.888054	0.000000	-0.345396

CH_2O

Energy: -114.500881 au

O	0.000000	0.000000	0.675895
C	0.000000	0.000000	-0.530828
H	0.000000	0.937979	-1.125705
H	0.000000	-0.937979	-1.125705

H_2O_2

Energy: -151.540163 au

O	-0.062381	0.007498	0.014743
O	0.037684	-0.050275	1.465257
H	0.879676	0.037752	-0.216428
H	-0.407144	0.780697	1.696428

O_2

Energy: -150.316605 au

O	0.000000	0.000000	0.132856
O	0.000000	0.000000	1.347144