

Supporting Information

Hiking on the potential energy surface of a functional tyrosinase model – implications of singlet, broken-symmetry and triplet description

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Computational details

Quantum chemical calculations were performed using Gaussian 09[1] with the TPSSh[2], BP86[3] and M06L [4] functionals and the 6-31g(d) sets implemented in Gaussian 09[1] or the tzvp[5] and def2-tzvp [6] basis set. In one case the DFT optimisation at a TPSSh/6-31g(d)/SMD[2] level of theory was accomplished within Gaussian 09[1]. Default convergence criteria were used in all calculations. Frequency calculations did not show imaginary values for minima and one imaginary value for the transition state which was found by QST3 calculations. After several conformational sampling, the conformer with both pyrazolyl donors in the equatorial direction has been chosen for the whole analysis. The largest difference between two conformers amounted at maximum 1 kcal/mol.

The energy of the open-shell singlet **P** species has been corrected by removing the error by spin contamination following the method of Yamaguchi et al.[7] The effect of spin contamination was found to be negligible (0.5 kcal/mol).

NBO calculations[8] were accomplished using the program suite Gaussian 09.[1] For the analysis of donation and back-donation, the CDA scheme was used as implemented in AOMix.[9]

Our benchmarking on page 10 shows that triple-zeta basis sets are not suited to reproduce the experimental Cu...Cu distance of 3.51 Å. Moreover, the oxo state is no stable minimum for tzvp or def2-tzvp calculations. In summary, the accordance is best with TPSSh/6-31g(d). M06L meets the Cu...Cu value similarly well but underestimates the broken-symmetry stabilization with a value of only 0.7 kcal/mol.

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Table S1: Key data of singlet minimum path, TPSSh/6-31g(d)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.808	-5535.00291	7.19
2.145	2.886	-5535.00489	5.95
2.013	2.98	-5535.00377	6.65
1.881	3.102	-5535.00182	7.87
1.749	3.261	-5535.00251	7.44
1.618	3.494	-5535.00818	3.89
1.488	3.574	-5535.01389	0.30
1.359	3.638	-5535.01026	2.58
Oxo			
2.137	2.890	-5535.00489	5.95
Peroxo			
1.453	3.559	-5535.01437	0

Table 2 S2: Key data of broken-symmetry minimum path, TPSSh/6-31g(d)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.806	-5535.00292	7.18
2.145	2.888	-5535.00507	5.84
2.013	2.98	-5535.00399	6.51
1.881	3.102	-5535.00182	7.88
1.749	3.261	-5535.00217	7.65
1.618	3.345	-5535.00451	6.19
1.488	3.494	-5535.01418	0.12
1.359	3.574	-5535.01962	-3.29
Oxo			
2.137	2.891	-5535.00491	5.94
Peroxo			
1.453	3.577	-5535.01969	-3.34

Table S3: Key data of triplet minimum path, TPSSh/6-31g(d)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.913	-5534.98670	17.36
2.145	2.997	-5534.98712	17.10
2.013	3.100	-5534.98518	18.31
1.881	3.190	-5534.97762	23.06
1.749	3.380	-5534.96922	28.33
1.618	3.442	-5535.00198	7.77
1.488	3.909	-5535.00921	3.24
1.359	3.979	-5535.00987	2.82
Oxo			
2.197	2.964	-5534.9874	16.93
Peroxo			
1.455	3.511	-5535.0085	3.69

Table S4: Key data of singlet minimum path, TPSSh/6-31g(d) with solvent model (DCM)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.804	-5535.15908	6.09
2.145	2.882	-5535.16063	5.11
2.013	2.977	-5535.15899	6.14
1.881	3.101	-5535.15662	7.63
1.749	3.256	-5535.15688	7.46
1.618	3.418	-5535.16219	4.13
1.488	3.530	-5535.16835	0.27
1.359	3.614	-5535.16470	2.56
Oxo			
2.155	2.874	-5535.16046	5.22
Peroxo			
1.454	3.554	-5535.16878	0

Table S5: Key data of singlet minimum path, TPSSh/tzvp

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.885	-5536.16272	21.38
2.145	2.976	-5536.16514	19.86
2.013	3.090	-5536.16637	19.07
1.881	3.236	-5536.16891	17.49
1.749	3.402	-5536.17585	13.14
1.618	3.537	-5536.18666	6.36
1.488	3.634	-5536.19547	0.83
1.359	3.719	-5536.19448	1.45
Oxo			
2.137	2.982	-5536.16523	19.80
Peroxo			
1.428	3.673	-5536.19679	0

Table S6: Key data of singlet minimum path, BP86/6-31g(d)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.852	-5535.32485	5.73
2.145	2.931	-5535.32665	4.60
2.013	3.032	-5535.32552	5.30
1.881	3.156	-5535.32362	6.50
1.749	3.309	-5535.32416	6.16
1.618	3.412	-5535.32908	3.07
1.488	3.584	-5535.33385	0.08
1.359	3.671	-5535.32884	3.22
Oxo			
2.139	2.935	-5535.32665	4.60
Peroxo			
1.468	3.598	-5535.33398	0

Table S7: Key data of singlet minimum path, M06L/6-31g(d)

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.825	-5534.47057	2.44
2.145	2.903	-5534.47158	3.06
2.013	3.000	-5534.46959	3.06
1.881	3.128	-5534.46686	4.76
1.749	3.277	-5534.46621	5.18
1.618	3.425	-5534.46972	2.97
1.488	3.534	-5534.47419	0.17
1.359	3.613	-5534.47021	2.67
Oxo			
2.173	2.885	-5534.47166	1.76
Peroxo			
1.458	3.554	-5534.47446	0

Table S8: Key data of singlet minimum path, TPSSh/def2tzvp

O...O distance [Å]	Cu...Cu distance [Å]	E [H]	$\Delta E = (E - E_{\text{peroxo of the Singlet}})$ in kcal/mol
2.277	2.853	-5536.26378	20.86
2.145	2.942	-5536.26615	18.72
2.013	3.054	-5536.26719	18.72
1.881	3.196	-5536.26929	17.40
1.749	3.364	-5536.27564	13.42
1.618	3.505	-5536.28628	6.74
1.488	3.606	-5536.29542	1.01
1.359	3.693	-5536.29510	1.21
Oxo*			
2.971	2.1370	-5536.26583	19.55
Peroxo			
1.422	3.650	-5536.29702	0

* The calculation of the oxo runs always into the peroxo. Thus, the O...O distance was fixed.

Table S9: NBO charges (in e⁻ units) of Singlet path and the oxo and peroxo with TPSSh/6-31g(d).

	Cu	O	N_{py}	N_{pz}
O...O distance [Å]				
2.277	1.201	-0.722 / -0.754	-0.476 / -0.480	-0.394 / -0.398
2.145	1.195	-0.697 / -0.728	-0.485 / -0.486	-0.401 / -0.399
2.103	1.182	-0.661 / -0.689	-0.492 / -0.494	-0.403 / -0.405
1.881	1.159	-0.612 / -0.635	-0.504 / -0.504	-0.407 / -0.408
1.749	1.128	-0.553 / -0.567	-0.514 / -0.514	-0.410 / -0.411
1.618	1.099	-0.503 / -0.509	-0.524 / -0.524	-0.412 / -0.414
1.488	1.080	-0.469 / -0.471	-0.530 / -0.532	-0.416 / -0.417
1.359	1.055	-0.429 / -0.429	-0.535 / -0.539	-0.417 / -0.419
oxo	1.194	-0.695 / -0.726	-0.485 / -0.486	-0.399 / -0.401
peroxo	1.075	-0.460 / -0.461	-0.531 / -0.534	-0.416 / -0.417

Table S10: Energy values for singlet PES for varying O-O distances in kcal/mol relative to the optimised singlet peroxo

	2.745	2.888	3.032	3.176	3.320	3.465	3.609	3.752
2.277	7.73	8.07	13.03	21.09	31.30	42.73	44.41	65.64
2.145	8.94	5.95	8.55	14.84	23.66	33.99	53.95	55.37
2.013	18.38	7.82	6.98	10.61	17.31	25.94	35.02	44.84
1.881	27.85	14.16	8.56	8.48	12.12	18.27	25.72	33.60
1.750	47.06	25.32	13.36	8.21	7.86	10.83	15.78	22.18
1.619	73.50	41.49	21.50	10.08	4.89	4.28	6.63	11.23
1.488	107.55	63.08	33.66	15.25	5.08	0.90	0.84	3.76
1.359	150.48	92.16	52.81	27.50	12.62	5.10	2.73	3.97

Table S11: Energy values for broken-symmetry PES for varying O-O distances in kcal/mol relative to the optimised singlet peroxo

	2.745	2.888	3.032	3.176	3.320	3.465	3.609	3.752
2.277	7.77	8.02	12.98	21.85	29.59	39.92	49.64	55.71
2.145	8.91	5.86	8.46	14.73	23.06	32.63	42.13	47.13
2.013	15.32	7.70	6.87	10.72	17.40	25.86	34.42	36.28
1.881	27.79	14.07	8.46	8.50	12.23	14.43	18.86	24.94
1.750	47.02	25.27	13.34	8.09	8.00	6.67	9.56	14.29
1.619	73.49	41.46	21.52	10.20	2.91	0.39	1.24	4.73
1.488	107.54	63.05	33.65	14.81	3.41	-2.09	-3.12	-0.86
1.359	150.48	92.07	52.74	27.31	11.88	3.51	0.59	1.40

Table S12: Spin expectation values S^2 for broken-symmetry PES for varying O-O distances

	2.745	2.888	3.032	3.176	3.320	3.465	3.609	3.752
2.277	0.00	0.00	0.05	0.33	0.99	0.80	1.08	1.89
2.145	0.00	0.00	0.00	0.20	0.36	0.56	0.08	0.85
2.013	0.00	0.00	0.00	0.00	0.09	0.08	0.44	0.82
1.881	0.00	0.00	0.00	0.18	0.00	0.62	0.73	0.82
1.750	0.00	0.00	0.00	0.18	0.00	0.60	0.68	0.73
1.619	0.00	0.00	0.00	0.00	0.45	0.56	0.63	0.70
1.488	0.00	0.00	0.00	0.23	0.40	0.49	0.55	0.59
1.359	0.00	0.00	0.00	0.12	0.27	0.36	0.42	0.46

Table S13: Energy values for triplet PES for varying O-O distances in kcal/mol relative to the optimised singlet peroxo

	2.745	2.888	3.032	3.176	3.320	3.465	3.609	3.752
2.277	22.60	19.37	20.09	29.13	35.89	40.81	45.50	49.92
2.145	27.62	20.29	18.74	25.68	31.88	39.32	38.63	47.28
2.013	37.69	26.34	21.28	26.06	24.08	30.56	47.42	41.79
1.881	55.80	41.20	27.90	29.52	24.22	27.03	27.33	32.25
1.750	85.53	56.45	37.88	28.71	20.79	17.65	18.30	20.86
1.619	112.73	75.25	50.42	31.74	18.63	12.78	10.97	12.90
1.488	152.05	100.58	64.99	37.69	21.61	13.04	9.79	9.97
1.359	200.11	135.14	87.74	53.85	34.62	22.30	16.07	13.71

Table S14: Spin expectation values S^2 for triplet PES for varying O-O distances

	2.745	2.888	3.032	3.176	3.320	3.465	3.609	3.752
2.277	2.05	2.13	2.26	2.03	2.04	2.80	2.78	2.83
2.145	2.05	2.12	2.25	2.10	2.02	2.03	2.28	2.70
2.013	2.06	2.13	2.23	2.02	2.51	2.52	2.74	2.78
1.881	2.06	2.01	2.21	2.01	2.27	2.27	2.17	2.04
1.750	2.01	2.05	2.08	2.06	2.03	2.01	2.00	2.00
1.619	2.04	2.05	2.02	2.01	2.00	2.00	2.00	2.00
1.488	2.02	2.02	2.01	2.00	2.00	2.00	2.00	2.01
1.359	2.01	2.01	2.01	2.00	2.00	2.00	2.01	2.01

Table S15: Structural benchmarking of peroxo in broken-symmetry

	b3lyp/ 6-31g(d) (DCM)	b3lyp/ 6-31g(d) (THF)	b3lyp/ def2svp	b3lyp/ def2tzvp	BP86/ def2svp	BP86/ def2tzvp
bond lengths [Å]						
Cu-O	1.936	1.936	2.007	1.987	2.011	2.001
	1.938	1.938	2.008	1.995	2.016	1.989
O-O	1.430	1.430	1.388	1.402	1.431	1.445
Cu-Npy	2.225	2.225	2.257	2.274	2.236	2.243
Cu-Npz	2.039	2.040	2.068	2.056	2.052	2.045
	2.005	2.006	2.076	2.068	2.056	2.035
bond angles [°]						
O-Cu-O	43.3	43.3	40.4	41.2	41.6	42.5
Cu-O-Cu	136.6	136.6	139.5	138.7	138.4	137.5
Npz-Cu-Npz	90.6	90.5	88.8	89.7	88.8	89.9
Npy-Cu-Npz	90.4	90.4	89.2	89	89.7	89.7
	89.7	89.7	88.6	89.3	89.2	90.3
Cu...Cu distance [Å]						
	3.601	3.601	3.768	3.727	3.764	3.719

	BP86/ 6-31g(d)	TPSSH/ 6-31g(d)	TPSSH/6-31g(d) (DCM)	TPSSH/ tzvp*	M06L/ 6-31g(d)
bond lengths [Å]					
Cu-O	1.961	1.930	1.949	1.990	1.963
	1.904	1.919	1.918	1.954	1.897
O-O	1.478	1.452	1.472	1.428	1.467
Cu-Npy	1.976	2.167	2.196	2.239	2.217
Cu-Npz	1.978	1.983	1.998	2.031	2.000
	2.274	2.046	1.992	2.044	1.984
bond angles [°]					
O-Cu-O	44.9	44.3	44.7	42.5	44.6
Cu-O-Cu	135.1	135.7	136.7	134.6	140.4
Npz-Cu-Npz	86.4	89.7	90.3	89.6	90.0
Npy-Cu-Npz	90.3	90.9	88.8	88.3	86.3
	94.5	90.3	91.3	91.0	91.0
Cu...Cu distance [Å]					
	3.572	3.567	3.564	3.673	3.571

* Always runs into singlet.

Coordinates of the compounds of the minimum paths

Table S16: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), Oxo

Cu	1.42995400	0.05498700	-0.25030700
Cu	-1.42061900	0.04410200	0.22567600
O	0.01272000	-0.98475600	0.01262600
O	-0.00553200	1.15116100	-0.05331100
N	4.18806100	0.76269700	-0.17709300
N	2.97963600	1.25330700	-0.60688500
N	3.74711900	-1.56329200	0.03423400
N	2.58645300	-1.46942300	-0.67853400
N	-2.55307400	-1.48916800	0.68954300
N	-3.70480100	-1.61445900	-0.03297900
N	-2.98975800	1.22545800	0.59298300
N	-4.19113000	0.70252000	0.17900000
C	4.29734700	-0.38915500	0.70780300
C	3.27272700	2.36410000	-1.32981300
C	4.66837900	2.56959900	-1.33264100
C	5.21319400	1.54371400	-0.59753200
C	2.23972900	3.25963100	-1.98291500
C	2.49734800	-2.60476400	-1.41738800
C	3.61046500	-3.42426400	-1.12491000
C	4.38635000	-2.72993300	-0.22598700
C	1.43787100	-2.89888300	-2.46852300
C	-4.28362500	-0.45159400	-0.70393700
C	-5.23266900	1.44466400	0.62820600
C	-4.70704800	2.47906500	1.36406700
C	-3.30498400	2.31955500	1.33318400
C	-2.30031800	3.26501200	1.96278500
C	-4.31775000	-2.79513500	0.22696200
C	-3.53279400	-3.46697900	1.13520300
C	-2.44292800	-2.61924700	1.43406900
C	-1.39233000	-2.87663000	2.50361200
H	5.36540800	-0.58074400	0.81386500
H	5.20481200	3.36668300	-1.82198400
H	3.83547300	-4.38881300	-1.55174500
H	-5.34844400	-0.66418600	-0.80215800
H	-5.26005900	3.25330500	1.87112800
H	-3.73810600	-4.43459600	1.56492200
C	3.70360000	-0.11623300	2.07535500
C	4.50578200	-0.13489600	3.21519100
N	2.39690000	0.18293700	2.08056400
C	3.91680400	0.18713600	4.44111300
H	5.56040600	-0.38682900	3.15299500
C	1.84765900	0.50413700	3.26130000
C	2.56420200	0.52082700	4.46105400
H	4.50550000	0.18525800	5.35285000
H	0.79692500	0.76357700	3.24132600
H	2.06649500	0.79324900	5.38562400
C	-3.70526100	-0.16874800	-2.07533700
C	-4.51700100	-0.18807700	-3.20825000
N	-2.40104900	0.14040100	-2.08980800
C	-3.94070700	0.14373100	-4.43756500
H	-5.56916700	-0.44804600	-3.13820700
C	-1.86413800	0.47104900	-3.27359400
C	-2.59077300	0.48732500	-4.46722800
H	-4.53686500	0.14132200	-5.34443800
H	-0.81567300	0.73927800	-3.26075000
H	-2.10265000	0.76681300	-5.39478800
H	6.23517800	1.30841700	-0.33673500
H	5.33624400	-2.96120000	0.23460500
H	-5.25842200	-3.05070800	-0.23967500
H	-6.25144300	1.17960600	0.38388300
C	-0.13237800	-3.54045800	1.90414800

H	0.56051800	-3.79229700	2.71522600
H	-0.38708300	-4.46631100	1.37752000
H	0.36792400	-2.86174500	1.20888900
C	-1.01498000	-1.55476100	3.19397900
H	-0.55517600	-0.86825100	2.47881500
H	-1.89176500	-1.07368600	3.64192200
H	-0.28811900	-1.75219300	3.98902100
C	-1.99162400	-3.83067600	3.56225300
H	-2.18637400	-4.82644400	3.15068600
H	-1.27202600	-3.95230200	4.37822100
H	-2.92209800	-3.43721900	3.98539700
C	0.21969800	-3.61363200	-1.84184500
H	-0.48219300	-3.88990900	-2.63701700
H	0.52349100	-4.53004900	-1.32483800
H	-0.28979100	-2.95696600	-1.13256700
C	0.99009400	-1.59451300	-3.14984200
H	0.50281200	-0.93363800	-2.42874600
H	1.83726400	-1.06999900	-3.60595500
H	0.26566600	-1.82555300	-3.93801400
C	2.05423400	-3.82678300	-3.54076800
H	2.29922600	-4.81382200	-3.13522300
H	1.32350300	-3.97803400	-4.34176200
H	2.95848300	-3.39455400	-3.98255200
C	1.48028500	4.00864500	-0.86535000
H	2.16594100	4.62357000	-0.27225900
H	0.72686500	4.66846800	-1.30929600
H	0.97748000	3.30079900	-0.19973800
C	1.26301500	2.42022300	-2.82551000
H	1.78940400	1.88197100	-3.62198200
H	0.73620100	1.70534400	-2.18756200
H	0.51843900	3.07850500	-3.28652800
C	2.93631200	4.28711900	-2.89716900
H	2.17598500	4.91141400	-3.37694400
H	3.59746800	4.95330400	-2.33266900
H	3.51862900	3.79973300	-3.68713400
C	-1.17595000	2.48859600	2.66906400
H	-1.58213500	1.83958700	3.45421700
H	-0.61096800	1.88932200	1.94959600
H	-0.48344400	3.19751600	3.13634300
C	-1.72110200	4.15049000	0.83454700
H	-2.51032500	4.74943500	0.36743100
H	-0.97284700	4.83558500	1.24809400
H	-1.24712900	3.53730300	0.06380600
C	-3.00630900	4.16670800	2.99641800
H	-2.26484300	4.82469700	3.46057700
H	-3.76292400	4.80723900	2.53140000
H	-3.48092700	3.57936000	3.79022500

Table S17: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), Peroxo

Cu	1.76443700	0.04678100	-0.01828100
Cu	-1.79373000	0.06484200	0.06388600
O	-0.01248600	-0.59015600	0.15281100
O	-0.02031000	0.85017400	-0.04149600
N	4.44330300	0.88773200	0.23745200
N	3.29671700	1.26096400	-0.40936400
N	4.09325100	-1.45650600	0.51921500
N	2.96789300	-1.53822700	-0.25488900
N	-3.02828200	-1.39983900	0.61800800
N	-4.17204600	-1.45575100	-0.12907600
N	-3.29537300	1.37030700	0.07674800
N	-4.43705300	0.88694600	-0.50025100
C	4.43405800	-0.20955000	1.19750600
C	3.64708100	2.28488300	-1.21813500
C	5.02615900	2.55408300	-1.07248900
C	5.49905700	1.64987500	-0.14830000
C	2.64832800	3.03403800	-2.07874200
C	3.07803800	-2.70091500	-0.94047000
C	4.27153300	-3.35789600	-0.56612000
C	4.89799400	-2.53500300	0.34130400
C	2.10577700	-3.14653000	-2.02100200
C	-4.45388100	-0.42949400	-1.12651700
C	-5.47180400	1.75310900	-0.35167200
C	-4.98859000	2.84206600	0.33897100
C	-3.62703300	2.57201100	0.59900100
C	-2.62767800	3.46629600	1.30629000
C	-5.00704100	-2.42987500	0.31479500
C	-4.38157800	-3.04082600	1.37759900
C	-3.15251300	-2.36692100	1.55556200
C	-2.11749800	-2.63263000	2.63441500
H	5.46319900	-0.32534200	1.53690200
H	5.60027600	3.31096100	-1.58346700
H	4.63414000	-4.30629600	-0.92942500
H	-5.48057500	-0.59813600	-1.45094800
H	-5.54556500	3.71993700	0.62641700
H	-4.76700900	-3.85983200	1.96426700
C	3.54806500	0.09762700	2.39229600
C	4.07725900	0.19469800	3.67712700
N	2.25137700	0.30475700	2.10816700
C	3.21563800	0.53395400	4.72440700
H	5.13253300	0.01637700	3.85987300
C	1.43468700	0.64208300	3.11732000
C	1.87201700	0.76929800	4.43664300
H	3.59155900	0.62026600	5.73881500
H	0.40303300	0.82361600	2.84458300
H	1.17149600	1.04972700	5.21582900
C	-3.53056600	-0.49921900	-2.33129800
C	-4.03141600	-0.72941100	-3.61059100
N	-2.22662800	-0.30439500	-2.07163800
C	-3.13154300	-0.75415700	-4.67991900
H	-5.09380400	-0.88268500	-3.77387400
C	-1.37115700	-0.32604000	-3.10442500
C	-1.77757300	-0.54537200	-4.42165900
H	-3.48515100	-0.92884700	-5.69098100
H	-0.33080900	-0.15729400	-2.85578900

H	-1.04602200	-0.54855600	-5.22250100
H	6.48506200	1.49034000	0.26420900
H	5.83699400	-2.62630800	0.86839700
H	-5.96370700	-2.60541900	-0.15622700
H	-6.45167000	1.52831000	-0.74803500
C	-0.89649800	-3.35851400	2.02737400
H	-0.18430900	-3.60402900	2.82345300
H	-1.19649600	-4.29230700	1.54006400
H	-0.38868300	-2.72730900	1.29387900
C	-1.67444400	-1.29557600	3.25874700
H	-1.24229600	-0.64271100	2.49355000
H	-2.51725100	-0.77563900	3.72696700
H	-0.91143300	-1.47746700	4.02333400
C	-2.73354900	-3.52224800	3.73248600
H	-2.99816600	-4.51349800	3.34894200
H	-2.00100400	-3.66629400	4.53315000
H	-3.62762300	-3.06575000	4.17102900
C	0.70108300	-3.40565900	-1.44047400
H	0.04091900	-3.76977900	-2.23609000
H	0.73782200	-4.16952700	-0.65680100
H	0.26522400	-2.49490100	-1.02277700
C	2.04518900	-2.04805000	-3.10579800
H	1.72187700	-1.09066400	-2.68242500
H	3.02618300	-1.89732800	-3.56897400
H	1.33778300	-2.33942200	-3.89025600
C	2.61592400	-4.44922700	-2.66964900
H	2.66271500	-5.26959700	-1.94511700
H	1.92635200	-4.74910400	-3.46514000
H	3.60643900	-4.31975100	-3.11920300
C	1.82593100	3.96621400	-1.15819000
H	2.47458100	4.69522500	-0.66102900
H	1.08674300	4.51630800	-1.75108200
H	1.29852300	3.39316700	-0.38906400
C	1.71442500	2.03992400	-2.79331100
H	2.27711700	1.38991400	-3.47275200
H	1.18620700	1.41869200	-2.06242500
H	0.96541600	2.58538800	-3.37737600
C	3.38787700	3.88244600	-3.13074800
H	2.65584000	4.39250500	-3.76502500
H	4.00973100	4.65361100	-2.66369100
H	4.02200000	3.26431000	-3.77565500
C	-1.83685100	2.64865900	2.34611200
H	-2.50017100	2.23869000	3.11563800
H	-1.30763500	1.82198200	1.86059600
H	-1.09373400	3.28903600	2.83358400
C	-1.66449800	4.05439000	0.24992200
H	-2.21066300	4.65404500	-0.48591600
H	-0.92826200	4.70193700	0.73889700
H	-1.13045800	3.26003100	-0.28053000
C	-3.36224600	4.61683900	2.02025100
H	-2.63327000	5.23962000	2.54844500
H	-3.89089900	5.26175500	1.31003300
H	-4.08231700	4.24266400	2.75632400

Table S18: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 2.277 Å

Cu	1.37858000	0.04124600	-0.28131900
Cu	-1.37476500	0.04740800	0.26167700
O	0.00479700	-1.06371600	0.01774700
O	-0.00295700	1.21248500	-0.05091400
N	4.13794000	0.72968400	-0.26493600
N	2.92473800	1.22704000	-0.67609700
N	3.67530700	-1.58145400	0.03135400
N	2.52478100	-1.48253600	-0.69697300
N	-2.50897400	-1.46380300	0.75519000
N	-3.65871900	-1.60327200	0.03237000
N	-2.92904800	1.23959800	0.62549600
N	-4.13909600	0.71381700	0.23914600
C	4.26099100	-0.39410700	0.65250200
C	3.21489200	2.31413900	-1.43752100
C	4.61298300	2.49741200	-1.48097200
C	5.16205800	1.48429900	-0.73251400
C	2.18687200	3.22066200	-2.08391600
C	2.40663500	-2.64246100	-1.39259000
C	3.49283500	-3.48124800	-1.05755000
C	4.28128600	-2.77545300	-0.17850400
C	1.35294800	-2.94579700	-2.44660400
C	-4.25596000	-0.44581600	-0.63305500
C	-5.17025500	1.46636900	0.69398600
C	-4.62987300	2.50903700	1.40653900
C	-3.22911100	2.34552100	1.35617900
C	-2.21658400	3.30009300	1.95809300
C	-4.25534800	-2.79183800	0.29378900
C	-3.46084000	-3.45321800	1.20146600
C	-2.38137100	-2.59218400	1.49961200
C	-1.32677400	-2.84041800	2.56676600
H	5.32989800	-0.59550900	0.72872900
H	5.14776200	3.27316800	-2.00494900
H	3.69426100	-4.46661400	-1.44716300
H	-5.32346700	-0.65828000	-0.69756800
H	-5.17216500	3.29210700	1.91144200
H	-3.65389900	-4.42265400	1.63285600
C	3.71944200	-0.07284400	2.03089600
C	4.56841000	-0.05087500	3.13648100
N	2.41344900	0.22486700	2.07819100
C	4.03014900	0.31262400	4.37391900
H	5.62026800	-0.30362500	3.03941000
C	1.91318600	0.58450600	3.26974100
C	2.67840400	0.64362700	4.43794000
H	4.65589000	0.34293400	5.26012600
H	0.86147800	0.84035800	3.28617400
H	2.21766900	0.94557400	5.37246600
C	-3.72153300	-0.17711700	-2.02489400
C	-4.57429000	-0.20293800	-3.12739200
N	-2.41670400	0.12239000	-2.08866100
C	-4.04106400	0.10994800	-4.38068400
H	-5.62509500	-0.45420500	-3.01614200
C	-1.92135600	0.43354900	-3.29581900
C	-2.69032300	0.44116500	-4.46298100
H	-4.66970400	0.10160400	-5.26531300
H	-0.87074000	0.69210200	-3.32617100

H	-2.23325700	0.70443100	-5.41089800
H	6.18696900	1.24210800	-0.49014500
H	5.22197600	-3.01502700	0.29654800
H	-5.19423800	-3.05884600	-0.17003200
H	-6.19356400	1.20207000	0.46853500
C	-0.10392400	-3.57750200	1.97542900
H	0.59423700	-3.82084500	2.78450100
H	-0.40357700	-4.51458800	1.49420600
H	0.40660500	-2.94812600	1.24253100
C	-0.88635200	-1.51020400	3.19966300
H	-0.40274600	-0.87469200	2.45413700
H	-1.73661300	-0.97451500	3.63693900
H	-0.16101400	-1.70837200	3.99582800
C	-1.94862300	-3.72683000	3.67139300
H	-2.18883200	-4.73017200	3.30503200
H	-1.22241300	-3.84357100	4.48223500
H	-2.85681400	-3.27957000	4.08949100
C	0.14254600	-3.67598300	-1.82205200
H	-0.55604900	-3.95775700	-2.61814500
H	0.45672400	-4.59058200	-1.30796800
H	-0.37276800	-3.02652100	-1.11039900
C	0.89165700	-1.64848900	-3.13088200
H	0.39326800	-0.99383800	-2.41206900
H	1.73385700	-1.11468900	-3.58579600
H	0.17310500	-1.89021600	-3.92112400
C	1.98547800	-3.86662900	-3.51658300
H	2.24197300	-4.85045500	-3.11057000
H	1.25941500	-4.02714400	-4.32005300
H	2.88578800	-3.42277400	-3.95478800
C	1.50546600	4.03561300	-0.96149600
H	2.23725800	4.65202300	-0.42797000
H	0.74985500	4.70052200	-1.39402100
H	1.01810200	3.36815600	-0.24533900
C	1.14474700	2.39410400	-2.85685600
H	1.62016700	1.79930000	-3.64560900
H	0.60355100	1.73632900	-2.17163500
H	0.41915500	3.06878700	-3.32458300
C	2.88156900	4.19065000	-3.06095000
H	2.12303100	4.82134900	-3.53514000
H	3.58305300	4.85570900	-2.54611000
H	3.41844100	3.65677600	-3.85298100
C	-1.09347400	2.53526800	2.67856400
H	-1.50015600	1.90791500	3.48099300
H	-0.53547000	1.91731900	1.96991100
H	-0.39593700	3.25198900	3.12594500
C	-1.64030200	4.15400400	0.80469800
H	-2.42915900	4.74779300	0.33020700
H	-0.88351400	4.84303500	1.19564000
H	-1.17782300	3.51768800	0.04603800
C	-2.91289800	4.23097200	2.97238000
H	-2.16522400	4.89622100	3.41568800
H	-3.66843900	4.86403900	2.49546800
H	-3.38597200	3.66667500	3.78369100

Table S19: XYZ coordinates for optimised structure: Singlet minimum path, TPSSH/6-31g(d), O...O = 2.145 Å

Cu	1.42527700	0.04677200	-0.25462200
Cu	-1.41898200	0.05087500	0.22743500
O	0.00696400	-0.98943800	0.01946400
O	-0.00265200	1.15383500	-0.06530800
N	4.18514700	0.74968000	-0.20283500
N	2.97630500	1.23533600	-0.63696500
N	3.73728500	-1.56887000	0.06781000
N	2.57932600	-1.48693800	-0.65101400
N	-2.55184500	-1.47091400	0.72563100
N	-3.70485100	-1.61187600	0.00837600
N	-2.98642200	1.24016300	0.57223900
N	-4.18867500	0.70924900	0.17080200
C	4.29431200	-0.38004000	0.70991600
C	3.26973900	2.32846100	-1.38635700
C	4.66615700	2.52824800	-1.40118100
C	5.21100300	1.51715300	-0.64595000
C	2.23713500	3.21484400	-2.05258800
C	2.48664900	-2.63967800	-1.36188400
C	3.59453600	-3.45735600	-1.04548100
C	4.37124400	-2.74483100	-0.16164500
C	1.42980000	-2.95331800	-2.41005300
C	-4.28368100	-0.46354800	-0.68697200
C	-5.22906600	1.46200500	0.60466400
C	-4.70191200	2.51191000	1.31714800
C	-3.30006800	2.35063600	1.28831500
C	-2.29347200	3.30854900	1.89503100
C	-4.31719100	-2.78667100	0.29520100
C	-3.53018100	-3.43860200	1.21613600
C	-2.43974000	-2.58455300	1.49417300
C	-1.38572100	-2.81970200	2.56526400
H	5.36218500	-0.57255600	0.81627500
H	5.20293500	3.31214300	-1.91100600
H	3.81589500	-4.43315400	-1.44799500
H	-5.34888000	-0.67713000	-0.77875000
H	-5.25372400	3.29763000	1.80757300
H	-3.73426000	-4.39673500	1.66709700
C	3.70747800	-0.06979300	2.07254800
C	4.51606900	-0.05487300	3.20790000
N	2.40063100	0.22872600	2.07626800
C	3.93383100	0.30278000	4.42717300
H	5.57049700	-0.30803100	3.14717900
C	1.85790500	0.58409800	3.25021600
C	2.58121600	0.63645300	4.44489700
H	4.52762700	0.32775800	5.33525700
H	0.80687600	0.84231200	3.22869200
H	2.08852200	0.93560300	5.36387700
C	-3.70768300	-0.21234100	-2.06548200
C	-4.52169600	-0.25975600	-3.19595200
N	-2.40350500	0.09652700	-2.09016700
C	-3.94794400	0.04113600	-4.43432600
H	-5.57369700	-0.51794200	-3.11732700
C	-1.86905200	0.39737200	-3.28301800
C	-2.59801800	0.38357900	-4.47531000
H	-4.54594900	0.01610800	-5.33964000
H	-0.82054400	0.66583700	-3.27924400

H	-2.11168900	0.63955200	-5.41056400
H	6.23340600	1.28398900	-0.38488900
H	5.31883100	-2.96919700	0.30706100
H	-5.25876300	-3.05238300	-0.16387200
H	-6.24829200	1.19262200	0.36705500
C	-0.13611400	-3.51239300	1.97682700
H	0.56036500	-3.74727800	2.78988200
H	-0.40298200	-4.45061400	1.47887000
H	0.36505500	-2.85846300	1.25893800
C	-0.99056300	-1.48297900	3.21550300
H	-0.52596000	-0.82267800	2.47914400
H	-1.85958500	-0.97943400	3.65374600
H	-0.26216500	-1.66590400	4.01260200
C	-1.98740400	-3.73709100	3.65476900
H	-2.19403100	-4.74264900	3.27395100
H	-1.26379600	-3.84165200	4.46956200
H	-2.91158700	-3.32284300	4.07187600
C	0.20664100	-3.64986100	-1.77250400
H	-0.49437300	-3.93848200	-2.56405300
H	0.50489400	-4.55733200	-1.23679100
H	-0.30173800	-2.97723200	-1.07745200
C	0.99050600	-1.66255600	-3.12207300
H	0.50467900	-0.98294700	-2.41764800
H	1.84192400	-1.15295200	-3.58716600
H	0.26730500	-1.90775000	-3.90706800
C	2.04689600	-3.90703800	-3.45901200
H	2.28693300	-4.88569900	-3.03079500
H	1.31870200	-4.07337300	-4.25932700
H	2.95429800	-3.48766800	-3.90664200
C	1.48941600	3.99206200	-0.94638300
H	2.18237300	4.61619100	-0.37170800
H	0.73622900	4.64591700	-1.39946100
H	0.98790400	3.30140200	-0.26206900
C	1.25020500	2.36310600	-2.87061100
H	1.76869400	1.80454100	-3.65831200
H	0.72269000	1.66583600	-2.21407800
H	0.50697400	3.01582800	-3.34161800
C	2.93317000	4.21870300	-2.99318800
H	2.17273400	4.83564900	-3.48224600
H	3.60029000	4.89409100	-2.44694400
H	3.50907600	3.71168500	-3.77543300
C	-1.17494600	2.54604600	2.62528200
H	-1.58648200	1.92290700	3.42836300
H	-0.61349000	1.92225200	1.92411600
H	-0.47827500	3.26370400	3.07245700
C	-1.70761100	4.16030600	0.74462500
H	-2.49306500	4.74952300	0.25904600
H	-0.95735300	4.85340700	1.14093600
H	-1.23420800	3.52401100	-0.00758200
C	-2.99842000	4.24104500	2.90162600
H	-2.25556400	4.90850900	3.34977400
H	-3.75110000	4.87173300	2.41708300
H	-3.47768200	3.67773700	3.70993700

Table S20: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 2.013 Å

Cu	1.47921000	0.05504100	-0.21169000
Cu	-1.47464300	0.05573500	0.18948000
O	0.00516900	-0.91191600	0.01301100
O	-0.00134600	1.09999800	-0.05078100
N	4.23993700	0.76126700	-0.11358600
N	3.03991700	1.24720800	-0.56826800
N	3.79817200	-1.56569200	0.10179900
N	2.63718300	-1.48933000	-0.61325000
N	-2.61293800	-1.48126100	0.67329800
N	-3.76987800	-1.60654600	-0.04116100
N	-3.05138200	1.24476300	0.51767300
N	-4.24493000	0.72016700	0.08693100
C	4.32542400	-0.38505100	0.78137500
C	3.34541100	2.34676800	-1.30103700
C	4.74156200	2.54995000	-1.28836100
C	5.27376400	1.53300100	-0.53104900
C	2.31644900	3.23168400	-1.97501400
C	2.57124500	-2.62575400	-1.35259300
C	3.69655100	-3.42776800	-1.05846000
C	4.45827000	-2.72118800	-0.15694500
C	1.51824100	-2.93153200	-2.40703900
C	-4.31598100	-0.46008800	-0.76358200
C	-5.29276200	1.47762900	0.49517000
C	-4.77760700	2.52643800	1.21908100
C	-3.37629900	2.35710200	1.22320100
C	-2.37062600	3.30137900	1.85209500
C	-4.41080500	-2.76211700	0.26160200
C	-3.63969100	-3.41903800	1.19228600
C	-2.52954800	-2.58638600	1.45727900
C	-1.47745400	-2.83017300	2.52857100
H	5.38968900	-0.57365300	0.92360800
H	5.28668600	3.33943500	-1.78059700
H	3.93753100	-4.38888100	-1.48426200
H	-5.37782600	-0.66879700	-0.89542100
H	-5.33714000	3.31574100	1.69503400
H	-3.86529700	-4.36649100	1.65531100
C	3.68483800	-0.10141600	2.12571000
C	4.44460400	-0.10381600	3.29412400
N	2.37765100	0.19382100	2.08154500
C	3.81040100	0.23181100	4.49370600
H	5.50137500	-0.35332800	3.27324900
C	1.78450900	0.52904200	3.23673800
C	2.45728300	0.56296900	4.46087400
H	4.36574300	0.24283900	5.42606200
H	0.73495800	0.78614500	3.17390600
H	1.92637300	0.84642900	5.36338000
C	-3.68256200	-0.22080000	-2.11923200
C	-4.44436200	-0.27604300	-3.28493200
N	-2.37835600	0.08869100	-2.08922300
C	-3.81542000	0.01843700	-4.49799200
H	-5.49858200	-0.53476100	-3.25204200
C	-1.79033200	0.38412400	-3.25776200
C	-2.46543000	0.36329900	-4.48087600
H	-4.37229800	-0.01240700	-5.42898600
H	-0.74371100	0.65470200	-3.20653200

H	-1.93870700	0.61590400	-5.39491800
H	6.29149500	1.29850100	-0.25345600
H	5.40966400	-2.93767100	0.30773600
H	-5.35696500	-3.01322500	-0.19624900
H	-6.30737100	1.21188600	0.23479400
C	-0.20631300	-3.47388800	1.93156600
H	0.48930800	-3.71527400	2.74351500
H	-0.44549800	-4.40330900	1.40399700
H	0.28655900	-2.78830200	1.23766700
C	-1.12194700	-1.50063200	3.21707100
H	-0.67617200	-0.80606200	2.50047800
H	-2.00646400	-1.03375600	3.66449700
H	-0.39063600	-1.68351300	4.01161800
C	-2.06116000	-3.79252500	3.58741500
H	-2.24172900	-4.79076300	3.17510200
H	-1.33937600	-3.90401200	4.40288200
H	-2.99675500	-3.41279100	4.01184900
C	0.26322500	-3.57359400	-1.77518700
H	-0.43455300	-3.85637900	-2.57179200
H	0.52262500	-4.47849800	-1.21552300
H	-0.23574500	-2.87096800	-1.10315900
C	1.13361200	-1.63805400	-3.14703300
H	0.67667000	-0.92359600	-2.45744900
H	2.00681100	-1.17233500	-3.61731100
H	0.40273900	-1.86752700	-3.92976200
C	2.11400600	-3.92512500	-3.42951700
H	2.31772700	-4.90170600	-2.97801300
H	1.38915800	-4.08449000	-4.23422600
H	3.03876700	-3.54444400	-3.87622900
C	1.54023000	3.98913100	-0.87462700
H	2.21595600	4.61316700	-0.27978000
H	0.78905300	4.64071900	-1.33422500
H	1.03190700	3.28781100	-0.20599300
C	1.35219000	2.37812500	-2.81849900
H	1.88850300	1.83591400	-3.60545000
H	0.82566400	1.66354200	-2.17957900
H	0.60611000	3.02629700	-3.29119000
C	3.01866900	4.25186100	-2.89266800
H	2.26201000	4.86923000	-3.38708300
H	3.67244700	4.92516400	-2.32801100
H	3.61071500	3.75765400	-3.67103000
C	-1.29097800	2.51874400	2.61911500
H	-1.73768200	1.91263100	3.41602500
H	-0.72937300	1.87320200	1.93774100
H	-0.58634800	3.22213500	3.07637200
C	-1.72897000	4.13146800	0.71588600
H	-2.48635400	4.72279200	0.19004800
H	-0.98734400	4.82126700	1.13355800
H	-1.23140400	3.48023300	-0.00808400
C	-3.08641600	4.25520100	2.82999900
H	-2.34511900	4.91245500	3.29554400
H	-3.81252300	4.89535000	2.31789800
H	-3.60084200	3.70795600	3.62762800

Table S21: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 1.881 Å

Cu	-1.54565000	0.05689900	0.14820000
Cu	1.54569500	0.05680600	-0.14843700
O	0.00002400	-0.83978900	0.00009900
O	0.00005600	1.04139400	-0.00050300
N	-4.30372900	0.76776700	-0.01469700
N	-3.11692000	1.26104400	0.46319400
N	-3.87047500	-1.56944700	-0.13055800
N	-2.71049700	-1.49064900	0.58699700
N	2.71062400	-1.49089000	-0.58632600
N	3.87056700	-1.56928800	0.13132000
N	3.11684900	1.26093300	-0.46384100
N	4.30373000	0.76786400	0.01408100
C	-4.35832500	-0.40959500	-0.87099100
C	-3.44201900	2.37000100	1.17084200
C	-4.83836700	2.57012400	1.12336000
C	-5.35041500	1.54051900	0.36864500
C	-2.42594900	3.26871900	1.84707900
C	-2.68217300	-2.59424800	1.37574800
C	-3.82810000	-3.37818500	1.11392800
C	-4.56527300	-2.69278600	0.17648500
C	-1.63590700	-2.88066700	2.44173300
C	4.35843600	-0.40899500	0.87105000
C	5.35034200	1.54051700	-0.36965800
C	4.83817300	2.56981500	-1.12471700
C	3.44183200	2.36962900	-1.17195600
C	2.42560900	3.26796000	-1.84847100
C	4.56523700	-2.69293800	-0.17485700
C	3.82802700	-3.37893100	-1.11184300
C	2.68220300	-2.59505200	-1.37428300
C	1.63600300	-2.88204500	-2.44018000
H	-5.41584700	-0.59691800	-1.05727500
H	-5.39701800	3.36561500	1.59028600
H	-4.09564400	-4.31359300	1.57923200
H	5.41597900	-0.59617300	1.05736500
H	5.39673800	3.36516000	-1.59199700
H	4.09551100	-4.31468600	-1.57648600
C	-3.65143700	-0.17734900	-2.19192600
C	-4.35073000	-0.21278900	-3.39660100
N	-2.34418200	0.10772100	-2.09443200
C	-3.65355400	0.07578300	-4.57323200
H	-5.40975600	-0.45187900	-3.42055500
C	-1.68935400	0.39740700	-3.22835600
C	-2.30005600	0.39550700	-4.48464000
H	-4.16179100	0.05990600	-5.53200700
H	-0.64211300	0.64730500	-3.11886300
H	-1.72234400	0.64306300	-5.36874200
C	3.65161000	-0.17602500	2.19189200
C	4.35099600	-0.21063700	3.39653700
N	2.34430900	0.10881900	2.09431600
C	3.65386700	0.07855000	4.57304400
H	5.41005700	-0.44956900	3.42056000
C	1.68953000	0.39910700	3.22811400
C	2.30032000	0.39803700	4.48435800
H	4.16217600	0.06331500	5.53179100
H	0.64224700	0.64880500	3.11855300

H	1.72264000	0.64604100	5.36835400
H	-6.36095700	1.29811200	0.07222800
H	-5.51875200	-2.90497700	-0.28589500
H	5.51868400	-2.90489200	0.28769700
H	6.36092600	1.29826800	-0.07325400
C	0.35943900	-3.49220500	-1.82147800
H	-0.33686500	-3.76115800	-2.62417200
H	0.59088200	-4.40072400	-1.25555100
H	-0.13256800	-2.77687700	-1.15742700
C	1.29082600	-1.57781400	-3.18207700
H	0.85735400	-0.84855200	-2.49221700
H	2.17850700	-1.13827600	-3.65008500
H	0.55413500	-1.78427000	-3.96591200
C	2.21722100	-3.88965900	-3.45575200
H	2.39923600	-4.86824200	-2.99908200
H	1.49458600	-4.03744200	-4.26463000
H	3.15179100	-3.52861400	-3.89843300
C	-0.35937500	-3.49112700	1.82326700
H	0.33698800	-3.75965600	2.62605000
H	-0.59084800	-4.39994700	1.25783400
H	0.13257200	-2.77614600	1.15880200
C	-1.29072300	-1.57603100	3.18291600
H	-0.85728800	-0.84712900	2.49265100
H	-2.17840000	-1.13625500	3.65070900
H	-0.55400800	-1.78204900	3.96684400
C	-2.21703000	-3.88775700	3.45787700
H	-2.39905600	-4.86658200	3.00172700
H	-1.49433600	-4.03510500	4.26678100
H	-3.15157400	-3.52650300	3.90044100
C	-1.66472200	4.04277400	0.74682000
H	-2.35163600	4.65999800	0.15793900
H	-0.91993000	4.70255700	1.20520200
H	-1.15011600	3.35368000	0.07052100
C	-1.44445700	2.42963000	2.68496000
H	-1.96976200	1.87622900	3.47159900
H	-0.90638900	1.72431200	2.04484100
H	-0.70822500	3.08886900	3.15778300
C	-3.14266100	4.27420400	2.76963000
H	-2.39567500	4.89953300	3.26886200
H	-3.80494800	4.94169400	2.20803600
H	-3.72955900	3.76718700	3.54354900
C	1.44462500	2.42840100	-2.68649500
H	1.97029500	1.87513700	-3.47298300
H	0.90675500	1.72291900	-2.04639100
H	0.70820300	3.08729200	-3.15950800
C	1.66383200	4.04183000	-0.74848100
H	2.35036300	4.65941200	-0.15952600
H	0.91887200	4.70124500	-1.20711700
H	1.14935200	3.35261100	-0.07220600
C	3.14217500	4.27361700	-2.77094100
H	2.39509400	4.89873100	-3.27029700
H	3.80420800	4.94128400	-2.20925600
H	3.72930900	3.76673800	-3.54477200

Table S22: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 1.749 Å

Cu	-1.62703900	0.05717200	0.10661000
Cu	1.62713600	0.05727800	-0.10688000
O	0.00014600	-0.76660300	-0.00012200
O	0.00004000	0.98324700	-0.00059500
N	-4.36777900	0.79158500	-0.11478700
N	-3.19209100	1.27497200	0.39542500
N	-3.95626800	-1.55431300	-0.18167500
N	-2.79805400	-1.49648800	0.54139400
N	2.79839200	-1.49635700	-0.54141000
N	3.95649900	-1.55395300	0.18180200
N	3.19204500	1.27521900	-0.39571200
N	4.36787400	0.79190100	0.11420600
C	-4.39890100	-0.39851600	-0.95506300
C	-3.52523000	2.38892300	1.08808800
C	-4.91804100	2.60302600	1.00145700
C	-5.41883800	1.57458100	0.23653100
C	-2.51055700	3.27288000	1.78613900
C	-2.80972300	-2.58474900	1.34930900
C	-3.97837300	-3.33850100	1.09844700
C	-4.68861800	-2.64919100	0.14308600
C	-1.76842700	-2.88003000	2.41713100
C	4.39917000	-0.39794300	0.95482300
C	5.41886200	1.57471800	-0.23770300
C	4.91785700	2.60299400	-1.00273700
C	3.52501200	2.38896100	-1.08881000
C	2.51006900	3.27264700	-1.78680500
C	4.68823300	-2.64965800	-0.14147200
C	3.97771600	-3.33969700	-1.09612800
C	2.80955500	-2.58557100	-1.34806600
C	1.76840700	-2.88126900	-2.41593500
H	-5.44871000	-0.57742200	-1.18710800
H	-5.48218100	3.40594600	1.44891700
H	-4.27534600	-4.25764500	1.57820100
H	5.44901600	-0.57672400	1.18680300
H	5.48188200	3.40578100	-1.45058000
H	4.27431400	-4.25949700	-1.57486100
C	-3.63043900	-0.19235800	-2.24694000
C	-4.27416000	-0.23891300	-3.48158600
N	-2.32434800	0.07997900	-2.09808000
C	-3.52153100	0.02247900	-4.62999000
H	-5.33378700	-0.46614400	-3.54997400
C	-1.61478500	0.34299200	-3.20544200
C	-2.16918000	0.32754200	-4.48717600
H	-3.98702600	-0.00304500	-5.61003600
H	-0.57055500	0.58205700	-3.05065000
H	-1.55017200	0.55353400	-5.34880200
C	3.63080700	-0.19141600	2.24670600
C	4.27471300	-0.23721900	3.48128600
N	2.32462100	0.08048700	2.09789200
C	3.52217300	0.02449700	4.62967200
H	5.33441200	-0.46413000	3.54963400
C	1.61514100	0.34381400	3.20523700
C	2.16971700	0.32911300	4.48690200
H	3.98780800	-0.00044100	5.60966700
H	0.57081700	0.58249800	3.05049800

H	1.55076700	0.55533100	5.34851000
H	-6.42309200	1.33969600	-0.08612200
H	-5.64440500	-2.84207800	-0.32298100
H	5.64392700	-2.84245200	0.32482300
H	6.42320800	1.33988000	0.08469800
C	0.47885800	-3.45841900	-1.79346000
H	-0.21547600	-3.73753500	-2.59440100
H	0.69257400	-4.35515300	-1.20246900
H	-0.01143300	-2.72083900	-1.15255200
C	1.44637700	-1.58389200	-3.18164500
H	1.02753400	-0.83401100	-2.50397100
H	2.34204600	-1.16760300	-3.65531200
H	0.70637800	-1.78995100	-3.96259500
C	2.34043800	-3.91559100	-3.40814600
H	2.51389300	-4.88503800	-2.92891800
H	1.61799600	-4.07484900	-4.21496800
H	3.27862800	-3.57259700	-3.85755200
C	-0.47886800	-3.45712100	1.79461800
H	0.21568300	-3.73579200	2.59552400
H	-0.69252900	-4.35411600	1.20400800
H	0.01113000	-2.71967300	1.15333200
C	-1.44657300	-1.58237700	3.18243900
H	-1.02798100	-0.83257800	2.50451100
H	-2.34228600	-1.16613900	3.65606900
H	-0.70645100	-1.78804100	3.96337700
C	-2.34012200	-3.91417500	3.40971700
H	-2.51349000	-4.88378300	2.93078800
H	-1.61751800	-4.07307100	4.21646500
H	-3.27829000	-3.57121500	3.85920000
C	-1.70825500	4.03260800	0.70495200
H	-2.36928400	4.66052200	0.09810400
H	-0.96445200	4.68034000	1.18183000
H	-1.18739200	3.33622700	0.04055000
C	-1.56354200	2.41665300	2.64735900
H	-2.11494000	1.88209500	3.42889800
H	-1.03374600	1.69040300	2.02328800
H	-0.81827000	3.06038600	3.12720600
C	-3.23175800	4.29113900	2.69040900
H	-2.48768800	4.90634500	3.20635400
H	-3.87101400	4.96688600	2.11221000
H	-3.84423600	3.79383100	3.45063800
C	1.56388100	2.41608500	-2.64862000
H	2.11586600	1.88208000	-3.43011900
H	1.03440400	1.68931600	-2.02488100
H	0.81833000	3.05945500	-3.12852100
C	1.70693700	4.03150300	-0.70563900
H	2.36738400	4.65956700	-0.09831200
H	0.96294400	4.67898500	-1.18255700
H	1.18620600	3.33458300	-0.04168900
C	3.23095700	4.29165600	-2.69046000
H	2.48670800	4.90675400	-3.20627200
H	3.86980200	4.96742100	-2.11182000
H	3.84380900	3.79499800	-3.45081700

Table S23: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 1.618 Å

Cu	-1.70913800	0.05849200	0.07333000
Cu	1.70900400	0.05840300	-0.07339700
O	-0.00004400	-0.68919200	0.00026200
O	-0.00009000	0.92961900	0.00072500
N	-4.42139100	0.82345200	-0.21160900
N	-3.25679100	1.29405200	0.33178300
N	-4.03879100	-1.53076400	-0.23031500
N	-2.88673100	-1.49525100	0.50459300
N	2.88642700	-1.49556400	-0.50383800
N	4.03822300	-1.53117700	0.23145900
N	3.25693500	1.29359800	-0.33206800
N	4.42140800	0.82294900	0.21153800
C	-4.43474000	-0.37937300	-1.03436000
C	-3.59494200	2.41276500	1.01170000
C	-4.98255400	2.64316500	0.88577400
C	-5.47396300	1.61822700	0.10927700
C	-2.58311300	3.28234200	1.73223500
C	-2.93582500	-2.57506700	1.32061600
C	-4.12122000	-3.30115200	1.06650800
C	-4.80322700	-2.60333200	0.09653400
C	-1.90580400	-2.88320800	2.39507100
C	4.43442500	-0.37943500	1.03493300
C	5.47426500	1.61704000	-0.11012700
C	4.98316400	2.64158200	-0.88734200
C	3.59543500	2.41164200	-1.01290100
C	2.58385400	3.28124300	-1.73375600
C	4.80246200	-2.60406100	-0.09484600
C	4.12056200	-3.30198100	-1.06482100
C	2.93547300	-2.57561200	-1.31955800
C	1.90581000	-2.88367100	-2.39437900
H	-5.47617300	-0.54806800	-1.30792500
H	-5.54982500	3.45404800	1.31473000
H	-4.44520300	-4.20889300	1.55058400
H	5.47580100	-0.54824800	1.30864400
H	5.55071300	3.45191400	-1.31697000
H	4.44444000	-4.20996500	-1.54851400
C	-3.60988500	-0.20557500	-2.29712300
C	-4.20105500	-0.26480300	-3.55705000
N	-2.30485000	0.04451300	-2.10089500
C	-3.39522800	-0.04375000	-4.67754000
H	-5.26127700	-0.47207900	-3.66625400
C	-1.54243900	0.26675900	-3.18184400
C	-2.04306100	0.23433900	-4.48489800
H	-3.81991500	-0.08045800	-5.67559500
H	-0.50050100	0.48508400	-2.98538200
H	-1.38378300	0.42667300	-5.32451700
C	3.60952700	-0.20475000	2.29752900
C	4.20056000	-0.26341000	3.55754400
N	2.30459600	0.04560400	2.10101400
C	3.39467300	-0.04146000	4.67781700
H	5.26071300	-0.47091900	3.66698600
C	1.54214600	0.26877700	3.18173300
C	2.04262000	0.23696300	4.48486600
H	3.81924100	-0.07771700	5.67593900
H	0.50033100	0.48741400	2.98497400

H	1.38331700	0.43001400	5.32430100
H	-6.47157700	1.39374400	-0.24024000
H	-5.75769700	-2.77717800	-0.37959700
H	5.75670800	-2.77805800	0.38167900
H	6.47182600	1.39243400	0.23945900
C	0.59699200	-3.41771200	-1.77401800
H	-0.09053300	-3.71066300	-2.57589800
H	0.78624400	-4.29833300	-1.15137300
H	0.10792900	-2.65276800	-1.16544300
C	1.62102300	-1.59890400	-3.19709900
H	1.22663100	-0.81661500	-2.54073100
H	2.52895400	-1.22156900	-3.67972800
H	0.87629600	-1.80434700	-3.97381100
C	2.47065200	-3.95421400	-3.35045900
H	2.62711600	-4.91096900	-2.84060800
H	1.75323900	-4.12714700	-4.15889400
H	3.41712300	-3.63753500	-3.80189600
C	-0.59754800	-3.41809900	1.77425500
H	0.09024400	-3.71103900	2.57591000
H	-0.78749600	-4.29887500	1.15203800
H	-0.10845400	-2.65360200	1.16514900
C	-1.61994600	-1.59828200	3.19715300
H	-1.22536000	-0.81651600	2.54029000
H	-2.52745400	-1.22023900	3.68002600
H	-0.87499600	-1.80384800	3.97361600
C	-2.47071700	-3.95311200	3.35181600
H	-2.62790500	-4.90997900	2.84239400
H	-1.75301300	-4.12611700	4.15997900
H	-3.41682100	-3.63579700	3.80357800
C	-1.75050600	4.03709900	0.67004600
H	-2.39203700	4.67518700	0.05300900
H	-1.00915500	4.67444000	1.16452400
H	-1.22420200	3.33871500	0.01186700
C	-1.66204300	2.41081100	2.60703700
H	-2.23280800	1.88661700	3.38153200
H	-1.13692000	1.67312600	1.99198000
H	-0.91182200	3.04152500	3.09622900
C	-3.30938200	4.30511600	2.62693300
H	-2.56894800	4.91000500	3.16006000
H	-3.92981900	4.99008900	2.03913700
H	-3.94222200	3.81121800	3.37252200
C	1.66166600	2.40963500	-2.60728800
H	2.23162700	1.88436000	-3.38164900
H	1.13629300	1.67285900	-1.99135100
H	0.91164600	3.04048500	-3.09661700
C	1.75235100	4.03755300	-0.67178800
H	2.39468300	4.67558200	-0.05553300
H	1.01130400	4.67511800	-1.16643400
H	1.22578700	3.34009100	-0.01284600
C	3.31039800	4.30266700	-2.62978600
H	2.57011300	4.90746100	-3.16322900
H	3.93148400	4.98786900	-2.04294500
H	3.94266800	3.80763600	-3.37510500

Table S24: XYZ coordinates for optimised structure: Singlet minimum path, TPSSH/6-31g(d), O...O = 1.488 Å

Cu	1.75002700	0.03863100	-0.01992100
Cu	-1.78388300	0.07014900	0.05906100
O	-0.01947100	-0.62019200	0.09469200
O	-0.01588800	0.86578900	0.01376600
N	4.43844100	0.87505700	0.21398800
N	3.29205200	1.24087800	-0.43741400
N	4.07026600	-1.45907700	0.54844100
N	2.94760200	-1.54729400	-0.22921200
N	-3.02890800	-1.38083200	0.64853200
N	-4.18022100	-1.44211800	-0.08566500
N	-3.27561000	1.38168600	0.06392100
N	-4.42596100	0.89641500	-0.49495900
C	4.42441600	-0.19992200	1.19839400
C	3.64903400	2.23438300	-1.28053600
C	5.03254400	2.49141700	-1.15184700
C	5.50093200	1.61119000	-0.20293500
C	2.65611800	2.97497200	-2.15555800
C	3.04985100	-2.72578600	-0.88936400
C	4.23475100	-3.38567600	-0.49392900
C	4.86460800	-2.54914400	0.39843700
C	2.08130300	-3.18767600	-1.96660300
C	-4.46211700	-0.43096000	-1.09770700
C	-5.44994100	1.77757600	-0.36318400
C	-4.95191500	2.87741400	0.29900500
C	-3.59236200	2.59914300	0.55944200
C	-2.58353400	3.49683600	1.24871500
C	-5.01923000	-2.39988100	0.38596800
C	-4.38783700	-2.99495100	1.45426500
C	-3.15140000	-2.32790200	1.60625900
C	-2.10810900	-2.57896800	2.68061400
H	5.45420100	-0.31748100	1.53526400
H	5.61258900	3.22494100	-1.68942700
H	4.59051000	-4.34481000	-0.83500800
H	-5.49369500	-0.59426300	-1.40909600
H	-5.49804600	3.76780200	0.56805900
H	-4.77411600	-3.79868500	2.06115200
C	3.54746400	0.14196200	2.38983200
C	4.08627300	0.27339600	3.66762100
N	2.25023300	0.34739400	2.10782800
C	3.23368800	0.64746000	4.71043100
H	5.14197200	0.09528300	3.84817300
C	1.44274600	0.71967400	3.11218100
C	1.88969300	0.88250200	4.42444900
H	3.61685200	0.76086000	5.71945300
H	0.41081700	0.90128000	2.84089100
H	1.19594800	1.18981300	5.19956600
C	-3.55145800	-0.53114500	-2.30965300
C	-4.06616000	-0.78620100	-3.57867700
N	-2.24385100	-0.33971200	-2.06643700
C	-3.17698000	-0.84059700	-4.65575100
H	-5.13103500	-0.93630100	-3.72817100
C	-1.39844400	-0.39137000	-3.10657000
C	-1.81917200	-0.63625300	-4.41481100
H	-3.54148600	-1.03495400	-5.65932600
H	-0.35391500	-0.22859000	-2.87196900

H	-1.09526100	-0.66271800	-5.22214400
H	6.48775400	1.45262300	0.20799000
H	5.80037700	-2.63766400	0.93170700
H	-5.98227100	-2.57627800	-0.07156300
H	-6.43401600	1.55402700	-0.74969200
C	-0.90224900	-3.33487400	2.08005000
H	-0.18845200	-3.57549800	2.87621900
H	-1.21850900	-4.27322800	1.61221500
H	-0.39065900	-2.72350800	1.33242900
C	-1.63951400	-1.23218600	3.26375400
H	-1.20405300	-0.60799400	2.47662900
H	-2.46959200	-0.68603100	3.72480600
H	-0.87181900	-1.40424200	4.02591400
C	-2.72325600	-3.43098500	3.80851600
H	-3.00326200	-4.42917400	3.45506600
H	-1.98428400	-3.56186000	4.60551900
H	-3.60760700	-2.95226500	4.24308900
C	0.67948700	-3.46028900	-1.38486500
H	0.02669500	-3.84490700	-2.17690800
H	0.72539300	-4.21239300	-0.59048300
H	0.22901100	-2.55002100	-0.98194400
C	2.00767300	-2.09742700	-3.05824200
H	1.67363700	-1.14162600	-2.63996900
H	2.98643900	-1.93879000	-3.52349400
H	1.30258700	-2.40194100	-3.83972900
C	2.60586900	-4.48885500	-2.60727800
H	2.65493800	-5.30630500	-1.87962200
H	1.92298600	-4.79725900	-3.40525800
H	3.59787500	-4.35294300	-3.05157400
C	1.90410000	3.99357800	-1.26599800
H	2.59848600	4.72081900	-0.83208600
H	1.16896400	4.54061400	-1.86672600
H	1.37919500	3.48900400	-0.44861600
C	1.65770800	1.98868600	-2.78825200
H	2.17164700	1.27609300	-3.44317300
H	1.11643300	1.43580100	-2.01333800
H	0.92170100	2.53720400	-3.38571600
C	3.39902300	3.72890500	-3.27562200
H	2.67030600	4.23653300	-3.91571600
H	4.06997700	4.49567600	-2.87411800
H	3.98337100	3.04608700	-3.90214000
C	-1.83137700	2.69926600	2.33226300
H	-2.51829000	2.33208400	3.10258200
H	-1.31361200	1.84367300	1.88665100
H	-1.08324200	3.34017000	2.81144500
C	-1.58911600	4.02538600	0.19016500
H	-2.10863300	4.61319600	-0.57409600
H	-0.84615400	4.67182000	0.67041100
H	-1.06508900	3.20231100	-0.30534500
C	-3.30310300	4.68870100	1.90818800
H	-2.56810400	5.31569400	2.42279100
H	-3.80937000	5.31656700	1.16710600
H	-4.03973800	4.35720300	2.64840100

Table S25: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), O...O = 1.359 Å

Cu	1.79203500	0.03961200	0.00209800
Cu	-1.82644600	0.06069600	0.05615100
O	-0.01614400	-0.55348000	0.12405700
O	-0.02351100	0.80155000	0.02657900
N	4.45684500	0.90906500	0.27199300
N	3.31588100	1.26595000	-0.39326900
N	4.12306100	-1.43873900	0.55187400
N	3.00193200	-1.53872200	-0.22700500
N	-3.09061400	-1.38803800	0.59851500
N	-4.23235800	-1.41163500	-0.15287100
N	-3.29619700	1.39537600	0.05143200
N	-4.43642400	0.93484400	-0.54648300
C	4.44267900	-0.18723100	1.23292300
C	3.67130300	2.27295400	-1.21999300
C	5.04924200	2.54749100	-1.06823600
C	5.51579400	1.66308900	-0.12215200
C	2.67908800	3.00774300	-2.10065900
C	3.12884000	-2.70488800	-0.90320600
C	4.32837400	-3.34528800	-0.51973900
C	4.94085800	-2.50920200	0.38517500
C	2.16290100	-3.17156900	-1.98022900
C	-4.47016900	-0.38656200	-1.16226700
C	-5.45489100	1.82370400	-0.42054800
C	-4.96143400	2.90441100	0.27601700
C	-3.61145300	2.60557800	0.56351000
C	-2.60631700	3.47755800	1.29029400
C	-5.10013500	-2.35629400	0.29296200
C	-4.49783200	-2.98168600	1.36106500
C	-3.24790700	-2.34667700	1.53838400
C	-2.21401800	-2.64413700	2.60945100
H	5.46752500	-0.29380800	1.58789500
H	5.62701600	3.29503200	-1.58878200
H	4.70344800	-4.29224100	-0.87403400
H	-5.49322000	-0.53396600	-1.50778600
H	-5.50453900	3.79530600	0.54960200
H	-4.91036600	-3.78584500	1.94997700
C	3.53714600	0.11158200	2.41565600
C	4.04978900	0.21955300	3.70626800
N	2.24011800	0.29847900	2.11693200
C	3.17144700	0.54671300	4.74337700
H	5.10561200	0.05829600	3.90116200
C	1.40687400	0.62408400	3.11679900
C	1.82741800	0.75966200	4.44052800
H	3.53478900	0.64051200	5.76169000
H	0.37573200	0.78950200	2.83217500
H	1.11365300	1.02909900	5.21151200
C	-3.52331500	-0.49043100	-2.34711800
C	-4.00395800	-0.72507500	-3.63338300
N	-2.21921900	-0.32759100	-2.06421100
C	-3.08405800	-0.79075400	-4.68371100
H	-5.06666000	-0.85179900	-3.81602300
C	-1.34391100	-0.39107700	-3.07887300
C	-1.72992800	-0.61842800	-4.40060300
H	-3.42225500	-0.97022900	-5.69918900
H	-0.30366900	-0.25311800	-2.81124800

H	-0.98257500	-0.65641300	-5.18580400
H	6.49880900	1.51292900	0.30088500
H	5.87788200	-2.58662200	0.91796700
H	-6.06004800	-2.50424000	-0.18093000
H	-6.43166700	1.61880900	-0.83494200
C	-1.02531500	-3.41017200	1.98745100
H	-0.30841400	-3.67460200	2.77317000
H	-1.36124000	-4.33559000	1.50774600
H	-0.51071900	-2.79650600	1.24370100
C	-1.71619200	-1.32147800	3.22314800
H	-1.27049500	-0.68774400	2.44906500
H	-2.53363000	-0.76955000	3.69958300
H	-0.94985800	-1.52760800	3.97816100
C	-2.84803200	-3.50955500	3.71598500
H	-3.15101000	-4.49157900	3.33714900
H	-2.11262600	-3.67756300	4.50933100
H	-3.72129400	-3.02166800	4.16262500
C	0.75511700	-3.41520300	-1.40097900
H	0.09733400	-3.79496900	-2.19119000
H	0.78646200	-4.16163500	-0.60049600
H	0.31930600	-2.49471200	-1.00554200
C	2.10972900	-2.09648100	-3.08881300
H	1.78578000	-1.12931000	-2.68834800
H	3.09333800	-1.95722900	-3.55002700
H	1.40632200	-2.40415700	-3.87071500
C	2.67412400	-4.48871200	-2.59785200
H	2.71822400	-5.29234400	-1.85464500
H	1.98718500	-4.80602400	-3.38884200
H	3.66608600	-4.36975900	-3.04708400
C	1.91675000	4.02342800	-1.21626600
H	2.60500800	4.75369800	-0.77775000
H	1.18355800	4.56728800	-1.82223600
H	1.38809700	3.51699600	-0.40234500
C	1.68872500	2.01513400	-2.73572600
H	2.20840700	1.30759100	-3.39162900
H	1.15199300	1.45628800	-1.96168600
H	0.94802100	2.55835200	-3.33216700
C	3.42341300	3.76392400	-3.21824600
H	2.69536600	4.26679600	-3.86290200
H	4.08823000	4.53482500	-2.81448500
H	4.01474800	3.08323900	-3.84048000
C	-1.86827100	2.64570600	2.35773500
H	-2.56423800	2.25830900	3.10983300
H	-1.34795100	1.80167200	1.89276300
H	-1.12266200	3.26902400	2.86327400
C	-1.59769400	4.03011200	0.25735000
H	-2.10634900	4.63822000	-0.49826900
H	-0.85895000	4.66242000	0.76222500
H	-1.07015700	3.21773200	-0.25181700
C	-3.32756500	4.65356700	1.97564700
H	-2.59576400	5.26251100	2.51588900
H	-3.82259600	5.30467600	1.24709800
H	-4.07431200	4.30473100	2.69750800

Table S26: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), Oxo

Cu	1.46123300	0.00593200	-0.26829100
Cu	-1.43727300	0.06758800	0.19201100
O	0.02356600	-0.98159000	0.16796500
O	-0.00203900	1.10648300	-0.29660400
N	4.18476500	0.84959700	-0.24467700
N	2.96420700	1.18005700	-0.79424400
N	3.84240100	-1.44943000	0.30642300
N	2.66324400	-1.53876100	-0.39216500
N	-2.59575200	-1.35183800	0.89769200
N	-3.76182000	-1.56544700	0.20482600
N	-2.98638100	1.31568600	0.33484900
N	-4.18705100	0.76879300	-0.07653800
C	4.32210400	-0.15771500	0.80586900
C	3.21985300	2.17845800	-1.69222100
C	4.60493800	2.47851200	-1.67690900
C	5.18343000	1.62326700	-0.75690200
C	2.16110800	2.85389700	-2.54844700
C	2.64174400	-2.78707000	-0.95119700
C	3.81453600	-3.48190000	-0.55578700
C	4.55734300	-2.60666700	0.21532100
C	1.58408500	-3.31446100	-1.91640700
C	-4.28084400	-0.54363700	-0.71129300
C	-5.23263900	1.59675600	0.20598200
C	-4.70945900	2.71680000	0.82039900
C	-3.30659400	2.51813400	0.90386500
C	-2.32394900	3.53033800	1.47839800
C	-4.43901400	-2.64010800	0.70053100
C	-3.68253600	-3.15122300	1.73952500
C	-2.54348200	-2.31440000	1.86772300
C	-1.49443500	-2.40525000	2.97126500
H	5.40522600	-0.28302500	0.95537400
H	5.11690800	3.22482600	-2.27896400
H	4.09719000	-4.49339600	-0.83600800
H	-5.35801200	-0.75000500	-0.80195300
H	-5.26838400	3.57615500	1.18167500
H	-3.93535300	-4.00467900	2.36339800
C	3.69656300	0.28565900	2.12113200
C	4.48908900	0.44799000	3.26611300
N	2.37464300	0.54318000	2.07512100
C	3.87366900	0.91757000	4.43730000
H	5.56053200	0.22087000	3.24796500
C	1.80009800	1.00560100	3.20367800
C	2.50469300	1.20971100	4.40147800
H	4.45676400	1.05950300	5.35266900
H	0.73215800	1.22785600	3.13899000
H	1.98427600	1.59335900	5.28405800
C	-3.66542600	-0.56814500	-2.10182500
C	-4.45908300	-0.83764200	-3.22542100
N	-2.35193500	-0.27237900	-2.15751400
C	-3.85448600	-0.78962600	-4.49125300
H	-5.52368500	-1.07343600	-3.12081700
C	-1.78835800	-0.21690600	-3.38100400
C	-2.49464500	-0.46504000	-4.56934500
H	-4.43861000	-0.99274600	-5.39434800
H	-0.72896900	0.04801600	-3.40648300

H	-1.98247100	-0.40000700	-5.53390500
H	6.21429900	1.50457700	-0.42451000
H	5.53048100	-2.70802900	0.69498600
H	-5.39860800	-2.94395500	0.28310000
H	-6.25426600	1.32364500	-0.05681500
C	-0.22783600	-3.14602100	2.47192900
H	0.48199600	-3.26413300	3.31028300
H	-0.47569600	-4.15259400	2.09242200
H	0.26317600	-2.57203400	1.66802400
C	-1.12090800	-0.98496700	3.44711600
H	-0.67341000	-0.40930000	2.62077500
H	-2.00245100	-0.44044600	3.82959100
H	-0.37568200	-1.04941200	4.25881300
C	-2.08630400	-3.19109300	4.16942900
H	-2.28361400	-4.24771700	3.91756200
H	-1.35651400	-3.18734100	4.99698400
H	-3.02154000	-2.73691800	4.54114200
C	0.36989400	-3.88679300	-1.14076900
H	-0.33747300	-4.34547500	-1.85483800
H	0.68249600	-4.66715200	-0.42506100
H	-0.15035000	-3.08577900	-0.58998300
C	1.12012300	-2.18405900	-2.86036100
H	0.63080500	-1.38038900	-2.28709500
H	1.96435400	-1.75983600	-3.43219500
H	0.38300000	-2.58150200	-3.57973100
C	2.20459800	-4.44993300	-2.77089700
H	2.46216500	-5.33458600	-2.16304700
H	1.46640700	-4.77852900	-3.52221400
H	3.10928900	-4.11566400	-3.30829200
C	1.22278000	3.67021400	-1.62649900
H	1.78246100	4.43015400	-1.05306900
H	0.46183200	4.19032100	-2.23512900
H	0.70457300	3.00106400	-0.91378800
C	1.35528800	1.78357200	-3.31884100
H	2.00593900	1.19284600	-3.98751700
H	0.85450200	1.10605100	-2.60711500
H	0.57808500	2.27198200	-3.93257200
C	2.83250000	3.80944100	-3.56294500
H	2.05480100	4.27494300	-4.19186700
H	3.38016400	4.62624500	-3.06106500
H	3.52986200	3.27559000	-4.23253200
C	-1.13984000	2.84040000	2.18518100
H	-1.49466500	2.21291900	3.02385800
H	-0.55695900	2.22159500	1.48189600
H	-0.46456100	3.60975900	2.59888000
C	-1.81798000	4.41245900	0.30482000
H	-2.65305100	4.95794700	-0.16823500
H	-1.09441500	5.15740500	0.68101100
H	-1.32244600	3.80194600	-0.46659800
C	-3.05186600	4.43344400	2.50639400
H	-2.32430500	5.13479300	2.94979900
H	-3.84337200	5.04470100	2.04016800
H	-3.49867400	3.84418800	3.32636900

Table S27: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), Peroxo

Cu	1.78058200	0.04263900	0.00948500
Cu	-1.81699200	0.05695700	0.06802900
O	-0.01296100	-0.60564100	0.17443600
O	-0.03178700	0.85369200	0.01445400
N	4.44560900	0.91494700	0.26413600
N	3.29260800	1.26568000	-0.40099100
N	4.11701300	-1.44425800	0.53175900
N	2.98024500	-1.53664800	-0.23978500
N	-3.07103200	-1.39245800	0.59051200
N	-4.22091400	-1.41228700	-0.16359900
N	-3.27838900	1.39391000	0.07797800
N	-4.42730100	0.94722600	-0.53154900
C	4.44242300	-0.19226400	1.22004400
C	3.64043400	2.28281400	-1.23523900
C	5.02360100	2.56649400	-1.08421000
C	5.50368100	1.68044600	-0.13549100
C	2.64302900	3.01872600	-2.11783900
C	3.10002900	-2.70419200	-0.93460200
C	4.30906900	-3.35045700	-0.56508700
C	4.93682500	-2.51952900	0.34561000
C	2.12804900	-3.15988400	-2.01842600
C	-4.46332600	-0.37177500	-1.16377400
C	-5.44661100	1.84476700	-0.39227900
C	-4.94308600	2.91697000	0.32500500
C	-3.58843100	2.60657100	0.61274700
C	-2.57994400	3.46803800	1.35778000
C	-5.08851400	-2.37104400	0.27488300
C	-4.47747900	-3.00842400	1.34078700
C	-3.22370500	-2.36868200	1.52782500
C	-2.18660700	-2.68106200	2.59908100
H	5.48068000	-0.30054900	1.56699100
H	5.59927300	3.32442000	-1.61014600
H	4.68269000	-4.30208100	-0.93452300
H	-5.49743600	-0.51697300	-1.50969900
H	-5.48569400	3.81373200	0.61449200
H	-4.88952500	-3.82725900	1.92582000
C	3.54801400	0.09631700	2.42111500
C	4.07594500	0.18454500	3.71512900
N	2.24202000	0.29357600	2.13515200
C	3.20488900	0.50234700	4.76967800
H	5.14181600	0.01477800	3.89973900
C	1.41596600	0.60922100	3.15333200
C	1.85221200	0.72564600	4.48120600
H	3.58149400	0.58137500	5.79433900
H	0.37318800	0.78401000	2.87781100
H	1.14126500	0.98985900	5.26942600
C	-3.52063300	-0.46219400	-2.36074800
C	-4.01245100	-0.67437200	-3.65480900
N	-2.20737800	-0.30706100	-2.08065300
C	-3.09525200	-0.72372600	-4.71683100
H	-5.08564800	-0.79605000	-3.83498800
C	-1.33515400	-0.35577200	-3.10787500
C	-1.73231400	-0.55905300	-4.43772400
H	-3.44341000	-0.88546800	-5.74183900
H	-0.28278100	-0.22444700	-2.84224700

H	-0.98398300	-0.58461400	-5.23513100
H	6.49791800	1.53679900	0.28667500
H	5.88695600	-2.60530600	0.87224900
H	-6.05628800	-2.52091300	-0.20301800
H	-6.43272800	1.65177400	-0.81380300
C	-0.99494500	-3.44012500	1.96125300
H	-0.26961100	-3.71925900	2.74643700
H	-1.33224800	-4.36637800	1.46421900
H	-0.47574100	-2.81215200	1.21902500
C	-1.68851700	-1.36375600	3.23693200
H	-1.23614900	-0.71163400	2.46983300
H	-2.51210700	-0.81488200	3.72647700
H	-0.91825800	-1.58352500	3.99676200
C	-2.82263100	-3.56786200	3.69483800
H	-3.12549800	-4.55383400	3.30104800
H	-2.08325600	-3.74914500	4.49367000
H	-3.70405500	-3.08703600	4.15437800
C	0.71027200	-3.38415500	-1.44256100
H	0.04411300	-3.76149900	-2.23904800
H	0.72706200	-4.13541000	-0.63411400
H	0.27794400	-2.45083800	-1.04637000
C	2.09747200	-2.08062100	-3.13160700
H	1.78457200	-1.09860800	-2.73362100
H	3.09268100	-1.95497100	-3.59321800
H	1.38934100	-2.37924500	-3.92492200
C	2.62445500	-4.48920300	-2.63535400
H	2.65810000	-5.30046100	-1.88700700
H	1.92962600	-4.80341200	-3.43281700
H	3.62523200	-4.38624700	-3.09022200
C	1.88392100	4.04108700	-1.22932500
H	2.57901600	4.77415800	-0.78409800
H	1.14851200	4.59592600	-1.83862700
H	1.34530700	3.53525100	-0.40961700
C	1.64562000	2.02370800	-2.75045500
H	2.16460700	1.30894100	-3.41392500
H	1.10456600	1.46121100	-1.96930200
H	0.89802700	2.57068400	-3.35092000
C	3.38849300	3.77384200	-3.24254900
H	2.65520000	4.28126600	-3.89264900
H	4.06089600	4.55286000	-2.84311500
H	3.98202300	3.08768100	-3.87204400
C	-1.84200300	2.61585900	2.41681600
H	-2.54355700	2.21135600	3.16757100
H	-1.31358700	1.77408000	1.93579100
H	-1.09285800	3.23541300	2.94042600
C	-1.56620100	4.03752300	0.33137300
H	-2.07518300	4.65528600	-0.42904300
H	-0.82686300	4.67475600	0.84816000
H	-1.02495300	3.22789400	-0.18730900
C	-3.30415800	4.63767000	2.06210600
H	-2.56888100	5.24342100	2.61876700
H	-3.80057100	5.30894400	1.33959300
H	-4.05936000	4.27859300	2.78340200

Table S28: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 2.277Å

Cu	1.40885600	-0.01774600	-0.30555800
Cu	-1.39208500	0.07940000	0.22090200
O	0.02171200	-1.04783300	0.22804800
O	-0.00864100	1.14954400	-0.36894200
N	4.13088400	0.82217100	-0.34020200
N	2.90461200	1.13322200	-0.89039700
N	3.78486000	-1.44639000	0.32078000
N	2.60807000	-1.55528800	-0.37854600
N	-2.54571300	-1.29849700	0.99206400
N	-3.71524700	-1.54163000	0.31522300
N	-2.93065200	1.33796900	0.33792600
N	-4.14010600	0.78257300	-0.03687700
C	4.28660400	-0.13761600	0.75120100
C	3.15306100	2.09488400	-1.83131500
C	4.53846300	2.39337300	-1.83879700
C	5.12449900	1.57463200	-0.89150800
C	2.09588100	2.73988300	-2.71291300
C	2.56866000	-2.82959900	-0.87481200
C	3.73008800	-3.51938200	-0.43890400
C	4.48232700	-2.61722600	0.29085900
C	1.51045400	-3.39254900	-1.81905200
C	-4.25696800	-0.55071500	-0.62208100
C	-5.17659000	1.62776400	0.22653500
C	-4.63955600	2.76626700	0.79203300
C	-3.23699000	2.56259500	0.86783500
C	-2.25012100	3.59254000	1.40326100
C	-4.37297900	-2.61298900	0.84271200
C	-3.59976600	-3.09049000	1.88528200
C	-2.46924600	-2.23780900	1.98309200
C	-1.40908900	-2.29654400	3.07833900
H	5.37279600	-0.26650800	0.87404900
H	5.04532400	3.11374400	-2.47569300
H	4.00107200	-4.54672900	-0.66869800
H	-5.33756900	-0.75370200	-0.67074900
H	-5.18886400	3.64171100	1.12843500
H	-3.83720600	-3.93061500	2.53302900
C	3.70966200	0.36884200	2.06565400
C	4.54663600	0.56629400	3.17341800
N	2.39102800	0.64453200	2.05538500
C	3.98227600	1.09353700	4.34557400
H	5.61347600	0.32206100	3.12588900
C	1.86637500	1.16233300	3.18451700
C	2.61734100	1.40528500	4.34657800
H	4.60074800	1.26415000	5.23238200
H	0.79983900	1.39823500	3.15159600
H	2.13482800	1.83339700	5.23028200
C	-3.68899300	-0.62934800	-2.03077800
C	-4.52449100	-0.93149100	-3.11548000
N	-2.37700700	-0.34514300	-2.14206000
C	-3.96582600	-0.93003000	-4.40320600
H	-5.58599300	-1.15641500	-2.96499200
C	-1.85831200	-0.33487100	-3.38652200
C	-2.60806200	-0.61707900	-4.54019400
H	-4.58309200	-1.15957600	-5.27746500
H	-0.79865500	-0.08027000	-3.46027300

H	-2.13001000	-0.58762200	-5.52384800
H	6.15830500	1.46835600	-0.56404800
H	5.45322000	-2.70761400	0.77725700
H	-5.33407700	-2.93688400	0.44419400
H	-6.20295900	1.35151300	-0.01356600
C	-0.18450800	-3.12686300	2.61385100
H	0.53123200	-3.22182500	3.45008600
H	-0.48276300	-4.14414600	2.30548100
H	0.31941700	-2.63109900	1.76761100
C	-0.96466700	-0.86842100	3.45676800
H	-0.49537800	-0.37220500	2.59229100
H	-1.81630400	-0.25959400	3.80956700
H	-0.21689500	-0.91684500	4.26714300
C	-2.02109800	-2.97569800	4.33135800
H	-2.26323100	-4.03756100	4.15229200
H	-1.28399500	-2.94662600	5.15199200
H	-2.93382700	-2.45912500	4.67614300
C	0.31584000	-3.97291400	-1.01871200
H	-0.39090500	-4.45698500	-1.71652900
H	0.65097500	-4.73509200	-0.29363300
H	-0.21105900	-3.17112300	-0.47581200
C	1.01413900	-2.29322200	-2.78247800
H	0.50564300	-1.49127400	-2.22410200
H	1.84454300	-1.86037700	-3.36813900
H	0.28484900	-2.72501300	-3.48982800
C	2.14542600	-4.53316500	-2.65704000
H	2.42430400	-5.40132200	-2.03522900
H	1.40694200	-4.88990700	-3.39518400
H	3.03939300	-4.19268500	-3.20825500
C	1.17956500	3.61958100	-1.82822300
H	1.75590800	4.40370100	-1.30629800
H	0.41720500	4.11316300	-2.45689000
H	0.66460100	2.99641200	-1.07312800
C	1.26774100	1.64421300	-3.42071800
H	1.90429700	1.00940700	-4.06234800
H	0.76017100	1.01450500	-2.67127400
H	0.49481100	2.11369800	-4.05421800
C	2.77232500	3.63096600	-3.78203800
H	1.99590200	4.06833100	-4.43219300
H	3.32895900	4.46988100	-3.32874600
H	3.46150900	3.05490300	-4.42455500
C	-1.04829300	2.92760600	2.10276100
H	-1.38407800	2.31868500	2.96284500
H	-0.47478100	2.29645300	1.40333200
H	-0.37185500	3.71189700	2.48537200
C	-1.77398000	4.45620700	0.20368200
H	-2.62204800	4.98791300	-0.26184900
H	-1.04813300	5.21225000	0.55229700
H	-1.28985600	3.83539200	-0.56636700
C	-2.96656000	4.51051900	2.42700400
H	-2.23478100	5.22204100	2.84659400
H	-3.76779100	5.11108400	1.96360600
H	-3.39783900	3.93376000	3.26400700

Table S29: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 2.145 Å

Cu	1.45895300	0.00106000	-0.26948900
Cu	-1.43486800	0.07019400	0.19328800
O	0.02188700	-0.98447000	0.17544700
O	-0.00018100	1.10568800	-0.30585400
N	4.18204900	0.84664500	-0.25793000
N	2.96063300	1.17065900	-0.80932600
N	3.84072600	-1.44563700	0.32017900
N	2.66152900	-1.54331900	-0.37739500
N	-2.59283300	-1.34093700	0.91608000
N	-3.75894000	-1.56343500	0.22625200
N	-2.98350900	1.32003700	0.32208500
N	-4.18458600	0.76735100	-0.08092200
C	4.32082000	-0.14824400	0.80419900
C	3.21478700	2.15878300	-1.71916000
C	4.59994400	2.45895300	-1.70938800
C	5.17990900	1.61427900	-0.78056000
C	2.15524400	2.82541700	-2.58128900
C	2.64029300	-2.79797100	-0.92202800
C	3.81335800	-3.48786900	-0.51879000
C	4.55592200	-2.60363900	0.24221900
C	1.58242200	-3.33731800	-1.88031600
C	-4.27950900	-0.55213200	-0.70063600
C	-5.23045700	1.59714400	0.19497100
C	-4.70734100	2.72438800	0.79605600
C	-3.30408400	2.52829900	0.87866200
C	-2.32194700	3.54920700	1.43859000
C	-4.43395400	-2.63421100	0.73299800
C	-3.67584700	-3.13368400	1.77655900
C	-2.53816000	-2.29367700	1.89562600
C	-1.48847800	-2.37154200	2.99962000
H	5.40414700	-0.27162500	0.95378900
H	5.11092300	3.19822300	-2.32092000
H	4.09635700	-4.50241800	-0.78736400
H	-5.35688000	-0.75929100	-0.78689500
H	-5.26641400	3.58717900	1.14879900
H	-3.92687400	-3.98106100	2.40942700
C	3.69722700	0.31091700	2.11494100
C	4.49235300	0.48987400	3.25567400
N	2.37490300	0.56616700	2.06853800
C	3.87923700	0.97476900	4.42180600
H	5.56405000	0.26387400	3.23798000
C	1.80260900	1.04351000	3.19201600
C	2.50985900	1.26492100	4.38520900
H	4.46437000	1.12995900	5.33372000
H	0.73426900	1.26374500	3.12691700
H	1.99115300	1.66026800	5.26363400
C	-3.66691800	-0.59310300	-2.09209300
C	-4.46276900	-0.87763500	-3.21047800
N	-2.35387600	-0.29690200	-2.15432200
C	-3.86099600	-0.84502100	-4.47816000
H	-5.52690900	-1.11316600	-3.10056600
C	-1.79306000	-0.25635500	-3.37966200
C	-2.50167400	-0.52005100	-4.56326800
H	-4.44687300	-1.06017500	-5.37732800
H	-0.73388700	0.00887400	-3.41093500

H	-1.99160500	-0.46665100	-5.52966300
H	6.21130400	1.49949300	-0.44839700
H	5.52915600	-2.69919300	0.72290700
H	-5.39346500	-2.94369800	0.31951500
H	-6.25231100	1.32016000	-0.06289900
C	-0.22317300	-3.12049300	2.50908300
H	0.48709200	-3.22823500	3.34847900
H	-0.47262500	-4.13178700	2.14339800
H	0.26790800	-2.55814500	1.69715100
C	-1.11283800	-0.94572700	3.45667300
H	-0.66647000	-0.38120500	2.62209600
H	-1.99324300	-0.39568100	3.83384100
H	-0.36608100	-1.00064100	4.26763100
C	-2.08083300	-3.14115900	4.20803000
H	-2.27963500	-4.20057800	3.96956000
H	-1.35077400	-3.12783800	5.03526400
H	-3.01537300	-2.68096800	4.57399100
C	0.36917800	-3.90124100	-1.09712400
H	-0.33794600	-4.36983100	-1.80501500
H	0.68312200	-4.67208400	-0.37176300
H	-0.15182000	-3.09377500	-0.55642800
C	1.11696900	-2.21871300	-2.83759100
H	0.62638000	-1.40907300	-2.27391800
H	1.96058200	-1.80011400	-3.41445000
H	0.38058500	-2.62590500	-3.55225900
C	2.20324000	-4.48251100	-2.72158400
H	2.46125100	-5.35983100	-2.10341700
H	1.46493700	-4.82027300	-3.46871400
H	3.10761500	-4.15418400	-3.26317500
C	1.21995600	3.65401000	-1.66719700
H	1.78170300	4.42075000	-1.10499500
H	0.45776700	4.16678400	-2.28047100
H	0.70345900	2.99406300	-0.94481900
C	1.34635500	1.74756000	-3.33785600
H	1.99506000	1.14791700	-4.00051400
H	0.84494400	1.07944800	-2.61778400
H	0.56935300	2.23037200	-3.95624900
C	2.82602000	3.76812200	-3.60822700
H	2.04787900	4.22631400	-4.24191400
H	3.37452400	4.59086100	-3.11701600
H	3.52242700	3.22596300	-4.27209300
C	-1.13487700	2.87079400	2.15135900
H	-1.48649600	2.25597700	3.00068500
H	-0.55396800	2.24185700	1.45554400
H	-0.45873300	3.64684000	2.55086700
C	-1.82084100	4.41797000	0.25292100
H	-2.65821300	4.95658700	-0.22394800
H	-1.09719400	5.16834000	0.61801900
H	-1.32674400	3.79921500	-0.51282000
C	-3.04932800	4.46356100	2.45705500
H	-2.32184500	5.17079000	2.89113700
H	-3.84224400	5.06857400	1.98507500
H	-3.49415600	3.88341200	3.28456500

Table S30: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 2.013 Å

Cu	1.51681900	0.04163300	-0.21869300
Cu	-1.49398100	0.03595300	0.14294000
O	0.02344200	-0.92962900	0.05732800
O	0.00053600	1.06821900	-0.18759800
N	4.22483900	0.92093400	-0.01895900
N	3.01625200	1.29421600	-0.56657800
N	3.92195400	-1.44085100	0.19260800
N	2.74208600	-1.47243900	-0.51038900
N	-2.65365600	-1.47513400	0.66036900
N	-3.81228000	-1.59499100	-0.06841300
N	-3.06186300	1.25409200	0.42643400
N	-4.24954900	0.75433500	-0.07085000
C	4.34725300	-0.22253000	0.88540700
C	3.27551700	2.41222700	-1.30716100
C	4.64885100	2.74351400	-1.19357000
C	5.21866600	1.78253700	-0.37773800
C	2.22935800	3.15110600	-2.12668600
C	2.76528600	-2.62740400	-1.24147100
C	3.96476700	-3.32871400	-0.95134300
C	4.67926400	-2.54575100	-0.06274300
C	1.71651100	-3.04258300	-2.26954200
C	-4.30644300	-0.46909000	-0.86780100
C	-5.30835400	1.53370700	0.29142300
C	-4.80532600	2.57450600	1.04724100
C	-3.40192400	2.37591700	1.12858300
C	-2.42658500	3.31075900	1.83199600
C	-4.50479100	-2.71535100	0.28342000
C	-3.76763200	-3.35470100	1.26364800
C	-2.62485400	-2.54876700	1.50709300
C	-1.59353500	-2.77725400	2.60824800
H	5.42564200	-0.34567300	1.06661900
H	5.16030900	3.57824800	-1.66602900
H	4.28111000	-4.27989100	-1.37214200
H	-5.37588800	-0.66884700	-1.03285600
H	-5.37820600	3.37972600	1.50004200
H	-4.03675600	-4.27660300	1.77294100
C	3.64835000	0.01958900	2.21599400
C	4.37304000	0.03240900	3.41562400
N	2.32467500	0.25960300	2.13310300
C	3.68313300	0.32279800	4.60351400
H	5.44900500	-0.17222000	3.42748800
C	1.67735200	0.54870700	3.27936700
C	2.31115900	0.59414100	4.53167100
H	4.21229100	0.34471400	5.56141700
H	0.60931700	0.75802900	3.18309100
H	1.73526400	0.84166600	5.42831800
C	-3.62165700	-0.31092500	-2.21640600
C	-4.34355100	-0.43250100	-3.41131900
N	-2.31087300	-0.00416200	-2.15609900
C	-3.66472200	-0.21173000	-4.62043900
H	-5.40889000	-0.68654100	-3.40373800
C	-1.67496600	0.21922200	-3.32293900
C	-2.30719000	0.12924300	-4.57334200
H	-4.19152400	-0.29561900	-5.57621300
H	-0.62075300	0.49306100	-3.24385500

H	-1.74117600	0.32683100	-5.48847000
H	6.24006800	1.64317100	-0.02469900
H	5.65691000	-2.68009800	0.39943300
H	-5.45951800	-2.95916900	-0.18190100
H	-6.32308000	1.28664200	-0.01954900
C	-0.28343800	-3.37148200	2.03375300
H	0.41076500	-3.60052200	2.86221200
H	-0.47579400	-4.30878900	1.48331300
H	0.20360600	-2.65286200	1.35228400
C	-1.30060700	-1.43552500	3.31585400
H	-0.87031300	-0.71194700	2.60407500
H	-2.21622100	-1.00209000	3.75578700
H	-0.56926000	-1.59367700	4.12762000
C	-2.17195800	-3.77213100	3.64578500
H	-2.32027500	-4.77769200	3.21522500
H	-1.45807000	-3.87882700	4.48031100
H	-3.13144300	-3.42191600	4.06496800
C	0.48781300	-3.68420100	-1.57640800
H	-0.21817100	-4.04435200	-2.34609500
H	0.78280800	-4.54763900	-0.95499100
H	-0.02977700	-2.94710900	-0.94036900
C	1.27430500	-1.80833700	-3.08615500
H	0.79912600	-1.06159900	-2.42923700
H	2.12814300	-1.33789400	-3.60494400
H	0.53248200	-2.11097600	-3.84552400
C	2.33864800	-4.08162100	-3.23626800
H	2.59209300	-5.02567900	-2.72311000
H	1.60473600	-4.32701300	-4.02269800
H	3.24659600	-3.69407000	-3.73071800
C	1.17268400	3.76332800	-1.17623700
H	1.63711400	4.44639400	-0.44346000
H	0.43251300	4.33769100	-1.76117100
H	0.63580000	2.96742700	-0.62306900
C	1.55985600	2.15913700	-3.10563600
H	2.29309300	1.73102700	-3.81147900
H	1.08763400	1.33688300	-2.54212600
H	0.77770500	2.67661300	-3.68866600
C	2.89705400	4.28874300	-2.93477200
H	2.13108600	4.80192100	-3.54058700
H	3.35709400	5.04595900	-2.27590700
H	3.66866400	3.90619100	-3.62607100
C	-1.25093700	2.53452000	2.45924400
H	-1.61559900	1.80586800	3.20682800
H	-0.66051400	2.00722100	1.69047600
H	-0.57805600	3.24236500	2.97486800
C	-1.90210200	4.32656000	0.78110700
H	-2.72958200	4.91785400	0.35205000
H	-1.19528900	5.02762200	1.25946700
H	-1.38094400	3.81203200	-0.04241400
C	-3.16444200	4.08347800	2.95385800
H	-2.44299900	4.73097700	3.48092200
H	-3.95691900	4.74095200	2.55736700
H	-3.61429500	3.40100600	3.69624800

Table S31: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 1.881 Å

Cu	1.59542200	0.06148900	-0.17803800
Cu	-1.54918400	0.03905300	0.08762200
O	0.02733700	-0.84853400	-0.05925600
O	0.01946300	1.03210900	-0.10363500
N	4.29662300	0.92328900	0.13940200
N	3.09965100	1.33941200	-0.39897600
N	4.00151500	-1.44863500	0.13345900
N	2.82134900	-1.44588800	-0.57028400
N	-2.72014800	-1.51271100	0.50571000
N	-3.86490000	-1.57731100	-0.25290800
N	-3.11931000	1.23830800	0.42469200
N	-4.29364600	0.77219100	-0.13083200
C	4.38822900	-0.29406900	0.94478700
C	3.37345400	2.50614500	-1.05129700
C	4.74756900	2.82009800	-0.89915500
C	5.30166200	1.79987400	-0.14570300
C	2.32862100	3.31647700	-1.80152800
C	2.86647700	-2.54213900	-1.38430500
C	4.07996300	-3.24096200	-1.15218800
C	4.78010100	-2.51599000	-0.20452400
C	1.80728000	-2.90419100	-2.42020000
C	-4.32207900	-0.40151100	-1.00100500
C	-5.36308600	1.52289500	0.26142200
C	-4.87858900	2.51251100	1.09548800
C	-3.47668600	2.31052900	1.19017300
C	-2.50427300	3.19294900	1.96063900
C	-4.58931700	-2.69659200	0.03323500
C	-3.88813600	-3.39404000	1.00044300
C	-2.73620700	-2.62241200	1.30432900
C	-1.74721000	-2.90180100	2.43256300
H	5.45689800	-0.42860700	1.16917800
H	5.26913000	3.68426200	-1.30294500
H	4.41280000	-4.15252900	-1.64231900
H	-5.38355700	-0.58454100	-1.22506800
H	-5.46243200	3.28624700	1.58766600
H	-4.18427100	-4.33389600	1.45969900
C	3.61685100	-0.17495600	2.25292200
C	4.27633800	-0.23399300	3.48776400
N	2.28931500	0.02257100	2.11993900
C	3.51395800	-0.06990300	4.65541700
H	5.35773200	-0.39873400	3.54226900
C	1.56971400	0.18462600	3.24786400
C	2.13614900	0.14918300	4.53197700
H	3.99197800	-0.10698700	5.63938600
H	0.49914600	0.35402200	3.10887900
H	1.50498500	0.29427400	5.41368400
C	-3.57683400	-0.16684500	-2.30641600
C	-4.24263500	-0.21278500	-3.53822000
N	-2.26772600	0.12631900	-2.17073700
C	-3.50744600	0.07116800	-4.70018000
H	-5.30864100	-0.45779500	-3.59404100
C	-1.57613300	0.40967800	-3.29220000
C	-2.15115700	0.39651300	-4.57272500
H	-3.99059500	0.04699800	-5.68203700
H	-0.52479100	0.66821900	-3.14793600

H	-1.54286200	0.64073700	-5.44857400
H	6.31753200	1.62910800	0.20954800
H	5.75895800	-2.66872900	0.24931000
H	-5.53684300	-2.90022600	-0.46502000
H	-6.37044800	1.29522500	-0.08614400
C	-0.35332400	-3.29586400	1.88694700
H	0.31870700	-3.53062000	2.73192800
H	-0.41815700	-4.19243600	1.24638300
H	0.09308100	-2.47525600	1.29936400
C	-1.64736400	-1.63648200	3.31906800
H	-1.31122800	-0.76471400	2.73177300
H	-2.62382800	-1.38758000	3.77089900
H	-0.92423300	-1.80618000	4.13612300
C	-2.27594100	-4.06848600	3.30294600
H	-2.32336200	-5.01559700	2.73754100
H	-1.58690700	-4.22704100	4.14983600
H	-3.27547400	-3.85446900	3.72036300
C	0.56893400	-3.53586800	-1.73546300
H	-0.15219400	-3.85871300	-2.50780700
H	0.84915200	-4.42172600	-1.13920000
H	0.07008000	-2.80543300	-1.07547800
C	1.39099900	-1.63426600	-3.19634700
H	0.94841500	-0.89200000	-2.51171600
H	2.25264300	-1.17474400	-3.71195400
H	0.63187000	-1.89300200	-3.95501200
C	2.39861700	-3.92917700	-3.41901500
H	2.64088300	-4.88939600	-2.93102300
H	1.65273500	-4.14196000	-4.20368700
H	3.30801000	-3.54528000	-3.91369400
C	1.30397900	3.87653100	-0.78489900
H	1.79579400	4.50794000	-0.02408800
H	0.55445400	4.49422800	-1.31048600
H	0.77414400	3.05448200	-0.26712500
C	1.61580000	2.40872000	-2.83020200
H	2.32600200	2.00203600	-3.57137900
H	1.12116300	1.57008400	-2.31105400
H	0.84309700	2.98499200	-3.36904500
C	3.00437500	4.49358900	-2.54244600
H	2.23955300	5.06529200	-3.09487200
H	3.49540700	5.19239000	-1.84265000
H	3.75368300	4.14363000	-3.27446200
C	-1.37778900	2.35440200	2.60000800
H	-1.78918000	1.63211800	3.32847400
H	-0.79979100	1.80997300	1.83359700
H	-0.68005400	3.02126300	3.13661400
C	-1.90953300	4.22477500	0.96466800
H	-2.70100000	4.86129000	0.53229800
H	-1.19276500	4.88141600	1.48906300
H	-1.38152700	3.72131400	0.13826500
C	-3.25835400	3.94924100	3.08144400
H	-2.53832400	4.55354000	3.65930400
H	-4.01442000	4.64511900	2.67906400
H	-3.75737000	3.25544000	3.78070200

Table S32: XYZ coordinates for optimised structure: Singlet minimum path, BP86-6-31g(d), O...O = 1.749 Å

Cu	-1.67431600	0.06844900	0.13535300
Cu	1.62931700	0.04385500	-0.04910800
O	-0.02408300	-0.76606300	0.10594100
O	-0.02521500	0.98321200	0.06272700
N	-4.35342100	0.93643700	-0.26996700
N	-3.17180500	1.36149900	0.29177200
N	-4.07703800	-1.43740400	-0.15111500
N	-2.90420800	-1.43180600	0.56555000
N	2.80407200	-1.52791500	-0.42179600
N	3.94769300	-1.55276200	0.34173600
N	3.19099100	1.24441600	-0.39703200
N	4.35527500	0.80106700	0.19401900
C	-4.41996700	-0.31464800	-1.02472100
C	-3.45799800	2.54307000	0.90744900
C	-4.82727000	2.85727000	0.71289500
C	-5.36486200	1.82036200	-0.03068700
C	-2.42143000	3.36555700	1.65668800
C	-2.98186000	-2.49529000	1.41747000
C	-4.20783800	-3.17734900	1.20085800
C	-4.88232200	-2.47485800	0.21787400
C	-1.93130200	-2.83725100	2.46844900
C	4.36336200	-0.35879700	1.08362300
C	5.42802200	1.55058400	-0.19345500
C	4.95286100	2.51842600	-1.05919100
C	3.55458000	2.30256400	-1.17593300
C	2.57752100	3.15377500	-1.97421800
C	4.70407700	-2.65590200	0.07322900
C	4.02536500	-3.38479000	-0.88693400
C	2.85403100	-2.64752400	-1.20246600
C	1.86754100	-2.96623700	-2.32165900
H	-5.47797000	-0.45247700	-1.29296300
H	-5.35663400	3.73253300	1.08148800
H	-4.56394900	-4.06395200	1.71967100
H	5.41641300	-0.52559700	1.35482100
H	5.54059300	3.28668600	-1.55555900
H	4.34549500	-4.32434000	-1.33051600
C	-3.58640600	-0.25893100	-2.29960700
C	-4.18589700	-0.36424700	-3.56134900
N	-2.26232200	-0.07493800	-2.11394900
C	-3.36580800	-0.26609500	-4.69687300
H	-5.26604500	-0.51497500	-3.66098400
C	-1.48575500	0.02204200	-3.21132300
C	-1.99129900	-0.06454900	-4.51781800
H	-3.79726400	-0.34094900	-5.70002600
H	-0.41991600	0.17847200	-3.02668800
H	-1.31651300	0.02778900	-5.37391200
C	3.56042100	-0.11161600	2.35333600
C	4.17101900	-0.12977000	3.61377300
N	2.25325600	0.16093100	2.15944300
C	3.38147800	0.15932700	4.73823800
H	5.23683400	-0.35793400	3.72008500
C	1.50784900	0.44960700	3.24472200
C	2.02705700	0.46217700	4.54850100
H	3.82190100	0.15622700	5.74027500
H	0.46058500	0.69092800	3.04836300

H	1.37832900	0.70903500	5.39403400
H	-6.37184400	1.64297500	-0.40736100
H	-5.85827200	-2.62594300	-0.24271300
H	5.65347700	-2.82851100	0.57956200
H	6.42980500	1.33837100	0.17911800
C	0.46681900	-3.31251000	-1.76247500
H	-0.20721200	-3.57923100	-2.59629900
H	0.51708800	-4.17719700	-1.07827300
H	0.02645700	-2.45988000	-1.21805300
C	1.79043200	-1.73902700	-3.26390700
H	1.47133600	-0.83481300	-2.71633300
H	2.77187000	-1.52754200	-3.72373700
H	1.06608300	-1.93096300	-4.07508500
C	2.38161200	-4.17882600	-3.13501800
H	2.42707800	-5.09576300	-2.52154300
H	1.68697500	-4.37608400	-3.96915800
H	3.37992700	-3.99357500	-3.56875400
C	-0.67262100	-3.44671000	1.80153900
H	0.04223400	-3.76036800	2.58348200
H	-0.92872700	-4.33471600	1.19780100
H	-0.17125700	-2.70838600	1.15215900
C	-1.54803300	-1.55511000	3.24319500
H	-1.12022500	-0.80397400	2.55798500
H	-2.42318900	-1.11273600	3.75077100
H	-0.78804300	-1.79313800	4.00789000
C	-2.51628500	-3.86898000	3.46274000
H	-2.74343700	-4.83154600	2.97195100
H	-1.77460900	-4.07265500	4.25377700
H	-3.43421100	-3.49638300	3.95026300
C	-1.38939700	3.91386300	0.63975500
H	-1.87696500	4.53955400	-0.12839500
H	-0.64144600	4.53550300	1.16285500
H	-0.85808400	3.08933000	0.13004800
C	-1.71333700	2.47354900	2.70286300
H	-2.42755900	2.07805600	3.44619500
H	-1.21567100	1.62525000	2.20171500
H	-0.94355600	3.05796200	3.23704200
C	-3.10652500	4.54988800	2.37609500
H	-2.34945800	5.13049700	2.93000700
H	-3.59182900	5.23887400	1.66271400
H	-3.86334400	4.20656700	3.10345700
C	1.49500900	2.27501600	-2.63705200
H	1.94537200	1.56949000	-3.35835900
H	0.92668400	1.70580200	-1.88122000
H	0.78043600	2.91535700	-3.18341400
C	1.92282300	4.16654800	-0.99653700
H	2.68136600	4.82845500	-0.54361200
H	1.19916400	4.79963100	-1.54027000
H	1.38923400	3.64707200	-0.18304700
C	3.33561600	3.93059000	-3.07705500
H	2.61369700	4.51309200	-3.67465700
H	4.06098000	4.64782500	-2.65588900
H	3.87203600	3.25043200	-3.76187500

Table S33: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 1.618 Å

Cu	-1.75533000	0.06532000	0.08476700
Cu	1.71495800	0.04027500	-0.01433700
O	-0.01634300	-0.69386500	0.13573400
O	-0.02998400	0.92159100	0.03302400
N	-4.38901200	0.95006300	-0.46604700
N	-3.22605000	1.39491300	0.11830500
N	-4.17291800	-1.41049100	-0.12359700
N	-3.01255800	-1.38440700	0.61359200
N	2.90641300	-1.54418300	-0.26735500
N	4.04561000	-1.47609400	0.50209900
N	3.25012600	1.24435800	-0.42934400
N	4.40775600	0.87453400	0.21872400
C	-4.44508300	-0.36310500	-1.10855800
C	-3.52249300	2.61089700	0.65556200
C	-4.88075400	2.92513000	0.39224500
C	-5.40126700	1.85243900	-0.31178600
C	-2.50227900	3.46988900	1.38689000
C	-3.14446000	-2.36560800	1.55033200
C	-4.39468000	-3.01566500	1.37602300
C	-5.02582000	-2.37854400	0.32201800
C	-2.10196900	-2.66705200	2.62028200
C	4.40803500	-0.22780900	1.17910900
C	5.47316200	1.61903200	-0.19951900
C	4.99565900	2.51049900	-1.14361800
C	3.60540100	2.25233000	-1.27326300
C	2.61640300	3.01157800	-2.14573300
C	4.83801800	-2.57195000	0.32126900
C	4.18989100	-3.39143600	-0.58542500
C	2.99766900	-2.71751300	-0.95910900
C	2.02385500	-3.15369800	-2.04971100
H	-5.48987500	-0.50492600	-1.42235800
H	-5.41426400	3.82477700	0.68944900
H	-4.79239800	-3.83984100	1.96330300
H	5.45283000	-0.35298800	1.49995000
H	5.57724200	3.25575900	-1.68084500
H	4.54099500	-4.35233000	-0.95286600
C	-3.54107500	-0.44241700	-2.33431100
C	-4.07125200	-0.64864100	-3.61418300
N	-2.22211100	-0.28189100	-2.09143000
C	-3.18590100	-0.68504400	-4.70341600
H	-5.14872700	-0.77528100	-3.76299900
C	-1.38106400	-0.31751000	-3.14444100
C	-1.81636800	-0.51340200	-4.46377500
H	-3.56349400	-0.84167000	-5.71876300
H	-0.32194500	-0.18202900	-2.90992000
H	-1.09211100	-0.52788000	-5.28342800
C	3.54996600	0.07997900	2.40002900
C	4.11172200	0.16348800	3.68023000
N	2.24280600	0.30034200	2.14297500
C	3.27246600	0.50207500	4.75388700
H	5.17852000	-0.02523400	3.83968300
C	1.44846100	0.63707300	3.17902200
C	1.91803000	0.75049700	4.49615300
H	3.67469000	0.57809400	5.76900500
H	0.40332000	0.83287800	2.92820300

H	1.23128100	1.03214300	5.29970000
H	-6.39562200	1.66179800	-0.71460200
H	-5.99924300	-2.53373700	-0.14253200
H	5.78678800	-2.67754700	0.84675600
H	6.47071200	1.45825800	0.20843500
C	0.60743200	-3.39882800	-1.47876400
H	-0.05668100	-3.76273600	-2.28324000
H	0.62859600	-4.16652000	-0.68610600
H	0.16984200	-2.47592900	-1.06246800
C	1.98988400	-2.05240500	-3.14037000
H	1.68115600	-1.07873500	-2.72008200
H	2.98340000	-1.91947100	-3.60359400
H	1.27728700	-2.33278800	-3.93624900
C	2.52405300	-4.46846600	-2.69535800
H	2.55490900	-5.29737800	-1.96649500
H	1.83207800	-4.76431800	-3.50224100
H	3.52658300	-4.35423000	-3.14359700
C	-0.89155500	-3.39805900	1.98619800
H	-0.17295100	-3.67882700	2.77701400
H	-1.20758800	-4.32108700	1.46956300
H	-0.37162800	-2.74802500	1.26310700
C	-1.63337200	-1.34470700	3.27001600
H	-1.18699200	-0.68018100	2.51043100
H	-2.47059200	-0.81356400	3.75599500
H	-0.86546600	-1.55470700	4.03497600
C	-2.72451800	-3.57375900	3.70799300
H	-3.00714000	-4.56264500	3.30651800
H	-1.98397800	-3.74607400	4.50768400
H	-3.61608000	-3.11297200	4.16850100
C	-1.46961400	3.99645700	0.35761900
H	-1.95960700	4.60550400	-0.42222400
H	-0.72295200	4.63139300	0.86661100
H	-0.93845800	3.16459800	-0.13715300
C	-1.79118400	2.62604100	2.47050400
H	-2.50720600	2.24989400	3.22217600
H	-1.27629500	1.76538100	2.00931800
H	-1.03500500	3.24145100	2.98896800
C	-3.20804500	4.66918000	2.05964200
H	-2.46388700	5.27477900	2.60438700
H	-3.69070600	5.33084100	1.31923300
H	-3.97090200	4.34057300	2.78741400
C	1.57556700	2.04744700	-2.75526500
H	2.06032800	1.30927100	-3.41919900
H	1.02270800	1.51205000	-1.96382100
H	0.84178100	2.61647400	-3.35221200
C	1.90880000	4.06635600	-1.25291300
H	2.63575300	4.78075900	-0.82887100
H	1.17882900	4.63871700	-1.85254300
H	1.37186700	3.58519300	-0.41771300
C	3.36716400	3.73276100	-3.28959400
H	2.63906900	4.25576800	-3.93314000
H	4.06906700	4.49518600	-2.90946200
H	3.92984300	3.02284500	-3.92107500

Table S34: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 1.488 Å

Cu	-1.81045300	0.05722000	0.06875600
Cu	1.77312500	0.04213300	0.00687800
O	-0.01158600	-0.62037400	0.15780600
O	-0.03423000	0.86216600	0.03108000
N	-4.42016700	0.95364000	-0.52726800
N	-3.26830800	1.39795400	0.07863100
N	-4.22185600	-1.40567000	-0.15486100
N	-3.06972500	-1.38754800	0.59566700
N	2.97036400	-1.53890100	-0.23697300
N	4.10616300	-1.44786600	0.53609000
N	3.28958200	1.26030700	-0.40659200
N	4.44222700	0.90897000	0.25888400
C	-4.46356100	-0.36663800	-1.15653300
C	-3.57249400	2.61444200	0.60858500
C	-4.92594600	2.92962600	0.32079200
C	-5.43501400	1.85654700	-0.39120700
C	-2.56075900	3.47445600	1.35090400
C	-3.22346800	-2.35942800	1.53728500
C	-4.48050300	-2.99469300	1.35664100
C	-5.09223700	-2.35886900	0.29022000
C	-2.18460000	-2.67159500	2.60692500
C	4.43711100	-0.19424600	1.21916100
C	5.50318400	1.66641300	-0.14841200
C	5.02544500	2.54804000	-1.10230000
C	3.64060500	2.26975400	-1.24883300
C	2.64595000	3.00545100	-2.13477600
C	4.92047500	-2.52849400	0.35808800
C	4.29041300	-3.36131900	-0.54926900
C	3.08566500	-2.71096800	-0.92538700
C	2.11542200	-3.16826900	-2.01025900
H	-5.49946400	-0.50831300	-1.49852000
H	-5.46411700	3.83011200	0.60694100
H	-4.89413100	-3.80951800	1.94614100
H	5.47574800	-0.30489700	1.56423200
H	5.60371800	3.29958600	-1.63448600
H	4.66021200	-4.31665000	-0.91288900
C	-3.52542800	-0.46343200	-2.35642900
C	-4.02227700	-0.67852900	-3.64809600
N	-2.21093200	-0.31114400	-2.08111900
C	-3.10879000	-0.73397200	-4.71300300
H	-5.09641000	-0.79784900	-3.82424700
C	-1.34228400	-0.36581400	-3.11106700
C	-1.74447900	-0.57226700	-4.43895300
H	-3.46081600	-0.89813100	-5.73630400
H	-0.28851900	-0.23742900	-2.84955300
H	-0.99889900	-0.60260200	-5.23877500
C	3.54643100	0.10204200	2.42086300
C	4.07771700	0.19468200	3.71322200
N	2.24065900	0.30198900	2.13656500
C	3.20998600	0.52013500	4.76818500
H	5.14350300	0.02261700	3.89622100
C	1.41800700	0.62540700	3.15501700
C	1.85746700	0.74655600	4.48147100
H	3.58903200	0.60272000	5.79166600
H	0.37540900	0.80310000	2.88083000

H	1.14908600	1.01683300	5.26995200
H	-6.42240900	1.66616300	-0.81091700
H	-6.06218300	-2.50645400	-0.18398000
H	5.86914400	-2.61605700	0.88706000
H	6.49755000	1.52100200	0.27284800
C	0.69690100	-3.39475300	-1.43691000
H	0.03367500	-3.77607100	-2.23395700
H	0.71368800	-4.14361800	-0.62629800
H	0.26103600	-2.46131800	-1.04480400
C	2.08535600	-2.09017800	-3.12444000
H	1.77233100	-1.10786000	-2.72744800
H	3.08079500	-1.96508200	-3.58570100
H	1.37756500	-2.38957100	-3.91774500
C	2.61432900	-4.49756800	-2.62550100
H	2.64567500	-5.30885500	-1.87708700
H	1.92205800	-4.81197400	-3.42509500
H	3.61653900	-4.39430400	-3.07710100
C	-0.99876600	-3.44014800	1.96961100
H	-0.27387300	-3.72110900	2.75454800
H	-1.34238200	-4.36587700	1.47596400
H	-0.47704800	-2.81715000	1.22490800
C	-1.67695400	-1.35360000	3.23567100
H	-1.22311500	-0.70881000	2.46324000
H	-2.49568800	-0.79700700	3.72463500
H	-0.90543400	-1.57343700	3.99417600
C	-2.82195200	-3.54890400	3.70950600
H	-3.13090400	-4.53553900	3.32218400
H	-2.08121200	-3.72936700	4.50724700
H	-3.69966300	-3.06104600	4.16874800
C	-1.53641400	4.02627700	0.32547200
H	-2.03580200	4.64248400	-0.44258300
H	-0.79429100	4.66114900	0.84116700
H	-0.99962600	3.20785300	-0.18405600
C	-1.83681000	2.62571500	2.42231000
H	-2.54658600	2.23360700	3.17185600
H	-1.31256800	1.77545600	1.95202600
H	-1.08617000	3.24382100	2.94555100
C	-3.27898600	4.65657400	2.04043900
H	-2.54141500	5.26200000	2.59437600
H	-3.76736200	5.32435500	1.30929800
H	-4.03965200	4.31016900	2.76220300
C	1.63241700	2.01494800	-2.74848600
H	2.13867600	1.28595500	-3.40634100
H	1.08870700	1.46861100	-1.95778100
H	0.88811400	2.56365800	-3.35138700
C	1.90501900	4.04840900	-1.25480700
H	2.61173300	4.77787700	-0.82222500
H	1.17328200	4.60507700	-1.86684500
H	1.36467400	3.55939600	-0.42610600
C	3.39324900	3.73682800	-3.27401500
H	2.66191700	4.24460800	-3.92605900
H	4.07763200	4.51291600	-2.88948900
H	3.97465900	3.03538900	-3.89796500

Table S35: XYZ coordinates for optimised structure: Singlet minimum path, BP86/6-31g(d), O...O = 1.359 Å

Cu	1.81786200	0.04261800	0.02607400
Cu	-1.85269600	0.04865900	0.06127300
O	-0.00781000	-0.55250600	0.16185800
O	-0.03956900	0.80146200	0.05497200
N	4.46877000	0.92281000	0.31500100
N	3.32032700	1.28394800	-0.35195300
N	4.15401800	-1.44711400	0.50516100
N	3.01645800	-1.53119500	-0.26631000
N	-3.11740700	-1.40464300	0.54052000
N	-4.26229900	-1.38974800	-0.22085800
N	-3.29574800	1.40290100	0.09403100
N	-4.44074200	0.98086700	-0.53947700
C	4.46091300	-0.21436000	1.23514100
C	3.67049500	2.31963600	-1.16076300
C	5.05176900	2.60470400	-0.99327400
C	5.52794300	1.69933200	-0.06081800
C	2.67507100	3.07039700	-2.03311700
C	3.14514600	-2.68076900	-0.98776900
C	4.36133600	-3.32450200	-0.63777500
C	4.98345400	-2.51017400	0.29184200
C	2.16799800	-3.12016700	-2.07311600
C	-4.47756500	-0.32422600	-1.20066800
C	-5.45293000	1.88587900	-0.39412000
C	-4.94755200	2.93748200	0.35212600
C	-3.59963100	2.60686700	0.64996300
C	-2.58930900	3.43986500	1.42465700
C	-5.14807900	-2.34382500	0.19184300
C	-4.55349600	-3.01389900	1.24729600
C	-3.29070500	-2.39837100	1.45433100
C	-2.25844900	-2.74940200	2.51780800
H	5.49488700	-0.32571500	1.59361400
H	5.62885000	3.37618600	-1.49764700
H	4.74240400	-4.26373600	-1.03073700
H	-5.50627300	-0.45188200	-1.56882800
H	-5.48481300	3.83346900	0.65390000
H	-4.98123900	-3.83893400	1.81203100
C	3.54754100	0.02803100	2.43321000
C	4.05759500	0.07579500	3.73638600
N	2.24238400	0.22339900	2.13860800
C	3.17059400	0.34806300	4.79032400
H	5.12261300	-0.09057700	3.92864600
C	1.40030700	0.49471400	3.15691000
C	1.81923300	0.56810900	4.49316200
H	3.53394300	0.39462900	5.82173100
H	0.35930200	0.66923800	2.87421300
H	1.09601000	0.79706200	5.28121400
C	-3.51391000	-0.39792200	-2.38309200
C	-3.98630200	-0.57677400	-3.68935700
N	-2.20280700	-0.26364700	-2.07934500
C	-3.05298500	-0.61362700	-4.73771000
H	-5.05768400	-0.68269700	-3.88898600
C	-1.31481700	-0.30030600	-3.09393100
C	-1.69294800	-0.47054600	-4.43366600
H	-3.38651600	-0.74942900	-5.77129900
H	-0.26521000	-0.18688800	-2.80963700

H	-0.93213700	-0.48775000	-5.21936500
H	6.51972600	1.54932900	0.36491000
H	5.93510500	-2.60033400	0.81499000
H	-6.11505800	-2.46811800	-0.29490200
H	-6.43560200	1.71215000	-0.83177600
C	-1.07762900	-3.50806500	1.85909800
H	-0.35089600	-3.80948800	2.63464500
H	-1.42725000	-4.42108700	1.34638900
H	-0.55636900	-2.87162900	1.12556800
C	-1.74237200	-1.45362100	3.18475000
H	-1.28488400	-0.78859000	2.43142300
H	-2.55778000	-0.90626000	3.68936500
H	-0.97227300	-1.70064000	3.93634300
C	-2.90512300	-3.65278100	3.59342800
H	-3.22209900	-4.62492200	3.17692000
H	-2.16779300	-3.86281200	4.38708300
H	-3.77949300	-3.17071500	4.06501800
C	0.75225000	-3.34309000	-1.49165400
H	0.07922300	-3.70885200	-2.28774500
H	0.76953300	-4.10228900	-0.69063700
H	0.32747600	-2.41144900	-1.08389500
C	2.13573300	-2.02701000	-3.17280000
H	1.82544900	-1.04966200	-2.76089700
H	3.12963300	-1.89663700	-3.63580700
H	1.42468000	-2.31429700	-3.96776900
C	2.65578600	-4.44422100	-2.70731400
H	2.69390500	-5.26271800	-1.96709800
H	1.95399300	-4.74915900	-3.50228900
H	3.65314300	-4.33919800	-3.16916400
C	1.92930600	4.09352900	-1.13383600
H	2.63316600	4.81606100	-0.68526000
H	1.19755700	4.66064400	-1.73627200
H	1.38806000	3.58705800	-0.31608500
C	1.66487100	2.08926600	-2.66721700
H	2.17305900	1.37660600	-3.34132100
H	1.12416800	1.52326700	-1.88804500
H	0.91731800	2.64773500	-3.25698800
C	3.42199400	3.82601800	-3.15664900
H	2.69049500	4.34362400	-3.80075800
H	4.10285000	4.59669100	-2.75547000
H	4.00732600	3.13848700	-3.79227700
C	-1.86874300	2.55429700	2.46820600
H	-2.58024900	2.14046700	3.20433700
H	-1.34667200	1.71774000	1.97098600
H	-1.11588300	3.15198700	3.01164300
C	-1.56039700	4.02422400	0.42143000
H	-2.05713000	4.66097200	-0.33139000
H	-0.82350500	4.64629200	0.95968100
H	-1.01784100	3.22245600	-0.10780000
C	-3.30847500	4.59909700	2.15088800
H	-2.57283300	5.18330600	2.72966500
H	-3.79055500	5.29328000	1.44035900
H	-4.07482000	4.23010900	2.85518200

Table S36: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, Oxo

Cu	1.42020500	0.06176000	-0.24225600
Cu	-1.40885700	0.04845300	0.26208200
O	0.01070800	-0.98855000	0.01287600
O	-0.00162800	1.16683900	-0.00038400
N	4.17224500	0.77826200	-0.17137100
N	2.96198600	1.26804300	-0.59537500
N	3.74346700	-1.55157800	-0.02230100
N	2.56651600	-1.45519200	-0.70543400
N	-2.53549200	-1.48826000	0.70448000
N	-3.67683000	-1.61530800	-0.03117700
N	-2.97228300	1.22617500	0.61563900
N	-4.17115400	0.69702500	0.20375800
C	4.28948100	-0.39583000	0.68374900
C	3.25103900	2.38486200	-1.31069400
C	4.64550800	2.59166200	-1.31559000
C	5.19448900	1.56015600	-0.58951800
C	2.21719100	3.29424900	-1.94363100
C	2.47149400	-2.57862300	-1.46267800
C	3.59967900	-3.38904600	-1.21325700
C	4.38969900	-2.70280200	-0.31865700
C	1.39040200	-2.86377000	-2.49349600
C	-4.26506800	-0.44995800	-0.68902900
C	-5.21505800	1.43094700	0.65494100
C	-4.69329700	2.46900800	1.39078100
C	-3.29156300	2.31862600	1.35618200
C	-2.28865400	3.27478600	1.97258600
C	-4.25709500	-2.82119700	0.16783500
C	-3.46167300	-3.50825600	1.05803900
C	-2.40100100	-2.64419900	1.40408800
C	-1.35944600	-2.90844800	2.47996300
H	5.35623300	-0.58754100	0.78613200
H	5.18087400	3.39413300	-1.79660400
H	3.82605200	-4.34194200	-1.66395900
H	-5.32831100	-0.66439000	-0.78421500
H	-5.25109300	3.24105700	1.89543100
H	-3.64505300	-4.49753700	1.44591900
C	3.69042300	-0.16063900	2.05528400
C	4.48407400	-0.23729600	3.19841100
N	2.39009500	0.16547100	2.06436800
C	3.89225300	0.05458000	4.43005200
H	5.53215700	-0.51034700	3.13093700
C	1.83920500	0.46018200	3.25133200
C	2.54779600	0.41972700	4.45455400
H	4.47435300	0.00694300	5.34439900
H	0.79528300	0.74460000	3.23484400
H	2.04881500	0.67165200	5.38380500
C	-3.68818400	-0.15944200	-2.05925100
C	-4.49631200	-0.20997600	-3.19354100
N	-2.39003900	0.17471900	-2.07470900
C	-3.92284000	0.11948600	-4.42432700
H	-5.54041700	-0.49571100	-3.12012100
C	-1.85680800	0.50347200	-3.26086700
C	-2.58063800	0.49190300	-4.45578500
H	-4.51633300	0.09243900	-5.33217200

H	-0.81376700	0.79102600	-3.25157500
H	-2.09422600	0.76996900	-5.38427600
H	6.21587500	1.32211200	-0.33220000
H	5.35373900	-2.92548500	0.11366300
H	-5.18467700	-3.07950700	-0.32115600
H	-6.23129100	1.15992400	0.40935800
C	-0.10446200	-3.58967400	1.89067100
H	0.58296600	-3.84273600	2.70639700
H	-0.36901000	-4.51443800	1.36663700
H	0.40598100	-2.92038200	1.19405500
C	-0.96776700	-1.59233000	3.16932800
H	-0.49494200	-0.91759700	2.45310800
H	-1.83948100	-1.09495100	3.60890200
H	-0.24573100	-1.79637500	3.96708000
C	-1.97842600	-3.85156800	3.53681500
H	-2.19282000	-4.84231800	3.12296200
H	-1.26188000	-3.98383200	4.35442200
H	-2.90330900	-3.43833800	3.95380000
C	0.16898800	-3.55544800	-1.84821400
H	-0.54890800	-3.81977400	-2.63357600
H	0.46625300	-4.47456400	-1.33179900
H	-0.31888000	-2.88844500	-1.13357000
C	0.95750000	-1.55558900	-3.17617800
H	0.50021900	-0.88001000	-2.45015300
H	1.80791300	-1.05152400	-3.64849000
H	0.21142600	-1.77385600	-3.94765600
C	1.97265500	-3.80883800	-3.56864500
H	2.21149900	-4.79502700	-3.15676200
H	1.22401000	-3.95311500	-4.35478200
H	2.87575500	-3.39185800	-4.02754900
C	1.52037500	4.08191400	-0.81154000
H	2.24440100	4.68789800	-0.25556400
H	0.76431700	4.75140200	-1.23690700
H	1.02753400	3.39686500	-0.11607800
C	1.18366300	2.47757200	-2.73667000
H	1.66453500	1.89718700	-3.53227000
H	0.64520500	1.80274400	-2.06635600
H	0.45405300	3.15509600	-3.19386500
C	2.90839200	4.28835400	-2.89793900
H	2.14561500	4.92098300	-3.36383200
H	3.60511900	4.94583900	-2.36689400
H	3.45386800	3.77043000	-3.69481400
C	-1.16543200	2.51713900	2.69960900
H	-1.57205600	1.88045500	3.49393300
H	-0.59748900	1.90592800	1.99343400
H	-0.47558700	3.23644900	3.15482000
C	-1.70415400	4.13928000	0.83162500
H	-2.49277700	4.72460500	0.34572500
H	-0.95914800	4.83366100	1.23626700
H	-1.22246700	3.51078300	0.07834600
C	-3.00006400	4.19569200	2.98452800
H	-2.25948200	4.86357900	3.43675900
H	-3.75946900	4.82149400	2.50375500
H	-3.47491700	3.62035500	3.78708100

Table S37: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, Peroxo

Cu	1.75765300	0.05525800	-0.00896500
Cu	-1.79566300	0.07667500	0.07274800
O	-0.01764800	-0.57117600	0.19520000
O	-0.02690500	0.86604100	-0.02255200
N	4.43818300	0.86706600	0.22507900
N	3.29500100	1.24861000	-0.42136400
N	4.06280100	-1.46566200	0.54585700
N	2.94594300	-1.54225800	-0.23996300
N	-3.02582100	-1.38131500	0.64052900
N	-4.16613800	-1.44848100	-0.10916900
N	-3.29267600	1.37833500	0.04864500
N	-4.42854700	0.88505200	-0.52864300
C	4.41868400	-0.21231700	1.20683400
C	3.65677100	2.25358700	-1.24752800
C	5.04075100	2.50076500	-1.11445800
C	5.50403800	1.60226800	-0.17793400
C	2.66218300	3.01212300	-2.10495600
C	3.04058700	-2.72280100	-0.89671600
C	4.21320100	-3.39552700	-0.48851300
C	4.84495700	-2.56380500	0.40922100
C	2.08125900	-3.16635100	-1.98967000
C	-4.44200200	-0.44356100	-1.13089600
C	-5.46127500	1.75584000	-0.41447600
C	-4.98184000	2.86044400	0.25682800
C	-3.62510500	2.59227000	0.53903100
C	-2.62750800	3.49285500	1.24043500
C	-4.99243200	-2.42970900	0.32902700
C	-4.36543000	-3.03243100	1.39764000
C	-3.14428900	-2.34701100	1.57972100
C	-2.11000700	-2.59576000	2.66316300
H	5.44520300	-0.33133800	1.54807700
H	5.62541600	3.24020400	-1.63843000
H	4.56223200	-4.35907200	-0.82358400
H	-5.46425600	-0.61766900	-1.46042400
H	-5.53975500	3.74610100	0.51677000
H	-4.74689700	-3.85303900	1.98435300
C	3.53095600	0.12518500	2.39162500
C	4.05374500	0.23833800	3.67745500
N	2.23771500	0.34068500	2.09817700
C	3.18803500	0.60379100	4.71222200
H	5.10529300	0.05204100	3.86740400
C	1.41746700	0.70356700	3.09524900
C	1.84840200	0.84864500	4.41410200
H	3.55881700	0.70202900	5.72702600
H	0.38982900	0.89192700	2.81368000
H	1.14504200	1.14788200	5.18305700
C	-3.50276300	-0.53785900	-2.32113500
C	-3.98535000	-0.80745300	-3.59933100
N	-2.20295100	-0.32971500	-2.05087200
C	-3.06953000	-0.86059100	-4.65362000
H	-5.04413400	-0.97044700	-3.76982000
C	-1.33251400	-0.37724400	-3.07023300
C	-1.71975100	-0.63881400	-4.38496500
H	-3.40859600	-1.06792600	-5.66309700

H	-0.29667400	-0.19616000	-2.81402900
H	-0.97605300	-0.66625400	-5.17352700
H	6.48752400	1.42713500	0.23235300
H	5.77352300	-2.65770000	0.95256300
H	-5.94419200	-2.61161100	-0.14808700
H	-6.43562200	1.52063900	-0.81630700
C	-0.88074500	-3.31654500	2.06722700
H	-0.16356200	-3.53801800	2.86619200
H	-1.17108000	-4.26121400	1.59471100
H	-0.38212900	-2.69179800	1.32237300
C	-1.67899400	-1.25292200	3.28265600
H	-1.23901600	-0.60524200	2.51870800
H	-2.53018500	-0.73082800	3.73291600
H	-0.92448600	-1.42481900	4.05791400
C	-2.72258000	-3.48355300	3.76413100
H	-2.98583600	-4.47606000	3.38228000
H	-1.98793800	-3.61991800	4.56473400
H	-3.61900200	-3.02665600	4.19798500
C	0.65066600	-3.35450600	-1.44734700
H	-0.00197900	-3.69936600	-2.25761300
H	0.63445900	-4.10782400	-0.65254400
H	0.24233200	-2.42160300	-1.05267800
C	2.10069900	-2.10837500	-3.11613100
H	1.82146100	-1.11871500	-2.74159500
H	3.10035800	-2.02916500	-3.55751500
H	1.39623400	-2.39193200	-3.90600100
C	2.55660300	-4.50989800	-2.57809100
H	2.55574100	-5.30283500	-1.82190000
H	1.87393000	-4.80976900	-3.38014500
H	3.56291100	-4.43220200	-3.00429100
C	1.89900500	4.00072500	-1.19189900
H	2.58756600	4.72202700	-0.73822300
H	1.15831300	4.55431800	-1.78014500
H	1.37783100	3.47044700	-0.38885600
C	1.67217500	2.03928800	-2.76970300
H	2.19180100	1.34831200	-3.44275700
H	1.13536900	1.46027400	-2.01220400
H	0.93170500	2.59882600	-3.35125800
C	3.40474400	3.80240400	-3.19888400
H	2.67377000	4.32613300	-3.82395000
H	4.07493600	4.55516700	-2.76995700
H	3.99153800	3.13815700	-3.84303300
C	-1.85723400	2.69179900	2.30757600
H	-2.53496000	2.29509200	3.07121900
H	-1.32489300	1.85521200	1.84481900
H	-1.11760600	3.33567100	2.79571500
C	-1.64456500	4.05533900	0.18858800
H	-2.17707200	4.64478600	-0.56578700
H	-0.90969700	4.70477600	0.67752300
H	-1.10846700	3.24857400	-0.32006600
C	-3.36426900	4.66114800	1.92132000
H	-2.63642800	5.29107900	2.44339300
H	-3.88618100	5.28930200	1.19113500
H	-4.09278700	4.30178000	2.65670100

Table S38: XYZ coordinates for optimised Structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 2.277 Å

Cu	-1.36518600	0.02223700	0.28212800
Cu	1.38510000	0.08205600	-0.25871700
O	0.02570900	-1.05378300	-0.02056500
O	-0.00657900	1.22206600	0.05248300
N	-4.13385000	0.63654500	0.30860500
N	-2.93335800	1.16311900	0.72010100
N	-3.60534400	-1.63682900	-0.12634600
N	-2.47896000	-1.53950900	0.63758000
N	2.53539200	-1.38979200	-0.81742200
N	3.70705600	-1.53086500	-0.13354100
N	2.91471300	1.31124600	-0.56143200
N	4.13166600	0.80258600	-0.17937900
C	-4.23356000	-0.43364500	-0.67356500
C	-3.25277400	2.19041900	1.55073600
C	-4.65533800	2.30302700	1.63925300
C	-5.17791600	1.30988600	0.84467900
C	-2.25617500	3.12477900	2.20960300
C	-2.31711800	-2.74639300	1.23978000
C	-3.34769400	-3.60726000	0.80658600
C	-4.15141800	-2.87122900	-0.03566800
C	-1.28527000	-3.07439400	2.30829500
C	4.26800600	-0.40987100	0.61649700
C	5.14644600	1.60749400	-0.56992900
C	4.58667100	2.67377500	-1.23433900
C	3.19291100	2.46443400	-1.22290700
C	2.15363700	3.40371600	-1.79995800
C	4.33546200	-2.68007100	-0.47261600
C	3.53868100	-3.31735700	-1.39738000
C	2.42458900	-2.47983700	-1.61981200
C	1.34449500	-2.70845100	-2.66544800
H	-5.29529300	-0.66072400	-0.75608000
H	-5.21300800	3.02182900	2.21718400
H	-3.50781800	-4.62968400	1.10958400
H	5.33749700	-0.60346200	0.68520700
H	5.11445700	3.50088200	-1.68066600
H	3.75176400	-4.25512000	-1.88489300
C	-3.70388000	-0.01608800	-2.02946400
C	-4.56118700	0.07332400	-3.12477100
N	-2.39950500	0.29067300	-2.06673500
C	-4.03235100	0.51807900	-4.33902300
H	-5.60950700	-0.19196000	-3.03423900
C	-1.90875400	0.72795600	-3.23626100
C	-2.68243900	0.85819400	-4.39235900
H	-4.66460000	0.60099500	-5.21685400
H	-0.85851900	0.98784200	-3.24616600
H	-2.22741300	1.21907000	-5.30823600
C	3.69956200	-0.24520400	2.01113100
C	4.52211200	-0.37101400	3.12934500
N	2.39661300	0.06529700	2.06736600
C	3.95773100	-0.15177500	4.38843000
H	5.57109200	-0.62711200	3.02271100
C	1.87189300	0.28812000	3.28162100
C	2.60974400	0.19233800	4.46414000
H	4.56254400	-0.23994900	5.28487600

H	0.82457700	0.55886900	3.30666700
H	2.12976700	0.38636900	5.41703600
H	-6.19504900	1.03215300	0.61116700
H	-5.06817100	-3.11281300	-0.55293000
H	5.29505800	-2.93305800	-0.04702400
H	6.17106500	1.35880700	-0.33799600
C	0.16237100	-3.50687700	-2.07154900
H	-0.55823200	-3.72749800	-2.86781400
H	0.50435800	-4.45669900	-1.64626100
H	-0.33801800	-2.92856300	-1.29149800
C	0.84391900	-1.36772200	-3.22687900
H	0.35628800	-0.78324700	-2.44386600
H	1.66460300	-0.78236400	-3.65660000
H	0.10510400	-1.55497300	-4.01338400
C	1.95343300	-3.52530100	-3.82847100
H	2.23770900	-4.53522300	-3.51532000
H	1.20221200	-3.62561100	-4.61897900
H	2.83351500	-3.02941400	-4.25222100
C	-0.02314200	-3.71670100	1.69062300
H	0.65836200	-4.01352000	2.49650200
H	-0.28052300	-4.61115000	1.11321600
H	0.48916600	-3.00733900	1.03631700
C	-0.90392400	-1.80638100	3.08761000
H	-0.42901600	-1.08311100	2.42243100
H	-1.78106200	-1.34394000	3.55382000
H	-0.18679800	-2.06112600	3.87501500
C	-1.91527400	-4.08449400	3.29548500
H	-2.12057000	-5.04816900	2.81793600
H	-1.20940500	-4.26526700	4.11308900
H	-2.84721000	-3.70023800	3.72421700
C	-1.70398900	4.06742200	1.11570000
H	-2.50971000	4.66964400	0.68140100
H	-0.96239100	4.74636700	1.55143700
H	-1.22736700	3.49392400	0.31713600
C	-1.11106800	2.34242800	2.87372100
H	-1.49709000	1.64832300	3.62944000
H	-0.54268600	1.78942100	2.12181600
H	-0.42785100	3.04251400	3.36762300
C	-2.96662400	3.96970700	3.28631100
H	-2.22993600	4.62344300	3.76461600
H	-3.74593600	4.60816500	2.85680600
H	-3.41630200	3.33910300	4.06149100
C	1.11860900	2.62590000	-2.62890100
H	1.59723400	2.09037400	-3.45679800
H	0.58790200	1.91475700	-1.99099900
H	0.38324800	3.32285100	-3.04581700
C	1.46405600	4.12902100	-0.62311900
H	2.19061300	4.71080100	-0.04488100
H	0.69996100	4.81487100	-1.00634600
H	0.98350800	3.40526400	0.04059800
C	2.83641200	4.44833700	-2.70532700
H	2.06929200	5.10549100	-3.12801200
H	3.53888500	5.07629000	-2.14675000
H	3.37315600	3.97513000	-3.53535200

Table S39: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 2.145 Å

Cu	1.42102300	0.03214000	-0.25860100
Cu	-1.42027500	0.07304800	0.22195500
O	-0.00495000	-0.98266500	0.03756900
O	0.00518300	1.15816800	-0.09520000
N	4.18276400	0.70298100	-0.24850100
N	2.97776200	1.19207400	-0.68719200
N	3.70654400	-1.59027400	0.14400400
N	2.55644700	-1.52749200	-0.58760400
N	-2.54982700	-1.42198400	0.79637400
N	-3.70878400	-1.59317200	0.09829500
N	-2.98121700	1.28011300	0.50693600
N	-4.18305100	0.73186700	0.13142100
C	4.28191700	-0.37786400	0.72343700
C	3.28117900	2.24419400	-1.48901300
C	4.68009300	2.41295200	-1.53366400
C	5.21667400	1.42535000	-0.74003000
C	2.25530800	3.12879500	-2.16839000
C	2.44391300	-2.72054000	-1.22627800
C	3.52997700	-3.53933700	-0.84965500
C	4.31609800	-2.78956700	-0.00361800
C	1.39175500	-3.07153600	-2.26749000
C	-4.27975800	-0.48516400	-0.66352000
C	-5.22306600	1.49935200	0.53198400
C	-4.69533500	2.58412200	1.19287900
C	-3.29467900	2.42356500	1.16880400
C	-2.28403000	3.40972300	1.72003800
C	-4.32354400	-2.74836900	0.44296800
C	-3.53001200	-3.35969200	1.38800100
C	-2.43474500	-2.49888600	1.61558500
C	-1.36912500	-2.68665400	2.68376200
H	5.34546900	-0.57821100	0.84128000
H	5.22600200	3.16292800	-2.08274700
H	3.73372900	-4.54195300	-1.18976900
H	-5.34306600	-0.70055200	-0.75284300
H	-5.24844000	3.39250500	1.64283100
H	-3.73364200	-4.29472800	1.88470400
C	3.69402600	0.01519200	2.06350300
C	4.50138300	0.09361500	3.19680800
N	2.38861800	0.32029900	2.04852300
C	3.91824400	0.52625500	4.39066600
H	5.55345100	-0.16788900	3.15031000
C	1.84555400	0.74872400	3.19776600
C	2.56754800	0.86813400	4.38768100
H	4.51103100	0.60098900	5.29629900
H	0.79648600	1.01106100	3.16104600
H	2.07353700	1.22287000	5.28554100
C	-3.68775300	-0.31160800	-2.04670300
C	-4.48729200	-0.44053500	-3.18104300
N	-2.38598000	0.00816500	-2.07749300
C	-3.89974600	-0.21486200	-4.42839800
H	-5.53632700	-0.70470200	-3.09553900
C	-1.83867900	0.23675600	-3.28067900
C	-2.55272100	0.13802900	-4.47728000
H	-4.48616400	-0.30558400	-5.33672400
H	-0.79311200	0.51511100	-3.28437700
H	-2.05561500	0.33654300	-5.42038400
H	6.23626400	1.18018400	-0.48199600
H	5.25501400	-2.99991700	0.48656100
H	-5.27210000	-3.02335600	0.00637500
H	-6.24044900	1.21430900	0.30927100
C	-0.13888300	-3.43020900	2.11761000
H	0.57031300	-3.62439800	2.93077300

H	-0.42797700	-4.39128100	1.67887700
H	0.35669600	-2.82613300	1.35394000
C	-0.94181600	-1.32413400	3.25289700
H	-0.47459800	-0.71750300	2.47446700
H	-1.79584600	-0.77811000	3.66882100
H	-0.20520600	-1.47358700	4.04959600
C	-1.96699700	-3.53014400	3.83289800
H	-2.20196300	-4.55067500	3.51276500
H	-1.22924200	-3.60005700	4.63913200
H	-2.87591000	-3.07239300	4.23843400
C	0.13993800	-3.69533900	-1.61115300
H	-0.55815700	-4.00778000	-2.39665600
H	0.40611900	-4.57719100	-1.01862200
H	-0.35870400	-2.97038800	-0.96343300
C	1.00028100	-1.81700200	-3.06555900
H	0.54097000	-1.07608800	-2.40805500
H	1.87089000	-1.36814300	-3.55641200
H	0.26765000	-2.08406400	-3.83450600
C	1.99574200	-4.10552100	-3.24475400
H	2.20645800	-5.05957200	-2.74999400
H	1.27196000	-4.30116300	-4.04291800
H	2.91986500	-3.73572700	-3.70219900
C	1.55567000	3.97151300	-1.07859800
H	2.27952700	4.60040500	-0.54832600
H	0.80533900	4.62308200	-1.54025500
H	1.05580300	3.32284300	-0.35355900
C	1.22319600	2.27905200	-2.92957400
H	1.70748200	1.65603600	-3.68998700
H	0.67419500	1.64274900	-2.23077600
H	0.50178200	2.93659000	-3.42740500
C	2.95671500	4.07491200	-3.16275100
H	2.20032100	4.69342800	-3.65699900
H	3.65775600	4.74780200	-2.65713400
H	3.49921700	3.51898300	-3.93561000
C	-1.17658300	2.68816600	2.50514300
H	-1.59618500	2.12395300	3.34617900
H	-0.62390600	2.01073400	1.84878800
H	-0.47018400	3.42530300	2.90270100
C	-1.68202200	4.18345500	0.52469600
H	-2.46088000	4.73891700	-0.00951500
H	-0.93343000	4.89874100	0.88412500
H	-1.19978800	3.49765200	-0.17669900
C	-2.98786000	4.40859600	2.66081600
H	-2.24121500	5.09844000	3.06779300
H	-3.73849400	5.00745300	2.13397300
H	-3.47258800	3.89809300	3.50055600

Table S40: XYZ coordinates for optimised structure: Singlet minimum path, TPSSH/6-31g(d), solvent model with dichloromethane, O...O = 2.013 Å

Cu	1.47363600	0.05777100	-0.21846700
Cu	-1.47578800	0.06004400	0.18653200
O	-0.00147000	-0.90741800	-0.01315000
O	-0.00108700	1.10529700	-0.04297000
N	4.22698000	0.76393000	-0.11858300
N	3.02900800	1.24684300	-0.57892800
N	3.77953600	-1.55714900	0.13585700
N	2.63073500	-1.48753600	-0.59758000
N	-2.60097300	-1.47687600	0.70199200
N	-3.77054900	-1.60834700	0.01204100
N	-3.04691000	1.25384900	0.50504000
N	-4.24247800	0.71841500	0.09567500
C	4.30924000	-0.36629800	0.79746500
C	3.33756000	2.32747900	-1.33707300
C	4.73420900	2.52097800	-1.33515900
C	5.26373700	1.51619500	-0.55757500
C	2.30859300	3.20679400	-2.01855600
C	2.55915900	-2.64687400	-1.30068600
C	3.66567700	-3.45446900	-0.96074200
C	4.42438200	-2.72924500	-0.06909300
C	1.52559700	-2.96203400	-2.37182200
C	-4.31948100	-0.47882000	-0.73162800
C	-5.28834700	1.47976800	0.49363400
C	-4.76971900	2.54755200	1.18929900
C	-3.36907300	2.38248800	1.18576900
C	-2.36025400	3.34887000	1.77439900
C	-4.40920100	-2.75655200	0.33619300
C	-3.62183700	-3.40612300	1.26029200
C	-2.50511900	-2.57505600	1.49487100
C	-1.43137800	-2.81108500	2.54586400
H	5.37088300	-0.55461800	0.94788000
H	5.28326700	3.29724200	-1.84328200
H	3.89972700	-4.43190000	-1.35107400
H	-5.37964300	-0.69088200	-0.85733500
H	-5.32874600	3.34713800	1.64779500
H	-3.84199100	-4.34753600	1.73744700
C	3.65743500	-0.05805400	2.13029600
C	4.40693300	-0.04966100	3.30487000
N	2.35199100	0.24310800	2.07129400
C	3.76302600	0.30497700	4.49327600
H	5.46090100	-0.30692300	3.29239600
C	1.75039300	0.59846200	3.21617600
C	2.41250700	0.64477400	4.44508700
H	4.30996100	0.32361100	5.43007600
H	0.70353000	0.86115900	3.14272100
H	1.87359700	0.94221500	5.33787400
C	-3.68435800	-0.26705400	-2.09030100
C	-4.44608900	-0.34602400	-3.25447500
N	-2.37855900	0.03739200	-2.06792500
C	-3.81308400	-0.08631400	-4.47288300
H	-5.50100800	-0.59723300	-3.21270100
C	-1.78657300	0.29843700	-3.24273400
C	-2.46053800	0.24898700	-4.46495900
H	-4.36941500	-0.13778500	-5.40289600

H	-0.73837300	0.56267900	-3.19991100
H	-1.92953700	0.47195700	-5.38375900
H	6.27923300	1.27967400	-0.27621300
H	5.36461900	-2.94043500	0.41866200
H	-5.36540500	-3.00250600	-0.10096800
H	-6.30225900	1.20237000	0.24626300
C	-0.16985300	-3.45410300	1.92915700
H	0.54457100	-3.68153800	2.72913700
H	-0.41712100	-4.38920400	1.41525500
H	0.30360000	-2.77296200	1.21819800
C	-1.06531200	-1.47899300	3.22218000
H	-0.63624800	-0.78825600	2.49305200
H	-1.94242500	-1.00987000	3.68135300
H	-0.31616300	-1.65453100	4.00166700
C	-1.98992100	-3.77159400	3.61889100
H	-2.17981200	-4.76964200	3.20983900
H	-1.24894200	-3.87865900	4.41809400
H	-2.91724500	-3.39040200	4.06022800
C	0.23607900	-3.55237700	-1.76079000
H	-0.44916500	-3.83182300	-2.56980100
H	0.45526900	-4.44976600	-1.17249800
H	-0.25889500	-2.81993400	-1.11849400
C	1.19728000	-1.68416800	-3.16380800
H	0.74371100	-0.93635600	-2.50933400
H	2.09623800	-1.25570100	-3.62031500
H	0.48025900	-1.91634400	-3.95842200
C	2.12250700	-4.00273100	-3.34476300
H	2.29735200	-4.96561400	-2.85305500
H	1.41096300	-4.17264800	-4.15959600
H	3.06527000	-3.65420800	-3.78023700
C	1.55724300	4.00128300	-0.92715200
H	2.24993200	4.62986600	-0.35664000
H	0.80589600	4.64910200	-1.39230800
H	1.05019600	3.32218700	-0.23547300
C	1.31913600	2.34974200	-2.82762800
H	1.83704500	1.76669200	-3.59728400
H	0.78027700	1.67106300	-2.16157900
H	0.58388600	2.99789100	-3.31700400
C	3.01108200	4.19584700	-2.96888200
H	2.25349100	4.81058600	-3.46617800
H	3.68384500	4.87003400	-2.42770400
H	3.58635500	3.67366200	-3.74164900
C	-1.26873500	2.60020000	2.55654700
H	-1.70286400	2.02129500	3.37993900
H	-0.71539900	1.93064400	1.89256100
H	-0.55916000	3.32106100	2.97749100
C	-1.73325900	4.14567100	0.60713400
H	-2.49946700	4.71589500	0.07023200
H	-0.98819300	4.84945200	0.99522600
H	-1.24030000	3.47361800	-0.10061600
C	-3.07078900	4.33025400	2.72795500
H	-2.32630900	5.00565700	3.16233400
H	-3.80994100	4.94558600	2.20389300
H	-3.57160100	3.80312500	3.54771300

Table S41: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 1.88 Å

Cu	-1.54291600	0.06599300	0.15387800
Cu	1.54295100	0.06577900	-0.15394600
O	-0.00001100	-0.82673300	0.00029500
O	0.00004800	1.05444900	-0.00040800
N	-4.30222200	0.75346500	0.00427400
N	-3.11633300	1.25813500	0.46990400
N	-3.84933000	-1.57894400	-0.10800800
N	-2.68775700	-1.48781300	0.60315300
N	2.68767400	-1.48837400	-0.60222600
N	3.84919300	-1.57917300	0.10906200
N	3.11645800	1.25762200	-0.47062900
N	4.30230200	0.75312400	-0.00469300
C	-4.35427200	-0.42709600	-0.84971700
C	-3.44385200	2.36724600	1.17491700
C	-4.84107200	2.55623500	1.13723100
C	-5.35131800	1.51783200	0.39056400
C	-2.42497900	3.27209300	1.83818400
C	-2.63681600	-2.59802300	1.38134300
C	-3.76969800	-3.39780900	1.11662500
C	-4.52320400	-2.71520100	0.18809500
C	-1.58581100	-2.86792800	2.44699900
C	4.35421500	-0.42688900	0.85005400
C	5.35146900	1.51717800	-0.39140200
C	4.84131900	2.55521200	-1.13864300
C	3.44409000	2.36628600	-1.17630100
C	2.42533500	3.27078800	-1.84021900
C	4.52291800	-2.71573400	-0.18622800
C	3.76936200	-3.39886700	-1.11433500
C	2.63665100	-2.59905900	-1.37972200
C	1.58563100	-2.86954600	-2.44522200
H	-5.40958600	-0.62581600	-1.03023200
H	-5.40309600	3.35005200	1.60252700
H	-4.02109200	-4.34115700	1.57438000
H	5.40950100	-0.62558000	1.03077500
H	5.40341600	3.34872400	-1.60436900
H	4.02062500	-4.34258400	-1.57140000
C	-3.65089100	-0.18814400	-2.17084600
C	-4.35313100	-0.22770500	-3.37340600
N	-2.34568700	0.10845000	-2.07686100
C	-3.65963400	0.06504500	-4.55069500
H	-5.41011200	-0.47179600	-3.39049400
C	-1.69549400	0.40444300	-3.21187600
C	-2.30842400	0.39524200	-4.46644200
H	-4.16970400	0.04435800	-5.50800400
H	-0.65086500	0.66541900	-3.10741100
H	-1.73274100	0.64550000	-5.35063900
C	3.65075500	-0.18692700	2.17095500
C	4.35289500	-0.22569200	3.37360000
N	2.34564000	0.10995000	2.07662800
C	3.65937400	0.06813600	4.55060700
H	5.40983200	-0.46995400	3.39096100
C	1.69543300	0.40699300	3.21136100
C	2.30825200	0.39859700	4.46598700
H	4.16936600	0.04809200	5.50797000

H	0.65087900	0.66815600	3.10662000
H	1.73256000	0.64968900	5.34994100
H	-6.35999700	1.26255600	0.10151500
H	-5.47577100	-2.93245200	-0.27152000
H	5.47540400	-2.93283600	0.27362400
H	6.36012100	1.26198400	-0.10218700
C	0.29486200	-3.45419200	-1.83215800
H	-0.40696800	-3.70041800	-2.63776000
H	0.50657700	-4.37050900	-1.27094200
H	-0.18097500	-2.73223400	-1.16397400
C	1.26884700	-1.56196200	-3.19294400
H	0.84347400	-0.82471700	-2.50766800
H	2.16862900	-1.13732300	-3.65129200
H	0.53401500	-1.75495300	-3.98175500
C	2.14967300	-3.89135000	-3.45556500
H	2.32029900	-4.86844100	-2.99104100
H	1.42205900	-4.03098400	-4.26193400
H	3.08926000	-3.54419500	-3.89892900
C	-0.29531000	-3.45362600	1.83437500
H	0.40654500	-3.69925100	2.64014000
H	-0.50739400	-4.37045000	1.27412700
H	0.18067500	-2.73250900	1.16538700
C	-1.26850300	-1.55975500	3.19346700
H	-0.84300100	-0.82328400	2.50743800
H	-2.16808100	-1.13440000	3.65155000
H	-0.53361700	-1.75225000	3.98234900
C	-2.15014700	-3.88858400	3.45833800
H	-2.32124100	-4.86602700	2.99472800
H	-1.42249000	-4.02778200	4.26474200
H	-3.08953300	-3.54063400	3.90150600
C	-1.67176900	4.04240000	0.73023200
H	-2.36442700	4.65557100	0.14329000
H	-0.92236100	4.70264000	1.18082600
H	-1.16155800	3.35073300	0.05354100
C	-1.43540600	2.44215600	2.67497900
H	-1.95384900	1.88553300	3.46353800
H	-0.89762900	1.73824400	2.03403600
H	-0.69869400	3.10499100	3.14184000
C	-3.13869200	4.28119400	2.75831000
H	-2.38890800	4.91474900	3.24377000
H	-3.81359500	4.93591800	2.19635200
H	-3.71465900	3.77463000	3.54084000
C	1.43597400	2.44041900	-2.67683500
H	1.95460500	1.88344000	-3.46501800
H	0.89809400	1.73678900	-2.03567100
H	0.69933300	3.10300300	-3.14416600
C	1.67187100	4.04162900	-0.73281300
H	2.36439200	4.65509800	-0.14602000
H	0.92255400	4.70163800	-1.18389700
H	1.16151800	3.35028900	-0.05589500
C	3.13922900	4.27944100	-2.76069200
H	2.38954700	4.91279500	-3.24657000
H	3.81406500	4.93440100	-2.19892900
H	3.71530500	3.77249300	-3.54289400

Table S42: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 1.749 Å

Cu	1.62415900	0.07122500	-0.11154300
Cu	-1.62416000	0.07126100	0.11152500
O	-0.00001100	-0.74769000	-0.00003800
O	0.00002000	1.00216000	0.00006400
N	4.36744400	0.77395600	0.09482100
N	3.19387200	1.27268800	-0.40241600
N	3.93044400	-1.56614100	0.16408900
N	2.77362600	-1.48956700	-0.55726700
N	-2.77365900	-1.48954400	0.55723500
N	-3.93047900	-1.56608400	-0.16412400
N	-3.19385300	1.27271800	0.40243600
N	-4.36743300	0.77401700	-0.09481000
C	4.39335900	-0.41658000	0.93670100
C	3.53293600	2.38214400	-1.09765100
C	4.92834500	2.57826100	-1.02584300
C	5.42420300	1.54145200	-0.26610900
C	2.51611000	3.27193900	-1.78447600
C	2.75493800	-2.58939800	-1.34870100
C	3.90161800	-3.37014100	-1.08501900
C	4.63116800	-2.68505700	-0.13895200
C	1.70996200	-2.86280800	-2.41880300
C	-4.39336800	-0.41650000	-0.93671800
C	-5.42417600	1.54153000	0.26613000
C	-4.92829900	2.57831400	1.02588700
C	-3.53289200	2.38217800	1.09767400
C	-2.51603900	3.27192000	1.78452700
C	-4.63122800	-2.68499100	0.13889700
C	-3.90170700	-3.37009100	1.08497300
C	-2.75500000	-2.58938700	1.34865200
C	-1.71004400	-2.86282800	2.41876400
H	5.44165600	-0.60490100	1.16409000
H	5.49853700	3.37455400	-1.47713300
H	4.17572200	-4.30312800	-1.55111000
H	-5.44166700	-0.60479100	-1.16412000
H	-5.49847600	3.37460700	1.47719600
H	-4.17584400	-4.30306700	1.55106800
C	3.62710800	-0.20120800	2.22796400
C	4.26994500	-0.26238900	3.46194000
N	2.32513100	0.09222500	2.08095700
C	3.52047800	0.00677900	4.61019800
H	5.32508100	-0.50576000	3.52550600
C	1.61967600	0.36517600	3.18849500
C	2.17350800	0.33553600	4.46964700
H	3.98521100	-0.03081600	5.58982300
H	0.58021000	0.62422800	3.03645100
H	1.55683800	0.56817900	5.33066400
C	-3.62709900	-0.20111500	-2.22796900
C	-4.26992100	-0.26226000	-3.46195400
N	-2.32511600	0.09228400	-2.08094400
C	-3.52043400	0.00690600	-4.61020000
H	-5.32506200	-0.50560400	-3.52553600
C	-1.61963800	0.36522800	-3.18847100
C	-2.17345600	0.33562100	-4.46962900
H	-3.98515800	-0.03066200	-5.58983100

H	-0.58016500	0.62424500	-3.03641400
H	-1.55676800	0.56825700	-5.33063500
H	6.42619800	1.28899300	0.04760300
H	5.58087000	-2.89232800	0.33127200
H	-5.58093000	-2.89223900	-0.33133800
H	-6.42617700	1.28908900	-0.04757600
C	-0.41139700	-3.43007800	1.80664500
H	0.28732400	-3.68359600	2.61264000
H	-0.61243700	-4.33866100	1.22926100
H	0.06729400	-2.69587700	1.15378500
C	-1.40597500	-1.55708300	3.17612900
H	-0.99162000	-0.80903900	2.49489300
H	-2.30980400	-1.14525100	3.63802100
H	-0.66753000	-1.74666500	3.96245800
C	-2.27143100	-3.89666200	3.41712700
H	-2.43696600	-4.86949100	2.94173200
H	-1.54635000	-4.04136500	4.22485800
H	-3.21411200	-3.55805000	3.86057000
C	0.41126000	-3.42989900	-1.80665400
H	-0.28746800	-3.68343400	-2.61263800
H	0.61221600	-4.33844500	-1.22918200
H	-0.06738500	-2.69559800	-1.15387000
C	1.40600900	-1.55708600	-3.17625500
H	0.99166900	-0.80897800	-2.49508200
H	2.30988400	-1.14533900	-3.63813100
H	0.66758600	-1.74666800	-3.96260500
C	2.27125800	-3.89675400	-3.41710100
H	2.43669000	-4.86957400	-2.94165200
H	1.54617000	-4.04142900	-4.22483100
H	3.21397600	-3.55826000	-3.86055300
C	1.71422900	4.02341400	-0.69780600
H	2.37651900	4.64750100	-0.08783900
H	0.96674100	4.67091300	-1.16959400
H	1.19586300	3.32197100	-0.03719900
C	1.56767700	2.42283400	-2.65071600
H	2.11738600	1.88980700	-3.43414100
H	1.04040800	1.69297700	-2.02968000
H	0.81960000	3.06747700	-3.12472200
C	3.23555900	4.29773700	-2.68044200
H	2.48909900	4.92137900	-3.18354500
H	3.88409700	4.96000400	-2.09660000
H	3.84110900	3.80422800	-3.44876200
C	-1.56757000	2.42273100	2.65064600
H	-2.11724000	1.88965400	3.43406300
H	-1.04035600	1.69290900	2.02952000
H	-0.81945000	3.06732300	3.12465400
C	-1.71420400	4.02348700	0.69788900
H	-2.37651900	4.64762600	0.08800300
H	-0.96669700	4.67094700	1.16970200
H	-1.19586300	3.32210200	0.03720000
C	-3.23544500	4.29764000	2.68061800
H	-2.48896000	4.92124200	3.18373300
H	-3.88401800	4.95995400	2.09686800
H	-3.84095000	3.80406200	3.44893000

Table S43: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 1.618 Å

Cu	-1.70766200	0.06541400	0.06800500
Cu	1.70761500	0.06540200	-0.06795400
O	-0.00000700	-0.67844600	0.00049900
O	-0.00003200	0.94036500	-0.00028500
N	-4.41729200	0.81784800	-0.21479000
N	-3.25509000	1.29524300	0.32494900
N	-4.02945600	-1.53293400	-0.22343800
N	-2.87660300	-1.49036700	0.50856400
N	2.87656600	-1.49053400	-0.50810900
N	4.02938400	-1.53287600	0.22396100
N	3.25502800	1.29509200	-0.32550500
N	4.41721600	0.81791300	0.21446600
C	-4.42801200	-0.38746100	-1.03577700
C	-3.59773800	2.41140300	1.00548300
C	-4.98658300	2.63196500	0.88525700
C	-5.47388900	1.60230900	0.10971800
C	-2.58492700	3.28443300	1.71963000
C	-2.91615100	-2.57189300	1.32250800
C	-4.09556100	-3.30583700	1.06799800
C	-4.78503600	-2.61061700	0.09940600
C	-1.88446000	-2.86777100	2.39867300
C	4.42795900	-0.38710800	1.03587200
C	5.47376200	1.60245600	-0.11002000
C	4.98644400	2.63191100	-0.88581400
C	3.59764200	2.41116200	-1.00619800
C	2.58484500	3.28393200	-1.72068100
C	4.78496100	-2.61068000	-0.09847000
C	4.09553100	-3.30621100	-1.06687100
C	2.91614400	-2.57233500	-1.32169200
C	1.88460300	-2.86848300	-2.39793200
H	-5.46653400	-0.55739200	-1.31306100
H	-5.55814800	3.43906300	1.31541100
H	-4.41347700	-4.21652000	1.55024400
H	5.46649100	-0.55694400	1.31317400
H	5.55797300	3.43899400	-1.31604700
H	4.41345900	-4.21705900	-1.54879700
C	-3.59661700	-0.21735100	-2.29375800
C	-4.18008200	-0.29919600	-3.55570200
N	-2.29529600	0.04961100	-2.09417100
C	-3.36913000	-0.08289200	-4.67303600
H	-5.23667600	-0.51988000	-3.66495000
C	-1.52903200	0.26956500	-3.17278200
C	-2.02162400	0.21488200	-4.47750600
H	-3.78728100	-0.13797000	-5.67260400
H	-0.49159400	0.50490300	-2.97490500
H	-1.35831800	0.40403600	-5.31416600
C	3.59661600	-0.21654700	2.29382700
C	4.18007700	-0.29825400	3.55578200
N	2.29535800	0.05067800	2.09419100
C	3.36919400	-0.08147900	4.67307400
H	5.23661900	-0.51917400	3.66506600
C	1.52916500	0.27110700	3.17275900
C	2.02176700	0.21661800	4.47748700
H	3.78734100	-0.13642900	5.67265100

H	0.49179000	0.50669400	2.97484500
H	1.35852900	0.40617200	5.31411200
H	-6.46872300	1.36526800	-0.23710700
H	-5.73823700	-2.78762000	-0.37657500
H	5.73813200	-2.78753700	0.37762700
H	6.46857700	1.36559100	0.23697800
C	0.56648200	-3.38577200	-1.78391300
H	-0.12453000	-3.66198700	-2.58904200
H	0.74210700	-4.27150200	-1.16425700
H	0.08842600	-2.61650400	-1.17269200
C	1.61975000	-1.58227600	-3.20438300
H	1.23395500	-0.79403100	-2.55127000
H	2.53612900	-1.21687400	-3.68022900
H	0.87515200	-1.77679700	-3.98390300
C	2.43869500	-3.94708200	-3.35056100
H	2.58702800	-4.90277500	-2.83606400
H	1.71856500	-4.11231500	-4.15867800
H	3.38958300	-3.63936100	-3.79933200
C	-0.56663800	-3.38574100	1.78457200
H	0.12449100	-3.66178000	2.58966000
H	-0.74266700	-4.27170300	1.16536100
H	-0.08850700	-2.61689700	1.17287600
C	-1.61901700	-1.58123600	3.20439000
H	-1.23308800	-0.79349200	2.55075600
H	-2.53517600	-1.21528700	3.68024200
H	-0.87430800	-1.77558800	3.98384500
C	-2.43863700	-3.94574200	3.35196100
H	-2.58729500	-4.90166400	2.83798500
H	-1.71840400	-4.11074100	4.16003500
H	-3.38937100	-3.63755300	3.80073600
C	-1.75134500	4.03394500	0.65519100
H	-2.39326700	4.67000200	0.03592900
H	-1.00675300	4.66964500	1.14725300
H	-1.22722400	3.33206500	-0.00042000
C	-1.66358100	2.41887100	2.59907600
H	-2.23411800	1.89304700	3.37233800
H	-1.13722900	1.68096800	1.98634300
H	-0.91337700	3.05054800	3.08681800
C	-3.31160200	4.31230600	2.60697400
H	-2.56988100	4.92379900	3.13156800
H	-3.93896700	4.98600400	2.01309700
H	-3.94028200	3.81985700	3.35718200
C	1.66358700	2.41806800	-2.59991700
H	2.23419100	1.89201800	-3.37297600
H	1.13721800	1.68034300	-1.98698400
H	0.91339600	3.04956700	-3.08790900
C	1.75117400	4.03373700	-0.65651800
H	2.39303400	4.67001100	-0.03741600
H	1.00657900	4.66925500	-1.14881200
H	1.22705200	3.33203200	-0.00072000
C	3.31154000	4.31155300	-2.60830200
H	2.56983100	4.92286200	-3.13312600
H	3.93885400	4.98545300	-2.01460100
H	3.94027900	3.81888700	-3.35831900

Table S44: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 1.488 Å

Cu	1.74425800	0.04578300	-0.01724300
Cu	-1.78484500	0.07989700	0.07291000
O	-0.02048000	-0.60435500	0.15254000
O	-0.02564700	0.87895700	0.03228000
N	4.43015400	0.85479100	0.20182600
N	3.28643700	1.23816100	-0.44328600
N	4.04442900	-1.47290700	0.54650400
N	2.92580100	-1.55776300	-0.23672400
N	-3.03575600	-1.35880200	0.65858100
N	-4.18038600	-1.41987000	-0.08433700
N	-3.26751700	1.39353300	0.03261400
N	-4.40672300	0.90933800	-0.54712200
C	4.40951800	-0.21481000	1.19295400
C	3.65220900	2.23572900	-1.27758400
C	5.03870900	2.47438000	-1.15055000
C	5.49944900	1.58011900	-0.20960600
C	2.66826800	3.00701400	-2.13672400
C	3.00972200	-2.75692600	-0.86344200
C	4.17616500	-3.42910400	-0.43787200
C	4.81527400	-2.58144600	0.43913300
C	2.05042300	-3.22933300	-1.94500600
C	-4.44014100	-0.43062800	-1.12474900
C	-5.42326100	1.80224200	-0.46304200
C	-4.93053200	2.91069600	0.19181300
C	-3.58284500	2.62300400	0.49602900
C	-2.58102800	3.51767600	1.19929300
C	-5.02352700	-2.37531700	0.37884600
C	-4.40243000	-2.96760400	1.45675000
C	-3.16729400	-2.30216700	1.61803100
C	-2.12968900	-2.54750500	2.69890500
H	5.43757900	-0.33636300	1.52884200
H	5.62649900	3.20614500	-1.68160800
H	4.51718500	-4.40337100	-0.74898200
H	-5.46413100	-0.59633100	-1.45327100
H	-5.47471900	3.81134900	0.42810000
H	-4.79616500	-3.76857900	2.06224600
C	3.53182300	0.13856800	2.38019600
C	4.06466900	0.26547200	3.66064000
N	2.23791700	0.35597300	2.09254200
C	3.20800500	0.64831100	4.69665700
H	5.11672100	0.07647300	3.84540300
C	1.42681800	0.73702800	3.09031900
C	1.86776900	0.89674800	4.40427900
H	3.58619800	0.75754800	5.70760900
H	0.39865100	0.92877900	2.81307400
H	1.17137600	1.20999100	5.17403700
C	-3.50122800	-0.56108200	-2.31176100
C	-3.98552100	-0.85251700	-3.58453300
N	-2.19956800	-0.36207500	-2.04435400
C	-3.06897000	-0.93984900	-4.63589900
H	-5.04617900	-1.00505900	-3.75333700
C	-1.32811300	-0.44354700	-3.06073100
C	-1.71683200	-0.72936900	-4.36996200
H	-3.40924500	-1.16483700	-5.64119000

H	-0.28997700	-0.27283300	-2.80658300
H	-0.97233100	-0.78409100	-5.15638900
H	6.48309800	1.40156700	0.19874200
H	5.74292100	-2.66988600	0.98498200
H	-5.98112100	-2.54916500	-0.08941300
H	-6.39784300	1.57863800	-0.87091700
C	-0.91890300	-3.30335500	2.10857800
H	-0.20176600	-3.52632500	2.90722600
H	-1.23041600	-4.24933400	1.65251000
H	-0.41249400	-2.69927900	1.35179800
C	-1.66563500	-1.20006600	3.28337200
H	-1.21669400	-0.58137500	2.50055600
H	-2.50159800	-0.64816800	3.72652200
H	-0.90909400	-1.36958600	4.05715700
C	-2.74999500	-3.39777100	3.82462400
H	-3.03543400	-4.39359400	3.46816600
H	-2.01163100	-3.52958600	4.62254000
H	-3.63400100	-2.91380700	4.25451900
C	0.61511700	-3.38619800	-1.40559100
H	-0.03474200	-3.75639600	-2.20687600
H	0.58785800	-4.10910100	-0.58341500
H	0.21055500	-2.43654000	-1.04913300
C	2.08676800	-2.21553000	-3.11085200
H	1.81647500	-1.20964100	-2.77662400
H	3.08922400	-2.16457400	-3.54987500
H	1.38298600	-2.52200400	-3.89273100
C	2.51446400	-4.59874100	-2.48133600
H	2.50167800	-5.36358000	-1.69673400
H	1.83175200	-4.92009800	-3.27490900
H	3.52305700	-4.54774400	-2.90598100
C	1.97887300	4.06400200	-1.24093400
H	2.71263900	4.76619000	-0.83053500
H	1.25026800	4.63234500	-1.83032000
H	1.45370500	3.58847100	-0.40676800
C	1.61261600	2.06538400	-2.74160700
H	2.08018800	1.31591900	-3.39004000
H	1.05162800	1.55481300	-1.95346400
H	0.89913200	2.64250500	-3.33953100
C	3.41796300	3.72157300	-3.27794800
H	2.69531200	4.25466700	-3.90481400
H	4.13257000	4.45900700	-2.89660600
H	3.95812500	3.00752200	-3.90957200
C	-1.85721600	2.72579700	2.30549000
H	-2.56386100	2.36176100	3.05903900
H	-1.33098300	1.86735700	1.87767300
H	-1.11791800	3.36598000	2.79909100
C	-1.55989100	4.03400200	0.16045300
H	-2.06017900	4.61806500	-0.61982200
H	-0.82345600	4.67865900	0.65333500
H	-1.02891100	3.20524300	-0.31719400
C	-3.30726800	4.71849700	1.83374800
H	-2.57739800	5.34533800	2.35661800
H	-3.79898500	5.33915300	1.07670200
H	-4.05941500	4.39329900	2.56123900

Table S45: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/6-31g(d), solvent model with dichloromethane, O...O = 1.359 Å

Cu	1.78803100	0.03816700	-0.00128600
Cu	-1.82502400	0.06886400	0.05804900
O	-0.01782400	-0.54505800	0.15471900
O	-0.02664400	0.80961700	0.05254600
N	4.45375200	0.88496200	0.24111400
N	3.31343500	1.25288000	-0.41817100
N	4.10278000	-1.45368500	0.55151100
N	2.98029100	-1.55829900	-0.22434000
N	-3.10109200	-1.35475100	0.63373800
N	-4.24448600	-1.37888900	-0.11319600
N	-3.27844800	1.41268400	0.00760700
N	-4.41553200	0.95203700	-0.59425600
C	4.43466200	-0.19757700	1.21846500
C	3.67493000	2.25783300	-1.24464700
C	5.05641300	2.51618500	-1.09967000
C	5.51827300	1.62573000	-0.15553200
C	2.68913100	3.01753700	-2.11206300
C	3.08999200	-2.74767400	-0.86384500
C	4.27852300	-3.39338200	-0.45883100
C	4.90270100	-2.53959100	0.42291600
C	2.12321100	-3.23640900	-1.93044200
C	-4.46188100	-0.39093200	-1.16406400
C	-5.41963300	1.85973500	-0.51764900
C	-4.91925600	2.95508600	0.15355700
C	-3.58112400	2.64302000	0.47602500
C	-2.57356900	3.51583200	1.19809600
C	-5.12533700	-2.29765800	0.35490000
C	-4.52943500	-2.90649200	1.43810900
C	-3.26983100	-2.28745800	1.59654300
C	-2.23286400	-2.56967800	2.66836200
H	5.45841100	-0.30541900	1.57136100
H	5.64028900	3.25817600	-1.62084800
H	4.64123100	-4.35525200	-0.78384600
H	-5.48085400	-0.54093400	-1.51430700
H	-5.45222600	3.86311000	0.38738700
H	-4.95326600	-3.68977100	2.04657900
C	3.53205200	0.12480400	2.39674800
C	4.04469600	0.24371100	3.68610800
N	2.23709900	0.32153800	2.09580700
C	3.16750800	0.59447900	4.71617400
H	5.09776100	0.07308600	3.88228800
C	1.40543400	0.67085100	3.08871700
C	1.82618700	0.81974900	4.41028200
H	3.53069200	0.69661300	5.73332800
H	0.37704100	0.84535800	2.80076400
H	1.11374800	1.10712000	5.17538600
C	-3.50174200	-0.54951400	-2.33128600
C	-3.97137100	-0.82697700	-3.61274200
N	-2.19841200	-0.39388900	-2.04014500
C	-3.03920400	-0.95133100	-4.64636700
H	-5.03359400	-0.94137400	-3.80100400
C	-1.31123700	-0.51510300	-3.03950800
C	-1.68541000	-0.79267700	-4.35447700
H	-3.36842400	-1.16691200	-5.65735900

H	-0.27147900	-0.38795000	-2.76669900
H	-0.92806100	-0.88168200	-5.12527100
H	6.49947300	1.45909300	0.26374100
H	5.83581100	-2.61156800	0.96162400
H	-6.08725100	-2.43819300	-0.11562500
H	-6.39147700	1.65496800	-0.94160100
C	-1.04720900	-3.34792800	2.05646200
H	-0.32218000	-3.58968000	2.84238200
H	-1.38529700	-4.28465600	1.60021100
H	-0.54075800	-2.75079900	1.29419700
C	-1.72866300	-1.23937400	3.25935000
H	-1.27586300	-0.62444100	2.47529700
H	-2.54507100	-0.67135700	3.71821300
H	-0.96607600	-1.43434100	4.02101900
C	-2.86460100	-3.41469900	3.79090800
H	-3.18084500	-4.39807200	3.42599700
H	-2.12286000	-3.57550300	4.58038400
H	-3.73099600	-2.91161400	4.23452400
C	0.69529300	-3.38497800	-1.37047600
H	0.03248300	-3.76231000	-2.15766700
H	0.67787800	-4.09787700	-0.53931100
H	0.29898900	-2.43016800	-1.01921000
C	2.14352500	-2.23634500	-3.10861300
H	1.86098100	-1.23004200	-2.78480000
H	3.14367800	-2.17783400	-3.55185700
H	1.44125400	-2.56070100	-3.88464500
C	2.58368400	-4.61195700	-2.45286200
H	2.58702200	-5.36374300	-1.65562400
H	1.88985900	-4.94862500	-3.23028900
H	3.58508600	-4.56433600	-2.89452800
C	1.99449400	4.07948300	-1.22610100
H	2.72528700	4.78567100	-0.81723700
H	1.26739900	4.64267300	-1.82229200
H	1.46641100	3.60828800	-0.39124500
C	1.63705400	2.06769300	-2.71012300
H	2.10722300	1.31662700	-3.35472900
H	1.07818600	1.55862600	-1.91939300
H	0.92082200	2.63826800	-3.31102200
C	3.43767400	3.72500300	-3.25858800
H	2.71399800	4.25009300	-3.89107400
H	4.14912600	4.46846800	-2.88300900
H	3.98140100	3.00743800	-3.88312800
C	-1.86740100	2.70214500	2.30004700
H	-2.58385200	2.33853700	3.04449000
H	-1.34829600	1.84188700	1.86680300
H	-1.12360700	3.32712600	2.80628000
C	-1.53860200	4.02990600	0.17177400
H	-2.02606000	4.62879900	-0.60543300
H	-0.79702600	4.65968300	0.67603600
H	-1.01608900	3.19895000	-0.31118100
C	-3.28922500	4.71831500	1.84113700
H	-2.55556600	5.33061900	2.37578800
H	-3.76835300	5.35301900	1.08770300
H	-4.05033000	4.39416900	2.55973500

Table S46: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, Oxo

Cu	1.83593200	0.03211400	-0.03224100
Cu	-1.83608000	0.03207900	0.03250400
O	0.00009800	-0.62759700	0.00017600
O	0.00007700	0.80053600	-0.00147000
N	4.48545200	0.99641600	0.36323100
N	3.33744100	1.37878500	-0.27016300
N	4.29212000	-1.38307800	0.32716800
N	3.15339100	-1.48207400	-0.41869800
N	-3.15350700	-1.48163900	0.41969100
N	-4.29239800	-1.38284800	-0.32591800
N	-3.33757100	1.37895400	0.26943000
N	-4.48542200	0.99663700	-0.36422700
C	4.54489700	-0.21786800	1.16620500
C	3.64670500	2.49397300	-0.95862000
C	5.00383700	2.81495400	-0.74878600
C	5.50420400	1.84584900	0.08420100
C	2.64144500	3.27530400	-1.77873000
C	3.32425200	-2.55544100	-1.21559700
C	4.57793100	-3.14328200	-0.94969900
C	5.16850800	-2.36963500	0.01775600
C	2.31479000	-2.99542400	-2.25686200
C	-4.54497100	-0.21841500	-1.16608700
C	-5.50404400	1.84649600	-0.08597300
C	-5.00365400	2.81595300	0.74658700
C	-3.64669900	2.49463100	0.95712600
C	-2.64141500	3.27621800	1.77694200
C	-5.16883100	-2.36914600	-0.01584300
C	-4.57815900	-3.14234700	0.95191900
C	-3.32436600	-2.55452200	1.21727000
C	-2.31471700	-2.99416700	2.25848400
H	5.57790900	-0.30675300	1.49686700
H	5.54715400	3.64699700	-1.16240300
H	5.00074300	-4.01401400	-1.42021000
H	-5.57798500	-0.30750500	-1.49669800
H	-5.54686300	3.64844000	1.15946000
H	-5.00099700	-4.01276600	1.42298800
C	3.64602700	-0.15238100	2.38650300
C	4.18605500	-0.19721700	3.66553300
N	2.33290800	-0.03824800	2.14936900
C	3.32073500	-0.11532700	4.75362600
H	5.25559200	-0.29113800	3.81388700
C	1.50815000	0.04484600	3.19937300
C	1.95803300	0.01067800	4.51511600
H	3.70709900	-0.14607800	5.76543700
H	0.45596200	0.14444600	2.96902500
H	1.25036500	0.08337000	5.33146500
C	-3.64602200	-0.15410500	-2.38638200
C	-4.18592200	-0.20025200	-3.66542000
N	-2.33294500	-0.03954900	-2.14924200
C	-3.32050000	-0.11928900	-4.75350000
H	-5.25543200	-0.29444900	-3.81377900
C	-1.50808300	0.04267000	-3.19923500
C	-1.95783800	0.00716100	-4.51498500
H	-3.70675400	-0.15107000	-5.76532200
H	-0.45594500	0.14269600	-2.96884000

H	-1.25010900	0.07917800	-5.33134100
H	6.48904300	1.69478200	0.49794200
H	6.12925900	-2.43853500	0.50365700
H	-6.12971600	-2.43813600	-0.50146300
H	-6.48878800	1.69551000	-0.49996800
C	-1.07222600	-3.59203600	1.57230200
H	-0.36937000	-3.94246300	2.33277200
H	-1.34309500	-4.44194400	0.94166000
H	-0.56845200	-2.84720700	0.95665900
C	-1.90956900	-1.78312300	3.11761400
H	-1.45256800	-1.00302300	2.50261000
H	-2.77444800	-1.35613400	3.63062500
H	-1.18153600	-2.09519600	3.87052000
C	-2.94332400	-4.06232300	3.16953800
H	-3.20175900	-4.96606400	2.61235200
H	-2.22285600	-4.34620400	3.93952100
H	-3.84062400	-3.69022000	3.67005500
C	1.07186400	-3.59245800	-1.57075900
H	0.36919800	-3.94318900	-2.33126700
H	1.34223000	-4.44201800	-0.93943400
H	0.56808400	-2.84702700	-0.95585600
C	1.91031600	-1.78471600	-3.11680500
H	1.45344200	-1.00410300	-2.50234900
H	2.77547200	-1.35829900	-3.62982000
H	1.18238300	-2.09694700	-3.86974000
C	2.94333000	-4.06434000	-3.16707300
H	3.20131100	-4.96781600	-2.60924800
H	2.22300600	-4.34847100	-3.93709900
H	3.84089700	-3.69284100	-3.66756200
C	1.73184800	4.06149300	-0.81145400
H	2.31638500	4.76001300	-0.20792600
H	0.99700800	4.63689700	-1.38038900
H	1.20025100	3.38637100	-0.13852000
C	1.79479000	2.33039700	-2.64761200
H	2.42477300	1.74215300	-3.31925200
H	1.19940200	1.65250800	-2.03042900
H	1.10355300	2.92004200	-3.25517600
C	3.37869900	4.26643500	-2.69554700
H	2.64804400	4.81522900	-3.29360500
H	3.94923500	5.00047700	-2.12209300
H	4.05787800	3.75230000	-3.38022500
C	-1.79391000	2.33160100	2.64529100
H	-2.42327900	1.74310400	3.31728300
H	-1.19856800	1.65395800	2.02777400
H	-1.10254500	2.92149900	3.25246400
C	-1.73265700	4.06299800	0.80936300
H	-2.31782600	4.76130500	0.20620600
H	-0.99783800	4.63868900	1.37803700
H	-1.20103900	3.38823900	0.13607900
C	-3.37873200	4.26682800	2.69428800
H	-2.64809500	4.81586500	3.29214500
H	-3.94987000	5.00071800	2.12123500
H	-4.05739300	3.75222600	3.37912900

Table S47: XYZ coordinates for Optimised structure: Singlet minimum path, TPSSh/tzvp, Peroxo

Cu	-1.83607200	0.03220000	0.03232800
Cu	1.83610400	0.03233700	-0.03248500
O	0.00018500	-0.62735500	-0.00083700
O	-0.00004900	0.80085400	0.00009000
N	-4.48543300	0.99656000	-0.36407900
N	-3.33730700	1.37938700	0.26886900
N	-4.29251300	-1.38290900	-0.32574600
N	-3.15363300	-1.48143400	0.41982200
N	3.15276900	-1.48222100	-0.41923400
N	4.29159900	-1.38370100	0.32650900
N	3.33804400	1.37839900	-0.26991800
N	4.48602300	0.99566500	0.36321200
C	-4.54502200	-0.21846400	-1.16597000
C	-3.64654000	2.49475500	0.95694900
C	-5.00378700	2.81550300	0.74731900
C	-5.50425500	1.84591100	-0.08502700
C	-2.64105700	3.27695200	1.77591000
C	-3.32443900	-2.55396800	1.21785600
C	-4.57826400	-3.14188500	0.95278900
C	-5.16899700	-2.36900500	-0.01520700
C	-2.31484100	-2.99310700	2.25931100
C	4.54498800	-0.21886600	1.16587500
C	5.50506600	1.84459700	0.08374700
C	5.00487700	2.81375600	-0.74928900
C	3.64753400	2.49329200	-0.95870800
C	2.64243500	3.27519000	-1.77841600
C	5.16707400	-2.37127100	0.01787100
C	4.57586800	-3.14500400	-0.94915000
C	3.32275000	-2.55621300	-1.21551300
C	2.31330800	-2.99568500	-2.25699800
H	-5.57803800	-0.30747800	-1.49658500
H	-5.54710700	3.64768800	1.16063600
H	-5.00114000	-4.01211500	1.42417500
H	5.57800400	-0.30836300	1.49636800
H	5.54851700	3.64547500	-1.16312500
H	4.99803400	-4.01632100	-1.41915300
C	-3.64605100	-0.15425100	-2.38624900
C	-4.18595300	-0.20042900	-3.66528900
N	-2.33297500	-0.03982500	-2.14914600
C	-3.32051400	-0.11951800	-4.75336200
H	-5.25545700	-0.29462300	-3.81368100
C	-1.50808700	0.04234500	-3.19910700
C	-1.95785200	0.00689400	-4.51485800
H	-3.70676500	-0.15130200	-5.76518400
H	-0.45594000	0.14224700	-2.96870300
H	-1.25014600	0.07893900	-5.33123200
C	3.64629100	-0.15309800	2.38629800
C	4.18645900	-0.19816000	3.66526100
N	2.33321700	-0.03833400	2.14934400
C	3.32129700	-0.11569900	4.75344300
H	5.25595200	-0.29269200	3.81352100
C	1.50860500	0.04531900	3.19940400
C	1.95864300	0.01106900	4.51510000
H	3.70775900	-0.14658000	5.76521300
H	0.45644300	0.14546400	2.96915900

H	1.25113900	0.08428500	5.33154500
H	-6.48917200	1.69457000	-0.49848200
H	-6.12991300	-2.43817400	-0.50073700
H	6.12779200	-2.44064300	0.50376300
H	6.48994900	1.69320200	0.49725800
C	1.06961400	-3.59165100	-1.57137800
H	0.36701900	-3.94186900	-2.33218300
H	1.33906400	-4.44138500	-0.93990600
H	0.56614200	-2.84580600	-0.95675000
C	1.91019700	-1.78484200	-3.11742100
H	1.45360500	-1.00376100	-2.50337000
H	2.77594600	-1.35920900	-3.63007800
H	1.18244700	-2.09669400	-3.87068700
C	2.94134100	-4.06533300	-3.16672400
H	3.19828600	-4.96891900	-2.60861600
H	2.22107300	-4.34898000	-3.93698000
H	3.83942800	-3.69472400	-3.66692500
C	-1.07214900	-3.59116400	1.57367400
H	-0.36947200	-3.94117200	2.33449300
H	-1.34281600	-4.44139800	0.94339100
H	-0.56825900	-2.84661600	0.95779800
C	-1.91001000	-1.78166000	3.11805200
H	-1.45271600	-1.00184300	2.50291800
H	-2.77509200	-1.35443200	3.63051300
H	-1.18231100	-2.09341100	3.87141600
C	-2.94344800	-4.06097000	3.17072900
H	-3.20168700	-4.96496700	2.61388300
H	-2.22303800	-4.34441600	3.94092200
H	-3.84086100	-3.68879400	3.67098000
C	-1.73173500	4.06196300	0.80736700
H	-2.31649500	4.75964400	0.20309300
H	-0.99682800	4.63817200	1.37539700
H	-1.20022600	3.38604000	0.13517300
C	-1.79413400	2.33317500	2.64576000
H	-2.42386900	1.74593200	3.31850400
H	-1.19899200	1.65437000	2.02934800
H	-1.10263200	2.92363100	3.25222700
C	-3.37796900	4.26924300	2.69173600
H	-2.64707900	4.81877600	3.28882300
H	-3.94870800	5.00257900	2.11759000
H	-4.05686800	3.75595200	3.37731700
C	1.79443100	2.33096000	-2.64672900
H	2.42349500	1.74237200	-3.31893000
H	1.19886800	1.65344400	-2.02931700
H	1.10324700	2.92122700	-3.25374300
C	1.73409500	4.06233800	-0.81072100
H	2.31960000	4.76036300	-0.20757800
H	0.99949100	4.63835600	-1.37933800
H	1.20222400	3.38777400	-0.13744300
C	3.37996200	4.26548400	-2.69597000
H	2.64937800	4.81463000	-3.29378400
H	3.95142100	4.99929200	-2.12315500
H	4.05834100	3.75056800	-3.38085100

Table S48: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 2.277 Å

Cu	1.43155800	0.03263100	-0.20925400
Cu	-1.42631000	0.03545900	0.18271200
O	0.00730900	-1.07545600	0.02676600
O	-0.00386900	1.19941400	-0.07669800
N	4.18805700	0.82236800	-0.03364600
N	3.00012300	1.27146000	-0.54943100
N	3.80755800	-1.50983100	0.21634400
N	2.68390500	-1.48959200	-0.55565700
N	-2.65542100	-1.47453900	0.65293000
N	-3.78132200	-1.56236200	-0.11140200
N	-3.01286400	1.27738000	0.47173000
N	-4.19578300	0.77525000	-0.00828700
C	4.28051000	-0.30166000	0.88556600
C	3.31066100	2.35293200	-1.30109600
C	4.69816100	2.58427800	-1.23524000
C	5.21830600	1.60379200	-0.43152400
C	2.31024500	3.20442900	-2.05204600
C	2.68090400	-2.64425800	-1.26045900
C	3.81314400	-3.40025500	-0.89524700
C	4.50903600	-2.64998800	0.01803200
C	1.68633100	-3.01236500	-2.34502900
C	-4.27608300	-0.40620100	-0.85306900
C	-5.24114600	1.55019400	0.36147900
C	-4.73762500	2.58235700	1.10762600
C	-3.34342300	2.38899100	1.17024000
C	-2.36774200	3.32299200	1.85508100
C	-4.46230500	-2.69953700	0.15996900
C	-3.75049400	-3.37970100	1.11475500
C	-2.63000800	-2.58360300	1.42770100
C	-1.62738000	-2.87062600	2.52941700
H	5.34477700	-0.45358000	1.05625500
H	5.24584500	3.36921700	-1.72669600
H	4.10063800	-4.36114200	-1.28566600
H	-5.33901100	-0.58380200	-1.00655100
H	-5.30024300	3.37774000	1.56409800
H	-4.02161900	-4.31912600	1.56472600
C	3.60516200	-0.02155600	2.20951200
C	4.34789100	0.02611400	3.38285300
N	2.29077800	0.20728400	2.14764800
C	3.68661600	0.34119400	4.56730300
H	5.41394700	-0.17108900	3.37723200
C	1.66956000	0.52157200	3.28916400
C	2.32380200	0.60125200	4.51573500
H	4.22840700	0.38964500	5.50437800
H	0.61046800	0.72315300	3.21632700
H	1.76930600	0.86374200	5.40817800
C	-3.61252300	-0.20461700	-2.19631100
C	-4.36271400	-0.23497400	-3.36543900
N	-2.29886400	0.03250600	-2.15768100
C	-3.70981900	0.00508300	-4.57186900
H	-5.42785300	-0.43539500	-3.34031400
C	-1.68540900	0.27326300	-3.32094400
C	-2.34728900	0.27093200	-4.54595000
H	-4.25737000	-0.00880200	-5.50674400
H	-0.62649900	0.48126700	-3.26752900

H	-1.79893800	0.47550300	-5.45713600
H	6.22748700	1.40151700	-0.10824700
H	5.44439900	-2.82576100	0.52619400
H	-5.39655200	-2.92218700	-0.33161900
H	-6.24842800	1.30668000	0.06150800
C	-0.39439000	-3.61114400	1.97422800
H	0.26398500	-3.88201700	2.80407500
H	-0.68727400	-4.53023900	1.46139400
H	0.15722100	-2.97658500	1.27982400
C	-1.19910300	-1.56050200	3.20432500
H	-0.68863200	-0.90870900	2.49359100
H	-2.05839500	-1.03235000	3.62523700
H	-0.50333600	-1.78313500	4.01670700
C	-2.30055300	-3.76946000	3.58698700
H	-2.54399400	-4.75599800	3.18675200
H	-1.60608900	-3.91800800	4.41653100
H	-3.21216300	-3.31637900	3.98382800
C	0.46190000	-3.73500000	-1.74902500
H	-0.19358300	-4.05744300	-2.56250600
H	0.76557600	-4.62154900	-1.18747800
H	-0.09681100	-3.07031900	-1.08949200
C	1.24345700	-1.75125900	-3.09980400
H	0.72087100	-1.06366100	-2.43269500
H	2.09764500	-1.23773200	-3.54821100
H	0.55415900	-2.03193000	-3.89947700
C	2.37500500	-3.96350200	-3.34559500
H	2.62895200	-4.92219200	-2.88790800
H	1.68603000	-4.16863400	-4.16761300
H	3.28255800	-3.52290700	-3.76516300
C	1.48702000	4.00370400	-1.02330800
H	2.13379600	4.64655200	-0.42113700
H	0.76534900	4.63777800	-1.54457900
H	0.94541600	3.32897000	-0.35810700
C	1.38550400	2.32646700	-2.90841700
H	1.95755600	1.73422100	-3.62750500
H	0.79562800	1.66371800	-2.27319300
H	0.69381900	2.96495200	-3.46351700
C	3.05306100	4.18851300	-2.97321500
H	2.31957400	4.78245300	-3.52231300
H	3.67763000	4.88334400	-2.40708400
H	3.67780200	3.66734100	-3.70309900
C	-1.28846600	2.54618200	2.62006700
H	-1.73824400	1.88803600	3.36884800
H	-0.67125200	1.96292100	1.93460500
H	-0.63698300	3.25500700	3.13749800
C	-1.72349600	4.21021600	0.76880900
H	-2.48237900	4.80245300	0.25171000
H	-1.01149300	4.89848900	1.23110100
H	-1.19635200	3.60131200	0.03418000
C	-3.12450500	4.22470900	2.84813700
H	-2.40637400	4.87267800	3.35491300
H	-3.84504700	4.87210100	2.34359500
H	-3.64761500	3.64038400	3.60922200

Table S49: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 2.145 Å

Cu	-1.47915800	0.03880400	0.16283300
Cu	1.47914400	0.03878700	-0.16284800
O	-0.00000500	-1.00080100	0.00006800
O	-0.00002000	1.14417000	-0.00006700
N	-4.24059100	0.81465100	-0.05427100
N	-3.06112100	1.28366900	0.46213000
N	-3.85967300	-1.52692800	-0.19862700
N	-2.72980400	-1.48695200	0.56374700
N	2.72969000	-1.48709700	-0.56362200
N	3.85952800	-1.52709900	0.19880200
N	3.06114400	1.28351100	-0.46225500
N	4.24058600	0.81445600	0.05419200
C	-4.31401000	-0.34712000	-0.92708400
C	-3.38675500	2.38142900	1.18205400
C	-4.77567100	2.60078500	1.09916000
C	-5.28122600	1.59623300	0.31591600
C	-2.39679100	3.26489600	1.91038300
C	-2.74120700	-2.60785800	1.32072500
C	-3.88677700	-3.36349100	0.99839300
C	-4.57741400	-2.64574800	0.05545600
C	-1.74127800	-2.93976800	2.41222000
C	4.31394600	-0.34723100	0.92712300
C	5.28125000	1.59602500	-0.31593800
C	4.77575600	2.60058500	-1.09920700
C	3.38683500	2.38127000	-1.18215600
C	2.39695500	3.26479000	-1.91054500
C	4.57727700	-2.64591500	-0.05530000
C	3.88665800	-3.36363900	-0.99825900
C	2.74110700	-2.60798400	-1.32062000
C	1.74119400	-2.93987800	-2.41213500
H	-5.37364900	-0.50493500	-1.11925000
H	-5.33388200	3.39385800	1.56516300
H	-4.18505900	-4.30205700	1.43260700
H	5.37357900	-0.50508500	1.11928400
H	5.33401000	3.39362900	-1.56520800
H	4.18492600	-4.30221500	-1.43246300
C	-3.60155600	-0.12458100	-2.24238000
C	-4.30740600	-0.12229600	-3.43892100
N	-2.28753800	0.09859100	-2.15221800
C	-3.60762600	0.13716100	-4.61477200
H	-5.37458500	-0.31212200	-3.45773800
C	-1.62812400	0.35776800	-3.28583100
C	-2.24450900	0.38873900	-4.53378600
H	-4.12062000	0.14919600	-5.56907100
H	-0.57009800	0.55353200	-3.18700500
H	-1.66162000	0.60773300	-5.41981100
C	3.60152700	-0.12453600	2.24241200
C	4.30739400	-0.12220600	3.43894100
N	2.28751800	0.09869400	2.15225100
C	3.60764500	0.13735400	4.61478900
H	5.37456500	-0.31208000	3.45775200
C	1.62813200	0.35795900	3.28586100
C	2.24453600	0.38897700	4.53380500
H	4.12065300	0.14942700	5.56907900
H	0.57011100	0.55375600	3.18704700

H	1.66166300	0.60804400	5.41982300
H	-6.28619100	1.37709100	-0.00950500
H	-5.51743300	-2.83154200	-0.44038300
H	5.51727200	-2.83173400	0.44057600
H	6.28619900	1.37685200	0.00951400
C	0.48593300	-3.61681000	-1.82796000
H	-0.17434900	-3.91431400	-2.64711500
H	0.75107300	-4.51422000	-1.26418700
H	-0.05484300	-2.93277500	-1.17276000
C	1.35191800	-1.65806400	-3.16325700
H	0.86210600	-0.94953900	-2.49275100
H	2.22739200	-1.17975800	-3.60937600
H	0.65077200	-1.90527300	-3.96382300
C	2.39860500	-3.91244400	-3.41165100
H	2.61797000	-4.87935800	-2.95322800
H	1.70537000	-4.09320200	-4.23579000
H	3.32169900	-3.50315800	-3.82905400
C	-0.48606300	-3.61676100	1.82801600
H	0.17423600	-3.91427600	2.64715300
H	-0.75125800	-4.51416800	1.26426400
H	0.05472000	-2.93275500	1.17279000
C	-1.35192800	-1.65796200	3.16331900
H	-0.86210300	-0.94946400	2.49279500
H	-2.22737100	-1.17961600	3.60945800
H	-0.65077100	-1.90519400	3.96386800
C	-2.39870300	-3.91229300	3.41176800
H	-2.61812600	-4.87920300	2.95336700
H	-1.70545100	-4.09306900	4.23589000
H	-3.32176600	-3.50295800	3.82919300
C	-1.62031900	4.08163700	0.85807200
H	-2.29901900	4.70551700	0.27154300
H	-0.90112800	4.73563000	1.35755700
H	-1.07978100	3.42042900	0.17945100
C	-1.42694500	2.42373700	2.75309900
H	-1.96627100	1.81513700	3.48383300
H	-0.82157600	1.77926200	2.11312900
H	-0.75015800	3.08940600	3.29450800
C	-3.15008700	4.23290900	2.84013100
H	-2.42401500	4.84769800	3.37606000
H	-3.80067700	4.90990200	2.28181100
H	-3.75070700	3.69872500	3.58070600
C	1.42684600	2.42370100	-2.75301700
H	1.96597600	1.81486300	-3.48369900
H	0.82137600	1.77947900	-2.11288900
H	0.75016900	3.08943300	-3.29448700
C	1.62076700	4.08186800	-0.85827900
H	2.29966000	4.70570800	-0.27193100
H	0.90165200	4.73592800	-1.35778800
H	1.08017100	3.42088700	-0.17948500
C	3.15034500	4.23250700	-2.84053300
H	2.42433200	4.84732300	-3.37651000
H	3.80109200	4.90949300	-2.28238700
H	3.75081600	3.69809000	-3.58106000

Table S50: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 2.013 Å

Cu	-1.54000900	0.03989300	0.12630000
Cu	1.53992600	0.03984500	-0.12628300
O	-0.00003100	-0.93039800	0.00035000
O	-0.00000400	1.08253800	-0.00012100
N	-4.28925200	0.84735800	-0.13689100
N	-3.11713600	1.29944300	0.40768400
N	-3.94181900	-1.50304600	-0.24287800
N	-2.80988200	-1.48910700	0.51767400
N	2.80991200	-1.48919100	-0.51706600
N	3.94196700	-1.50276800	0.24331700
N	3.11702100	1.29939900	-0.40799300
N	4.28915400	0.84764300	0.13677300
C	-4.35272800	-0.32449100	-0.99722900
C	-3.44447400	2.39929400	1.12151900
C	-4.82854100	2.63696600	1.00930900
C	-5.32922500	1.63978700	0.21283100
C	-2.45358300	3.26262600	1.87257500
C	-2.85958300	-2.59850300	1.28874600
C	-4.02956300	-3.32121700	0.97886500
C	-4.69666800	-2.59403500	0.02605900
C	-1.86314400	-2.94483400	2.37873000
C	4.35272200	-0.32399800	0.99740600
C	5.32901800	1.64018500	-0.21302300
C	4.82821300	2.63713600	-1.00971500
C	3.44420400	2.39917600	-1.12202200
C	2.45321000	3.26217800	-1.87331700
C	4.69728200	-2.59335800	-0.02597900
C	4.03034600	-3.32067200	-0.97878900
C	2.85999600	-2.59841500	-1.28836000
C	1.86350000	-2.94505900	-2.37819000
H	-5.40718300	-0.46825100	-1.22514900
H	-5.38723000	3.43623300	1.46419700
H	-4.35607800	-4.24518500	1.42383900
H	5.40718500	-0.46760200	1.22538500
H	5.38680000	3.43641800	-1.46470200
H	4.35713100	-4.24446300	-1.42393000
C	-3.59023000	-0.13070600	-2.28948100
C	-4.25109200	-0.13370700	-3.51122400
N	-2.27536100	0.06841500	-2.15713800
C	-3.50365400	0.09146000	-4.66457400
H	-5.32056300	-0.30204000	-3.56644400
C	-1.56850400	0.29254700	-3.26942700
C	-2.13881900	0.31431600	-4.53911800
H	-3.98174300	0.09828400	-5.63688400
H	-0.51056000	0.46581900	-3.13329500
H	-1.52003600	0.50424900	-5.40729900
C	3.59019200	-0.12999400	2.28961100
C	4.25107300	-0.13266600	3.51134500
N	2.27529700	0.06894600	2.15724000
C	3.50363400	0.09267000	4.66466200
H	5.32056400	-0.30087200	3.56657600
C	1.56843900	0.29323200	3.26949700
C	2.13877300	0.31534700	4.53917600
H	3.98173700	0.09975400	5.63696200
H	0.51046800	0.46635200	3.13336400

H	1.51997400	0.50540400	5.40731800
H	-6.32965400	1.43277000	-0.13380500
H	-5.64110800	-2.75676900	-0.46944600
H	5.64184000	-2.75578500	0.46940300
H	6.32945200	1.43341400	0.13374300
C	0.58306100	-3.56250700	-1.78444400
H	-0.07796000	-3.87083900	-2.59899400
H	0.81509700	-4.44490400	-1.18369100
H	0.05424600	-2.83918100	-1.16188500
C	1.51907400	-1.67644100	-3.17471400
H	1.04861700	-0.93060900	-2.53056000
H	2.41230600	-1.23855800	-3.62670700
H	0.81658400	-1.92656000	-3.97328700
C	2.50036300	-3.96966600	-3.33663700
H	2.69687900	-4.92237200	-2.83937400
H	1.80597400	-4.16671200	-4.15601100
H	3.43340000	-3.59790100	-3.76699300
C	-0.58267600	-3.56240600	1.78517300
H	0.07830900	-3.87059700	2.59980700
H	-0.81467400	-4.44490500	1.18455400
H	-0.05382500	-2.83918300	1.16251900
C	-1.51874700	-1.67603700	3.17496900
H	-1.04830800	-0.93033900	2.53065800
H	-2.41199000	-1.23810000	3.62689300
H	-0.81625000	-1.92598400	3.97359000
C	-2.50004900	-3.96922200	3.33739700
H	-2.69646100	-4.92207700	2.84038200
H	-1.80572900	-4.16600700	4.15689200
H	-3.43315200	-3.59738600	3.76754500
C	-1.63803000	4.06761200	0.84113000
H	-2.29095500	4.70714300	0.24234400
H	-0.91684700	4.70531400	1.35863400
H	-1.09539500	3.39983100	0.17036400
C	-1.51813800	2.39925400	2.73256300
H	-2.08383800	1.80087900	3.45148200
H	-0.91463900	1.74064100	2.10475200
H	-0.83685400	3.04849800	3.28804600
C	-3.20773000	4.24125000	2.79008300
H	-2.48253500	4.84356300	3.34119600
H	-3.83714400	4.92908400	2.22086200
H	-3.83069700	3.71490200	3.51768100
C	1.51807800	2.39846000	-2.73330400
H	2.08398800	1.80013100	-3.45209300
H	0.91469500	1.73978800	-2.10544200
H	0.83668100	3.04745600	-3.28894000
C	1.63730700	4.06707000	-0.84208600
H	2.28997000	4.70685100	-0.24327900
H	0.91602300	4.70452200	-1.35976000
H	1.09475900	3.39921800	-0.17131400
C	3.20723800	4.24087300	-2.79084600
H	2.48197200	4.84298500	-3.34208500
H	3.83645800	4.92888500	-2.22162800
H	3.83037800	3.71458400	-3.51833900

Table S51: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 1.881 Å

Cu	1.61522200	0.03854100	-0.09144500
Cu	-1.61521900	0.03850900	0.09144100
O	0.00000900	-0.86373100	-0.00004100
O	-0.00000700	1.01745200	0.00000300
N	4.33861800	0.89963000	0.22948200
N	3.17556000	1.32495600	-0.35179400
N	4.04396700	-1.46184700	0.28851500
N	2.91205000	-1.48629800	-0.47239700
N	-2.91201600	-1.48633900	0.47243400
N	-4.04392700	-1.46193200	-0.28848700
N	-3.17558800	1.32490400	0.35174400
N	-4.33862200	0.89954200	-0.22955800
C	4.39800500	-0.28499700	1.07281200
C	3.50008600	2.42841100	-1.05877100
C	4.87554300	2.69550000	-0.90825400
C	5.37338200	1.71054200	-0.09428300
C	2.50787100	3.26368900	-1.83970600
C	3.00953300	-2.58501600	-1.25245100
C	4.20821700	-3.26270200	-0.95104000
C	4.84390500	-2.51827900	0.01018400
C	2.01832900	-2.95923800	-2.33750300
C	-4.39796700	-0.28512000	-1.07284100
C	-5.37340900	1.71045100	0.09413400
C	-4.87560600	2.69547100	0.90804800
C	-3.50016700	2.42836400	1.05869600
C	-2.50802800	3.26369400	1.83967400
C	-4.84385500	-2.51836200	-0.01011500
C	-4.20816500	-3.26273500	0.95114800
C	-3.00948500	-2.58502900	1.25252800
C	-2.01826800	-2.95919900	2.33758700
H	5.44592900	-0.40791400	1.33957000
H	5.43109400	3.50482500	-1.34918200
H	4.57063600	-4.16986400	-1.40261300
H	-5.44588300	-0.40807100	-1.33961900
H	-5.43117900	3.50482800	1.34889100
H	-4.57057800	-4.16988100	1.40275900
C	3.58212100	-0.13438500	2.33897700
C	4.19555500	-0.14755100	3.58510100
N	2.26672400	0.02863200	2.16392900
C	3.39850500	0.02376700	4.71422500
H	5.26695300	-0.28401500	3.67740700
C	1.51033700	0.19861600	3.25310900
C	2.03209200	0.20390800	4.54345700
H	3.83972400	0.02067800	5.70382900
H	0.45274400	0.33904500	3.07928800
H	1.37560200	0.34846900	5.39244100
C	-3.58205800	-0.13452500	-2.33899100
C	-4.19544700	-0.14783700	-3.58513400
N	-2.26668800	0.02867600	-2.16390700
C	-3.39838000	0.02350800	-4.71424200
H	-5.26682700	-0.28443100	-3.67746800
C	-1.51028600	0.19869100	-3.25307000
C	-2.03199500	0.20383200	-4.54343700
H	-3.83956400	0.02030600	-5.70386100
H	-0.45271700	0.33926900	-3.07922000

H	-1.37549400	0.34842300	-5.39240800
H	6.36783700	1.52376900	0.27995300
H	5.79217900	-2.64864900	0.50789000
H	-5.79212600	-2.64876200	-0.50781900
H	-6.36784700	1.52365400	-0.28013900
C	-0.71890000	-3.51883100	1.72955600
H	-0.05599200	-3.84705800	2.53475400
H	-0.92471200	-4.37810400	1.08724300
H	-0.20041400	-2.75689700	1.14511700
C	-1.71091100	-1.71517000	3.18864900
H	-1.26382600	-0.92796400	2.57707800
H	-2.61730000	-1.32133600	3.65446600
H	-1.00337800	-1.97733000	3.97891400
C	-2.63842600	-4.03754000	3.24519100
H	-2.82112800	-4.96751700	2.70150400
H	-1.94208400	-4.26339700	4.05539000
H	-3.57687100	-3.70094500	3.69252400
C	0.71892800	-3.51878000	-1.72946100
H	0.05603000	-3.84705100	-2.53465000
H	0.92469700	-4.37800700	-1.08707300
H	0.20045000	-2.75678200	-1.14509600
C	1.71104100	-1.71526800	-3.18867400
H	1.26397500	-0.92799400	-2.57717800
H	2.61745700	-1.32150800	-3.65450200
H	1.00351700	-1.97746500	-3.97893500
C	2.63847400	-4.03767300	-3.24500700
H	2.82111900	-4.96761600	-2.70124400
H	1.94214900	-4.26356100	-4.05521100
H	3.57694700	-3.70114900	-3.69233400
C	1.65897500	4.06917600	-0.83556200
H	2.28882500	4.72940100	-0.23454100
H	0.93587100	4.68620600	-1.37511800
H	1.11590900	3.40309800	-0.16315400
C	1.60247000	2.37196600	-2.70365200
H	2.19085600	1.77357200	-3.40390400
H	0.99842600	1.70971900	-2.07954400
H	0.91990800	3.00099300	-3.28046400
C	3.26179500	4.24173000	-2.75788400
H	2.53748100	4.82565000	-3.32962900
H	3.87120700	4.94627200	-2.18741200
H	3.90523800	3.71492200	-3.46705600
C	-1.60283300	2.37206700	2.70393400
H	-2.19138600	1.77381100	3.40416500
H	-0.99868800	1.70969900	2.08005600
H	-0.92036300	3.00116000	3.28078400
C	-1.65891500	4.06898100	0.83555100
H	-2.28862500	4.72916000	0.23433200
H	-0.93586000	4.68604200	1.37513700
H	-1.11578400	3.40277100	0.16332900
C	-3.26205800	4.24192100	2.75756600
H	-2.53781300	4.82585600	3.32938300
H	-3.87129200	4.94643900	2.18687500
H	-3.90569400	3.71526200	3.46667400

Table S52: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 1.749 Å

Cu	1.69976000	0.03729400	-0.06476300
Cu	-1.69976100	0.03730500	0.06476300
O	-0.00000400	-0.79516900	-0.00001000
O	0.00000400	0.95468100	0.00000500
N	4.39591400	0.93831800	0.29734500
N	3.24099900	1.34716800	-0.30894700
N	4.14115500	-1.43115600	0.31043300
N	3.00796100	-1.48380500	-0.44755600
N	-3.00797000	-1.48377100	0.44765100
N	-4.14116800	-1.43116200	-0.31033200
N	-3.24099600	1.34719300	0.30885900
N	-4.39590400	0.93831500	-0.29743000
C	4.45151000	-0.26039500	1.12173100
C	3.56264500	2.45579600	-1.00626900
C	4.93086600	2.74381100	-0.82665900
C	5.42634500	1.76421300	-0.00413100
C	2.56820200	3.27143400	-1.80550900
C	3.13753600	-2.57169000	-1.23580100
C	4.35800100	-3.21496500	-0.94606500
C	4.97303600	-2.46014300	0.02074300
C	2.14292100	-2.96752400	-2.30957200
C	-4.45150400	-0.26046100	-1.12172400
C	-5.42633100	1.76424400	0.00396700
C	-4.93085500	2.74389600	0.82643400
C	-3.56264400	2.45587300	1.00609800
C	-2.56821100	3.27155400	1.80530800
C	-4.97306500	-2.46011200	-0.02055800
C	-4.35803200	-3.21487500	0.94629800
C	-3.13755700	-2.57159400	1.23598000
C	-2.14293400	-2.96737000	2.30976500
H	5.49293500	-0.37007900	1.41806100
H	5.48377000	3.56241400	-1.25379400
H	4.74590500	-4.10765800	-1.40524500
H	-5.49292800	-0.37015700	-1.41805500
H	-5.48375800	3.56253700	1.25349800
H	-4.74594400	-4.10753000	1.40554500
C	3.59634700	-0.14738200	2.36712100
C	4.17405400	-0.17710900	3.62995900
N	2.28240700	-0.00407100	2.16129500
C	3.34289500	-0.04626300	4.73973800
H	5.24477100	-0.29607900	3.74967800
C	1.49196700	0.12658700	3.23186100
C	1.97810300	0.11164100	4.53563700
H	3.75684100	-0.06361000	5.74090800
H	0.43689300	0.25048000	3.03018100
H	1.29613900	0.22369700	5.36929100
C	-3.59633000	-0.14755200	-2.36711600
C	-4.17402500	-0.17739000	-3.62995700
N	-2.28239200	-0.00422000	-2.16129000
C	-3.34285500	-0.04663800	-4.73973900
H	-5.24474000	-0.29637400	-3.74967700
C	-1.49194200	0.12634700	-3.23186000
C	-1.97806500	0.11128700	-4.53563900
H	-3.75679200	-0.06407300	-5.74091200
H	-0.43687000	0.25025900	-3.03018000

H	-1.29609400	0.22327300	-5.36929700
H	6.41577500	1.59080400	0.38937800
H	5.92514100	-2.56716600	0.51667400
H	-5.92517600	-2.56715800	-0.51647300
H	-6.41575500	1.59082100	-0.38955100
C	-0.84939000	-3.51573900	1.67993600
H	-0.17721800	-3.85644600	2.47211100
H	-1.06086000	-4.36394300	1.02489700
H	-0.33620400	-2.74457600	1.10374000
C	-1.82593600	-1.73808600	3.17969500
H	-1.38468600	-0.93957000	2.57787100
H	-2.72749200	-1.35126300	3.66042100
H	-1.11162100	-2.01459800	3.95896700
C	-2.75853600	-4.06035700	3.20158100
H	-2.95369800	-4.97711000	2.63996000
H	-2.05532000	-4.30779700	3.99947700
H	-3.68986600	-3.72754800	3.66629300
C	0.84935900	-3.51582800	-1.67972600
H	0.17719200	-3.85657700	-2.47188800
H	1.06080500	-4.36399200	-1.02462700
H	0.33617500	-2.74461900	-1.10358900
C	1.82596100	-1.73829400	-3.17959500
H	1.38473300	-0.93971900	-2.57783300
H	2.72753100	-1.35153400	-3.66034400
H	1.11164400	-2.01484400	-3.95885000
C	2.75851600	-4.06058600	-3.20130200
H	2.95365900	-4.97729900	-2.63961200
H	2.05530500	-4.30807400	-3.99918700
H	3.68985600	-3.72782300	-3.66603000
C	1.69328700	4.07114700	-0.81853600
H	2.30461300	4.74582400	-0.21444300
H	0.96784400	4.67299000	-1.37195100
H	1.15145000	3.40312100	-0.14680900
C	1.68719100	2.36051800	-2.67549800
H	2.29359300	1.76659700	-3.36388300
H	1.08404800	1.69114600	-2.05756400
H	1.00316700	2.97557800	-3.26557600
C	3.31993600	4.25410400	-2.72027500
H	2.59566200	4.82569700	-3.30444600
H	3.91357900	4.96920300	-2.14635400
H	3.97889500	3.73127600	-3.41801900
C	-1.68722900	2.36069000	2.67538100
H	-2.29365400	1.76682100	3.36379000
H	-1.08407600	1.69126900	2.05750900
H	-1.00321600	2.97578400	3.26543300
C	-1.69326700	4.07119500	0.81830300
H	-2.30457400	4.74584100	0.21415500
H	-0.96782900	4.67306400	1.37169400
H	-1.15142400	3.40312200	0.14662700
C	-3.31995800	4.25429100	2.71999100
H	-2.59569200	4.82591500	3.30414200
H	-3.91358000	4.96935800	2.14601000
H	-3.97893800	3.73151400	3.41775400

Table S53: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 1.618 Å

Cu	-1.76796500	0.03584200	0.04842500
Cu	1.76796800	0.03584100	-0.04842900
O	0.00000100	-0.72522400	0.00000800
O	0.00000300	0.89358700	0.00001500
N	-4.44209900	0.96524300	-0.33257900
N	-3.29111000	1.36181800	0.28758200
N	-4.21526200	-1.40904200	-0.31988000
N	-3.07972300	-1.48269000	0.43327000
N	3.07972300	-1.48268900	-0.43326900
N	4.21526300	-1.40904000	0.31988000
N	3.29111000	1.36181900	-0.28758000
N	4.44209900	0.96524500	0.33258000
C	-4.49787700	-0.24155100	-1.14600500
C	-3.60741300	2.47376000	0.98009500
C	-4.97039400	2.77729700	0.78460800
C	-5.46745400	1.80231800	-0.04299400
C	-2.60840600	3.27359100	1.78981900
C	-3.22893000	-2.56369900	1.22589200
C	-4.46486700	-3.18182200	0.94652900
C	-5.06806100	-2.41869100	-0.02132100
C	-2.22773900	-2.97972300	2.28545500
C	4.49787700	-0.24155000	1.14600600
C	5.46745400	1.80231800	0.04299100
C	4.97039500	2.77729300	-0.78461500
C	3.60741200	2.47375900	-0.98009700
C	2.60840300	3.27359000	-1.78981800
C	5.06806200	-2.41868800	0.02131900
C	4.46486800	-3.18181900	-0.94653200
C	3.22893100	-2.56369700	-1.22589300
C	2.22773900	-2.97971900	-2.28545500
H	-5.53508800	-0.34204400	-1.45981900
H	-5.51926100	3.60246700	1.20441300
H	-4.86929900	-4.06435600	1.41108500
H	5.53508800	-0.34204200	1.45982000
H	5.51926200	3.60246100	-1.20442500
H	4.86930100	-4.06435100	-1.41108900
C	-3.62004400	-0.15142500	-2.37860700
C	-4.17761800	-0.18963900	-3.65024800
N	-2.30690700	-0.02058800	-2.15577800
C	-3.32804000	-0.08177300	-4.74847500
H	-5.24759300	-0.29786500	-3.78539300
C	-1.49802900	0.08810600	-3.21527600
C	-1.96459000	0.06279700	-4.52573900
H	-3.72697100	-0.10652400	-5.75556300
H	-0.44474600	0.20212600	-2.99791900
H	-1.26891100	0.15666300	-5.35022800
C	3.62004400	-0.15142400	2.37860800
C	4.17761700	-0.18964100	3.65024900
N	2.30690800	-0.02058400	2.15577900
C	3.32803900	-0.08177600	4.74847600
H	5.24759200	-0.29787000	3.78539400
C	1.49802900	0.08811000	3.21527600
C	1.96458900	0.06279800	4.52573900
H	3.72697000	-0.10653000	5.75556400
H	0.44474700	0.20213500	2.99791800

H	1.26891000	0.15666500	5.35022800
H	-6.45441600	1.63930300	-0.44700100
H	-6.02395200	-2.50852000	-0.51334900
H	6.02395400	-2.50851700	0.51334700
H	6.45441700	1.63930300	0.44699700
C	0.95754200	-3.55306300	-1.63036300
H	0.27296400	-3.90024300	-2.40887000
H	1.19719700	-4.40107900	-0.98480200
H	0.44552100	-2.79457600	-1.03794700
C	1.86823300	-1.75804900	-3.14968500
H	1.41690600	-0.97001500	-2.54118900
H	2.75278000	-1.34981800	-3.64405000
H	1.14873800	-2.05166500	-3.91792300
C	2.85107300	-4.05980000	-3.18679900
H	3.07594100	-4.97134600	-2.62780100
H	2.14028500	-4.32373200	-3.97265400
H	3.76709300	-3.70741700	-3.66724200
C	-0.95754500	-3.55307500	1.63036100
H	-0.27296700	-3.90025500	2.40886800
H	-1.19720600	-4.40109200	0.98480300
H	-0.44552300	-2.79459200	1.03794100
C	-1.86822500	-1.75805300	3.14968100
H	-1.41689400	-0.97002300	2.54118300
H	-2.75277000	-1.34981600	3.64404600
H	-1.14873100	-2.05167100	3.91791800
C	-2.85107600	-4.05979900	3.18680100
H	-3.07594800	-4.97134500	2.62780700
H	-2.14028900	-4.32373100	3.97265700
H	-3.76709500	-3.70741100	3.66724400
C	-1.71540000	4.06600100	0.81265100
H	-2.31314600	4.75183000	0.20752700
H	-0.98598300	4.65560300	1.37395200
H	-1.17766100	3.39424400	0.14131500
C	-1.74512400	2.34713200	2.66175600
H	-2.36398300	1.75738700	3.34245600
H	-1.14534400	1.67210300	2.04630100
H	-1.05798000	2.95073500	3.26006700
C	-3.35424100	4.26145900	2.70352400
H	-2.62746500	4.82286900	3.29446900
H	-3.93628400	4.98501200	2.12833000
H	-4.02359900	3.74348700	3.39493700
C	1.74510200	2.34712800	-2.66173400
H	2.36394700	1.75737200	-3.34243600
H	1.14532600	1.67211000	-2.04626400
H	1.05795500	2.95073000	-3.26004200
C	1.71541500	4.06601800	-0.81264800
H	2.31317300	4.75184800	-0.20753800
H	0.98599700	4.65562000	-1.37394800
H	1.17767800	3.39427200	-0.14129900
C	3.35423600	4.26144200	-2.70354300
H	2.62745800	4.82285000	-3.29448700
H	3.93629100	4.98499700	-2.12836400
H	4.02358200	3.74345600	-3.39495800

Table S54: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 1.488 Å

Cu	1.81638300	0.03274000	-0.03671000
Cu	-1.81637700	0.03295700	0.03690100
O	-0.00015200	-0.65912800	-0.00003800
O	0.00011000	0.82905900	-0.00053300
N	4.47199100	0.99094500	0.35634600
N	3.32310000	1.37450500	-0.27494500
N	4.27233300	-1.38719700	0.32774900
N	3.13482600	-1.48093400	-0.42057700
N	-3.13452000	-1.48093900	0.42155400
N	-4.27214000	-1.38771000	-0.32666400
N	-3.32333400	1.37445000	0.27431300
N	-4.47211600	0.99036100	-0.35685200
C	4.53172400	-0.22070500	1.16291500
C	3.63331900	2.48787700	-0.96655300
C	4.99152900	2.80623000	-0.76023000
C	5.49169800	1.83770300	0.07339900
C	2.62953800	3.27139600	-1.78634000
C	3.30140600	-2.55670700	-1.21569300
C	4.55089200	-3.15126500	-0.94521800
C	5.14360000	-2.37928600	0.02217900
C	2.29483000	-2.99283600	-2.26149000
C	-4.53171100	-0.22182000	-1.16263000
C	-5.49191100	1.83725800	-0.07463400
C	-4.99191800	2.80639300	0.75839400
C	-3.63371800	2.48825200	0.96512900
C	-2.63010500	3.27250400	1.78439500
C	-5.14315700	-2.37986700	-0.02067100
C	-4.55021200	-3.15135300	0.94698300
C	-3.30083700	-2.55641900	1.21712800
C	-2.29416500	-2.99184300	2.26312700
H	5.56597600	-0.31137600	1.48921100
H	5.53557300	3.63636300	-1.17666700
H	4.96995700	-4.02496800	-1.41354000
H	-5.56598100	-0.31284900	-1.48877400
H	-5.53608400	3.63674400	1.17423800
H	-4.96905600	-4.02494300	1.41571500
C	3.63809400	-0.14901800	2.38623600
C	4.18232300	-0.19057800	3.66358600
N	2.32497700	-0.03233500	2.15215000
C	3.32043500	-0.10224100	4.75393000
H	5.25207000	-0.28682600	3.80899900
C	1.50373400	0.05716800	3.20420200
C	1.95742900	0.02676300	4.51884800
H	3.70964300	-0.13027400	5.76473300
H	0.45124300	0.15907100	2.97660100
H	1.25240500	0.10464200	5.33701900
C	-3.63818900	-0.15089700	-2.38605400
C	-4.18250000	-0.19366500	-3.66333300
N	-2.32509500	-0.03370100	-2.15215800
C	-3.32069900	-0.10608000	-4.75380400
H	-5.25223800	-0.29024600	-3.80859600
C	-1.50393600	0.05510100	-3.20433200
C	-1.95770700	0.02343800	-4.51892300
H	-3.70996500	-0.13507900	-5.76455900
H	-0.45146500	0.15749600	-2.97686300

H	-1.25275400	0.10076400	-5.33720900
H	6.47704500	1.68541600	0.48547900
H	6.10295800	-2.45251100	0.51019800
H	-6.10254200	-2.45347800	-0.50857900
H	-6.47721100	1.68458200	-0.48668400
C	-1.04761500	-3.58983400	1.58457600
H	-0.34936400	-3.93958400	2.34959500
H	-1.31450000	-4.44018800	0.95284900
H	-0.54012800	-2.84512000	0.97179800
C	-1.89502600	-1.77823500	3.12126400
H	-1.43623500	-0.99922500	2.50643100
H	-2.76297300	-1.35145700	3.62925100
H	-1.17005400	-2.08742400	3.87826700
C	-2.92490200	-4.05899300	3.17414700
H	-3.17819200	-4.96509500	2.61844500
H	-2.20747200	-4.33872400	3.94846800
H	-3.82557700	-3.68769400	3.66917200
C	1.04850100	-3.59092800	-1.58261000
H	0.35030300	-3.94121200	-2.34743200
H	1.31568500	-4.44093400	-0.95054000
H	0.54082900	-2.84610500	-0.97011800
C	1.89526500	-1.77972800	-3.12012000
H	1.43624800	-1.00058900	-2.50561500
H	2.76304500	-1.35289200	-3.62834200
H	1.17035300	-2.08948400	-3.87694700
C	2.92586400	-4.06017700	-3.17208600
H	3.17941200	-4.96597900	-2.61601000
H	2.20851500	-4.34044700	-3.94628800
H	3.82643400	-3.68882400	-3.66726100
C	1.72237500	4.05980900	-0.81873800
H	2.30888500	4.75712800	-0.21573600
H	0.98844900	4.63669400	-1.38734600
H	1.18980900	3.38602200	-0.14530400
C	1.78060100	2.32868500	-2.65522200
H	2.40912800	1.73957400	-3.32747900
H	1.18427500	1.65199700	-2.03783000
H	1.09035400	2.92008500	-3.26220100
C	3.36875100	4.26097900	-2.70334300
H	2.63898000	4.81121900	-3.30113200
H	3.94096100	4.99392400	-2.13015500
H	4.04656800	3.74546400	-3.38834400
C	-1.78044600	2.33060200	2.65344800
H	-2.40849600	1.74148100	3.32615300
H	-1.18387800	1.65392600	2.03626800
H	-1.09035300	2.92263000	3.25998400
C	-1.72362000	4.06098000	0.81619700
H	-2.31067500	4.75770800	0.21304300
H	-0.98982600	4.63850900	1.38432300
H	-1.19088900	3.38717000	0.14290900
C	-3.36955500	4.26205700	2.70124500
H	-2.63989900	4.81278700	3.29872500
H	-3.94216700	4.99460400	2.12794900
H	-4.04703200	3.74644900	3.38650700

Table S55: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/tzvp, O...O = 1.359 Å

Cu	1.85917200	0.03084900	-0.02771000
Cu	-1.85914900	0.03091300	0.02781200
O	-0.00012600	-0.59179800	0.00000700
O	0.00016300	0.76675400	-0.00000600
N	4.50153000	1.00262500	0.37059700
N	3.35426800	1.38449800	-0.26416000
N	4.31517300	-1.37843100	0.32378700
N	3.17486500	-1.48312000	-0.41881600
N	-3.17467800	-1.48321300	0.41914200
N	-4.31496500	-1.37890000	-0.32351700
N	-3.35440000	1.38439600	0.26389500
N	-4.50161200	1.00212500	-0.37076000
C	4.56047600	-0.21543600	1.16823300
C	3.66235200	2.50221100	-0.94825400
C	5.01851400	2.82561100	-0.73495300
C	5.51933900	1.85496100	0.09609000
C	2.65526400	3.28258700	-1.76706700
C	3.34973000	-2.55404100	-1.21749200
C	4.60790100	-3.13474900	-0.95704400
C	5.19673600	-2.35922100	0.01011800
C	2.33646500	-2.99772400	-2.25332800
C	-4.56042500	-0.21607800	-1.16817000
C	-5.51955100	1.85439700	-0.09652500
C	-5.01889800	2.82538000	0.73422100
C	-3.66268300	2.50225000	0.94764300
C	-2.65572700	3.28308200	1.76619100
C	-5.19638400	-2.35975100	-0.00964200
C	-4.60745000	-3.13495100	0.95772800
C	-3.34939600	-2.55395400	1.21809900
C	-2.33610000	-2.99720800	2.25408500
H	5.59203800	-0.30282000	1.50378900
H	5.56104100	3.66005900	-1.14479700
H	5.03451400	-4.00226100	-1.43010500
H	-5.59198900	-0.30363200	-1.50367500
H	-5.56154900	3.65986100	1.14383300
H	-5.03393200	-4.00242800	1.43097100
C	3.65581800	-0.15790000	2.38528500
C	4.19160100	-0.20714700	3.66596000
N	2.34256100	-0.04656100	2.14535700
C	3.32293300	-0.13306900	4.75190000
H	5.26093200	-0.29859400	3.81716700
C	1.51434600	0.02879100	3.19346100
C	1.96050500	-0.01023900	4.51019300
H	3.70654300	-0.16745400	5.76463800
H	0.46236900	0.12589700	2.96066300
H	1.25024300	0.05626500	5.32479700
C	-3.65580000	-0.15872700	-2.38525000
C	-4.19156300	-0.20854300	-3.66591000
N	-2.34257100	-0.04704000	-2.14535100
C	-3.32289800	-0.13470000	-4.75186700
H	-5.26087600	-0.30024600	-3.81709400
C	-1.51435600	0.02807600	-3.19347100
C	-1.96049400	-0.01153000	-4.51019300
H	-3.70649000	-0.16952200	-5.76459700
H	-0.46240000	0.12547900	-2.96070100

H	-1.25024000	0.05481000	-5.32481700
H	6.50376300	1.70464200	0.51108400
H	6.15919400	-2.42345000	0.49326000
H	-6.15882100	-2.42424700	-0.49278900
H	-6.50394800	1.70378900	-0.51148000
C	-1.09537900	-3.58954200	1.55986000
H	-0.38755400	-3.94051300	2.31545200
H	-1.36722100	-4.43814600	0.92788400
H	-0.59692100	-2.84147700	0.94379100
C	-1.92915500	-1.78915700	3.11687900
H	-1.47632500	-1.00520700	2.50339000
H	-2.79247600	-1.36568300	3.63536500
H	-1.19741000	-2.10321100	3.86538900
C	-2.95981400	-4.07025600	3.16247500
H	-3.22067000	-4.97102000	2.60161000
H	-2.23581700	-4.35801200	3.92769700
H	-3.85493100	-3.70109600	3.66903600
C	1.09579900	-3.58995400	-1.55890700
H	0.38803400	-3.94128100	-2.31438800
H	1.36773000	-4.43829700	-0.92662200
H	0.59723500	-2.84172600	-0.94311900
C	1.92939200	-1.78998300	-3.11649200
H	1.47645200	-1.00591100	-2.50324400
H	2.79267300	-1.36655800	-3.63508700
H	1.19770100	-2.10433800	-3.86492900
C	2.96026400	-4.07101100	-3.16137500
H	3.22126100	-4.97154900	-2.60021500
H	2.23626700	-4.35911300	-3.92646700
H	3.85531500	-3.70192200	-3.66810600
C	1.74597800	4.06814100	-0.79877700
H	2.33065500	4.76685600	-0.19563200
H	1.01041500	4.64334800	-1.36699100
H	1.21506600	3.39279300	-0.12541700
C	1.80807500	2.33665600	-2.63447700
H	2.43752200	1.74857900	-3.30674000
H	1.21379800	1.65822500	-2.01656200
H	1.11547100	2.92548200	-3.24127900
C	3.39035100	4.27412500	-2.68516000
H	2.65856900	4.82228000	-3.28244400
H	3.96107700	5.00868100	-2.11256400
H	4.06915600	3.76033400	-3.37045000
C	-1.80817300	2.33761200	2.63374500
H	-2.43737600	1.74954700	3.30625200
H	-1.21377400	1.65915800	2.01597000
H	-1.11565900	2.92678400	3.24031100
C	-1.74678000	4.06868300	0.79760900
H	-2.33173800	4.76710400	0.19439900
H	-1.01130000	4.64421200	1.36560500
H	-1.21578000	3.39334100	0.12431600
C	-3.39099900	4.27463100	2.68412400
H	-2.65931100	4.82313800	3.28119900
H	-3.96199000	5.00889200	2.11141400
H	-4.06959200	3.76081300	3.36960300

Table S56: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), Oxo

Cu	-1.41776800	0.11641000	0.26946800
Cu	1.40987400	0.07387800	-0.30323500
O	-0.01364200	-0.94428500	0.00691500
O	0.00369800	1.22734700	-0.06757400
N	-4.21421600	0.67508800	0.26015100
N	-3.01848300	1.26317900	0.58223900
N	-3.66014500	-1.63141800	0.15429900
N	-2.50227400	-1.42488200	0.83677500
N	2.48252700	-1.52426900	-0.69609200
N	3.60312300	-1.68333400	0.05839000
N	3.02538100	1.16373300	-0.69471600
N	4.20973200	0.58233000	-0.32215000
C	-4.28206300	-0.52362800	-0.55941100
C	-3.33130000	2.40315800	1.22948900
C	-4.72799400	2.54151400	1.29748200
C	-5.25355600	1.43696500	0.67375500
C	-2.28280600	3.36376900	1.72413300
C	-2.28570200	-2.53371500	1.57553600
C	-3.31868400	-3.45485700	1.32351400
C	-4.17748800	-2.84817800	0.43778000
C	-1.17094400	-2.67306800	2.58791400
C	4.25643800	-0.51224700	0.63288400
C	5.26275300	1.27702600	-0.81356600
C	4.75721000	2.32378100	-1.54413300
C	3.35825300	2.22356000	-1.45721200
C	2.32582500	3.14226000	-2.05426400
C	4.06014500	-2.95336100	-0.01893000
C	3.20224800	-3.64115300	-0.84497400
C	2.23244700	-2.71765300	-1.27596300
C	1.17038900	-2.94367100	-2.33065300
H	-5.34429600	-0.77276900	-0.64191900
H	-5.27850100	3.35023500	1.75706900
H	-3.44482600	-4.42911900	1.77452400
H	5.31389300	-0.77292800	0.73974300
H	5.32190000	3.07062400	-2.08428900
H	3.29454000	-4.67558500	-1.14623100
C	-3.70997700	-0.28650500	-1.93723900
C	-4.51079500	-0.36630000	-3.06915700
N	-2.41671700	0.05640500	-1.96117900
C	-3.93788500	-0.06136000	-4.30215500
H	-5.55817400	-0.65310500	-2.99466000
C	-1.88646100	0.36942800	-3.14652500
C	-2.60399300	0.32396800	-4.33967200
H	-4.53031300	-0.11143300	-5.21254500
H	-0.84310700	0.67763800	-3.13160700
H	-2.12143100	0.59164200	-5.27605000
C	3.70000900	-0.09109700	1.97264500
C	4.52064600	-0.00125500	3.08960100
N	2.40468900	0.24432100	1.96714500
C	3.96758100	0.48057600	4.27416200
H	5.56805000	-0.29303500	3.03893200
C	1.89443900	0.72895400	3.10300700
C	2.63260500	0.86442700	4.27644900
H	4.57459300	0.56339200	5.17243100
H	0.84845000	1.02571900	3.06419600

H	2.16456100	1.26614600	5.17130200
H	-6.27481300	1.13073500	0.48419300
H	-5.11672400	-3.17021100	0.00551000
H	4.96507500	-3.25268900	0.49533300
H	6.27843100	0.97084400	-0.59594400
C	-0.12797500	-3.49514000	-1.72273700
H	-0.82476400	-3.75319600	-2.53026900
H	0.05659900	-4.40561400	-1.13937300
H	-0.60652100	-2.75443800	-1.07298800
C	0.88802800	-1.63560700	-3.07056200
H	0.46782500	-0.88603400	-2.39125800
H	1.79605900	-1.22446900	-3.53007900
H	0.15374200	-1.80718100	-3.86683400
C	1.71136100	-3.97187000	-3.33429100
H	1.85057300	-4.95823200	-2.87778000
H	0.99417900	-4.09680600	-4.15288200
H	2.66676000	-3.65737600	-3.76991900
C	0.06328600	-3.34168500	1.96452100
H	0.83617200	-3.47253200	2.73278500
H	-0.17858500	-4.33357500	1.56276800
H	0.47557500	-2.72793800	1.15645600
C	-0.79810400	-1.29925100	3.14704700
H	-0.37000100	-0.65848100	2.36868700
H	-1.66589800	-0.78987200	3.58611000
H	-0.04060100	-1.41086200	3.93216500
C	-1.67393300	-3.55195600	3.74170100
H	-1.88046900	-4.57876200	3.41892700
H	-0.90500700	-3.61060600	4.51978700
H	-2.58387600	-3.14729000	4.20006400
C	-1.58785600	3.97154500	0.49860100
H	-2.29898000	4.53167100	-0.12084300
H	-0.80096300	4.66581600	0.81809500
H	-1.12548100	3.19370900	-0.12302600
C	-1.27016000	2.61998400	2.59851200
H	-1.74462200	2.19545300	3.49261900
H	-0.79297700	1.81235500	2.03182300
H	-0.47903600	3.30627900	2.92530800
C	-2.94050700	4.47631100	2.54084100
H	-2.17574700	5.17087000	2.90413500
H	-3.64826400	5.05977200	1.94023600
H	-3.47221700	4.08298400	3.41567100
C	1.31500900	2.32346600	-2.86129800
H	1.79820000	1.79482600	-3.69285000
H	0.81487300	1.59084500	-2.21741700
H	0.54216000	2.98207100	-3.27641000
C	1.62379700	3.87761200	-0.90481400
H	2.33415300	4.48897000	-0.33503500
H	0.84961900	4.54524300	-1.30258500
H	1.14208000	3.17294300	-0.21418300
C	3.00384100	4.16122100	-2.97069700
H	2.25065900	4.82572400	-3.40711200
H	3.71408600	4.79292900	-2.42435200
H	3.53775800	3.67798900	-3.79788200

Table S57: XYZ coordinates for Optimised structure: Singlet minimum path, M06L/6-31g(d), Peroxo

Cu	1.77295700	0.10271900	-0.11974700
Cu	-1.77294000	0.10317200	0.12049300
O	-0.00017300	-0.51708000	-0.00098100
O	0.00041400	0.94074000	0.00285800
N	4.50862300	0.74377100	0.18780500
N	3.35499600	1.26764600	-0.31748100
N	4.04581700	-1.59524700	0.13007900
N	2.87299500	-1.50554000	-0.56078400
N	-2.87249200	-1.50525400	0.56367900
N	-4.04505200	-1.59687200	-0.12717300
N	-3.35534800	1.26756400	0.31546900
N	-4.50879600	0.74188100	-0.18852200
C	4.47507500	-0.48501700	0.96770000
C	3.70026400	2.40871100	-0.93525000
C	5.08650600	2.61239000	-0.81175300
C	5.56733200	1.53995500	-0.09651100
C	2.65657700	3.28645600	-1.57867200
C	2.86467400	-2.54511000	-1.41470200
C	4.03325800	-3.30895200	-1.23997500
C	4.76767400	-2.66979800	-0.27048000
C	1.77986200	-2.73670500	-2.44880300
C	-4.47487600	-0.48813600	-0.96646200
C	-5.56775700	1.53858400	0.09328200
C	-5.08745600	2.61305200	0.80581300
C	-3.70121200	2.41014400	0.93019800
C	-2.65818900	3.28968200	1.57221500
C	-4.76605000	-2.67156100	0.27456600
C	-4.03122500	-3.30882000	1.24503800
C	-2.86337100	-2.54370300	1.41898200
C	-1.77841700	-2.73260300	2.45338700
H	5.51103000	-0.69883200	1.24553700
H	5.66490600	3.43843000	-1.20226100
H	4.31454300	-4.20390400	-1.77721400
H	-5.51080500	-0.70276200	-1.24378500
H	-5.66621200	3.44000500	1.19384200
H	-4.31187800	-4.20326700	1.78342700
C	3.64358500	-0.32133700	2.22417900
C	4.21403000	-0.44244300	3.48424300
N	2.35199100	-0.01562100	2.03097200
C	3.40717500	-0.22603200	4.59940600
H	5.26653200	-0.69470400	3.59801400
C	1.59051700	0.20653400	3.10553200
C	2.07312800	0.11242400	4.40755300
H	3.82131200	-0.31199300	5.60113200
H	0.55623200	0.47630800	2.89779000
H	1.41428500	0.30761000	5.24969700
C	-3.64368100	-0.32631300	-2.22332300
C	-4.21452200	-0.44982100	-3.48300700
N	-2.35204000	-0.02018900	-2.03099500
C	-3.40803200	-0.23575900	-4.59885700
H	-5.26708500	-0.70223200	-3.59588200
C	-1.59092000	0.19951100	-3.10632800
C	-2.07386100	0.10276500	-4.40801400
H	-3.82249700	-0.32362400	-5.60027700
H	-0.55647200	0.46939000	-2.89975100

H	-1.41508000	0.29592600	-5.25067300
H	6.56532500	1.27962100	0.23349100
H	5.73496800	-2.88576000	0.16588400
H	-5.73313900	-2.88886300	-0.16160000
H	-6.56555200	1.27713600	-0.23643300
C	-0.47486700	-3.22423000	1.81160900
H	0.27052800	-3.41388500	2.59471100
H	-0.62630600	-4.16086800	1.26215000
H	-0.05484900	-2.48136200	1.12471300
C	-1.53584400	-1.38721800	3.14399000
H	-1.18914300	-0.63994600	2.41714100
H	-2.44771900	-1.00258100	3.61718600
H	-0.76562500	-1.49059600	3.91786700
C	-2.24289700	-3.75908300	3.48818000
H	-2.38560200	-4.75026900	3.04187400
H	-1.48716000	-3.86455000	4.27398900
H	-3.18247900	-3.46074800	3.96818900
C	0.47639000	-3.22752500	-1.80630700
H	-0.26891500	-3.41859700	-2.58914700
H	0.62793000	-4.16320000	-1.25523800
H	0.05603800	-2.48372500	-1.12062600
C	1.53686300	-1.39289500	-3.14231100
H	1.18933200	-0.64445200	-2.41711000
H	2.44874800	-1.00865700	-3.61581000
H	0.76710000	-1.49830100	-3.91636900
C	2.24505900	-3.76528400	-3.48117100
H	2.38868400	-4.75520100	-3.03235200
H	1.48934900	-3.87333900	-4.26664300
H	3.18435800	-3.46734300	-3.96197400
C	1.79815200	3.90554500	-0.46513400
H	2.40441400	4.52291500	0.20821000
H	1.02230100	4.54611200	-0.90184400
H	1.30014000	3.13305700	0.13707700
C	1.77052300	2.44269000	-2.50091500
H	2.34844900	1.99068300	-3.31651900
H	1.28088700	1.63845300	-1.93680800
H	0.98185600	3.06457600	-2.94168200
C	3.33278600	4.39527800	-2.38293200
H	2.57689600	5.02499300	-2.86428200
H	3.93940400	5.04797900	-1.74413500
H	3.97855600	3.99082300	-3.17156300
C	-1.77391700	2.44834200	2.49842400
H	-2.35334800	1.99939800	3.31465200
H	-1.28410300	1.64193600	1.93759600
H	-0.98546500	3.07111500	2.93832200
C	-1.79790800	3.90504400	0.45808100
H	-2.40297000	4.52045300	-0.21813700
H	-1.02264600	4.54683200	0.89402500
H	-1.29913900	3.13056000	-0.14091600
C	-3.33518400	4.40125800	2.37199300
H	-2.57976000	5.03204300	2.85267100
H	-3.94039300	5.05237900	1.73023000
H	-3.98249000	3.99963900	3.16081400

Table S58: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 2.277 Å

Cu	-1.38765300	0.10590800	0.27438500
Cu	1.37468000	0.06384700	-0.31660300
O	-0.01645800	-1.01171500	0.00571300
O	0.00005000	1.26372400	-0.08312000
N	-4.18298000	0.66863300	0.29188800
N	-2.98409700	1.26010100	0.59898400
N	-3.62882500	-1.63565600	0.17217200
N	-2.47416500	-1.42266500	0.85804600
N	2.45769300	-1.52150000	-0.70610800
N	3.57048600	-1.67812700	0.06051600
N	2.98501500	1.16185200	-0.71264100
N	4.17236800	0.58356800	-0.34225300
C	-4.26203700	-0.52686900	-0.53037600
C	-3.29321600	2.39932200	1.25132000
C	-4.68951100	2.53272400	1.33589000
C	-5.21921700	1.42738400	0.71810800
C	-2.24876300	3.37035000	1.73396200
C	-2.24944100	-2.53227200	1.59366800
C	-3.27608200	-3.45933900	1.33796500
C	-4.13803100	-2.85638300	0.45275600
C	-1.13651700	-2.66895500	2.60765500
C	4.23020900	-0.50307200	0.62046600
C	5.22234900	1.27497100	-0.84383300
C	4.71307700	2.31546700	-1.57993300
C	3.31466900	2.21579300	-1.48656200
C	2.28570700	3.13310600	-2.09137700
C	4.02535000	-2.94938800	-0.00651300
C	3.17282900	-3.64048000	-0.83538200
C	2.20837000	-2.71821600	-1.28025600
C	1.15717100	-2.95010500	-2.34414200
H	-5.32532400	-0.77627700	-0.59715300
H	-5.23623200	3.33980700	1.80261300
H	-3.39643200	-4.43523500	1.78712900
H	5.28919200	-0.76259100	0.71493000
H	5.27443100	3.05849700	-2.12865100
H	3.26566000	-4.67687100	-1.12975900
C	-3.71243700	-0.28569300	-1.91598200
C	-4.53423000	-0.35676900	-3.03330700
N	-2.41814100	0.05183400	-1.96071700
C	-3.98298000	-0.04888300	-4.27527600
H	-5.58139600	-0.63930700	-2.94056400
C	-1.90893700	0.36725000	-3.15481200
C	-2.64821800	0.33017000	-4.33499700
H	-4.59200000	-0.09230000	-5.17493000
H	-0.86434400	0.67059700	-3.15907200
H	-2.18129500	0.59956100	-5.27876100
C	3.69367300	-0.07306100	1.96459400
C	4.53577000	0.03196900	3.06425300
N	2.39656100	0.25517500	1.97947700
C	4.00416400	0.52246800	4.25478200
H	5.58348200	-0.25533500	2.99552900
C	1.90719600	0.74733600	3.12166000
C	2.66750700	0.89877100	4.27900900
H	4.62816800	0.61722500	5.14014400
H	0.85879600	1.03626500	3.10359200

H	2.21419500	1.30616400	5.17881700
H	-6.24168000	1.11825700	0.53995100
H	-5.07548500	-3.18301500	0.02006500
H	4.92630600	-3.24700400	0.51565000
H	6.23909200	0.97123900	-0.62770800
C	-0.13493900	-3.52966800	-1.74943300
H	-0.82368500	-3.78896800	-2.56329800
H	0.06213500	-4.44474500	-1.17741500
H	-0.62692100	-2.80491200	-1.09209000
C	0.85900800	-1.64104600	-3.07538900
H	0.42322200	-0.90364500	-2.39303300
H	1.76334100	-1.21233200	-3.52642300
H	0.13242800	-1.81787000	-3.87751000
C	1.72278600	-3.96019400	-3.35317800
H	1.87569600	-4.94808000	-2.90454400
H	1.01296000	-4.08978900	-4.17746100
H	2.67541000	-3.62567200	-3.77978100
C	0.08417000	-3.37056300	1.99431600
H	0.85981400	-3.49268500	2.76116600
H	-0.17496000	-4.36908300	1.62082500
H	0.49836000	-2.78358000	1.16753900
C	-0.74016200	-1.29249900	3.14225000
H	-0.30361200	-0.67238600	2.35225800
H	-1.59829000	-0.76226200	3.57590100
H	0.01784200	-1.40388700	3.92692700
C	-1.65373600	-3.51765000	3.77813300
H	-1.88130200	-4.54586700	3.47485200
H	-0.88374500	-3.57726800	4.55515400
H	-2.55430000	-3.08721200	4.23160700
C	-1.58401100	3.99239500	0.49889800
H	-2.31364500	4.54857700	-0.10227000
H	-0.79853600	4.69319100	0.80743700
H	-1.12669200	3.22270700	-0.13578200
C	-1.21322600	2.63795600	2.59029400
H	-1.66833600	2.20797900	3.49199200
H	-0.73522000	1.83792100	2.01440800
H	-0.42556600	3.33381400	2.90497800
C	-2.90729500	4.47180400	2.56543300
H	-2.14428100	5.17208700	2.92135800
H	-3.62899300	5.05181700	1.97825200
H	-3.42253600	4.06899400	3.44586200
C	1.26911100	2.31122300	-2.88740200
H	1.74803800	1.77455400	-3.71639600
H	0.76885800	1.58675300	-2.23507600
H	0.49742800	2.96929400	-3.30551800
C	1.59359800	3.88727800	-0.94825900
H	2.31011000	4.50518300	-0.39338200
H	0.81858400	4.55111700	-1.35068700
H	1.11573800	3.19381300	-0.24438600
C	2.96682100	4.13764300	-3.02169000
H	2.21513500	4.80024000	-3.46354300
H	3.68106200	4.77289100	-2.48477800
H	3.49611300	3.64251400	-3.84480200

Table S59: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 2.145 Å

Cu	-1.42694900	0.12011300	0.26674600
Cu	1.42008700	0.07622000	-0.29877400
O	-0.01323800	-0.92563000	0.01005900
O	0.00493300	1.21789800	-0.06645700
N	-4.22352600	0.67642100	0.24821200
N	-3.02917200	1.26460800	0.57420500
N	-3.66849200	-1.63062400	0.14974500
N	-2.51050500	-1.42454700	0.83223500
N	2.49054400	-1.52535800	-0.69033900
N	3.61358000	-1.68350100	0.06068600
N	3.03647800	1.16431200	-0.68979400
N	4.22015100	0.58349800	-0.31489600
C	-4.28724000	-0.52428400	-0.56895100
C	-3.34384300	2.40434200	1.22041900
C	-4.74073400	2.54268200	1.28439700
C	-5.26430900	1.43793400	0.65903800
C	-2.29490500	3.36302900	1.71801500
C	-2.29582100	-2.53287000	1.57225600
C	-3.32944400	-3.45339600	1.32058400
C	-4.18714000	-2.84672900	0.43373000
C	-1.18192500	-2.67116500	2.58600300
C	4.26381900	-0.51261100	0.63877200
C	5.27385200	1.27962000	-0.80306800
C	4.76909600	2.32696700	-1.53355400
C	3.36999600	2.22537300	-1.44977300
C	2.33635800	3.14286300	-2.04682300
C	4.07335700	-2.95237200	-0.02018700
C	3.21514500	-3.64031600	-0.84576800
C	2.24236100	-2.71789200	-1.27244800
C	1.17774100	-2.94315900	-2.32479200
H	-5.34897800	-0.77390600	-0.65619600
H	-5.29294600	3.35128500	1.74219000
H	-3.45680700	-4.42709300	1.77245400
H	5.32091900	-0.77283200	0.74993400
H	5.33457400	3.07488400	-2.07142000
H	3.30901000	-4.67390400	-1.14940800
C	-3.70811700	-0.29014400	-1.94454300
C	-4.50215100	-0.37481800	-3.08087800
N	-2.41535900	0.05489100	-1.96241700
C	-3.92253200	-0.07245100	-4.31141800
H	-5.54941000	-0.66328900	-3.01168900
C	-1.87862900	0.36566200	-3.14537000
C	-2.58918200	0.31545800	-4.34247000
H	-4.50959200	-0.12632800	-5.22508500
H	-0.83591100	0.67594300	-3.12488300
H	-2.10179600	0.58143900	-5.27683100
C	3.70085000	-0.09339800	1.97669800
C	4.51481800	-0.00688300	3.09875800
N	2.40590500	0.24331900	1.96479400
C	3.95490500	0.47257500	4.28114000
H	5.56227300	-0.29929200	3.05370500
C	1.88894400	0.72570500	3.09847400
C	2.62018900	0.85753900	4.27661200
H	4.55667300	0.55282600	5.18316200
H	0.84353900	1.02392600	3.05338100

H	2.14730800	1.25753400	5.16970700
H	-6.28498600	1.13155100	0.46665800
H	-5.12620700	-3.16846500	0.00086800
H	4.97993700	-3.25088500	0.49163900
H	6.28930600	0.97395400	-0.58371200
C	-0.12206000	-3.48730000	-1.71339200
H	-0.82142900	-3.74406800	-2.51914500
H	0.05920100	-4.39714500	-1.12802900
H	-0.59646600	-2.74280900	-1.06484900
C	0.89914400	-1.63563300	-3.06725100
H	0.48232500	-0.88309600	-2.38901500
H	1.80805800	-1.22852800	-3.52852100
H	0.16330500	-1.80626700	-3.86230400
C	1.71267500	-3.97605600	-3.32663000
H	1.84891200	-4.96170300	-2.86765100
H	0.99356100	-4.10044000	-4.14359800
H	2.66852100	-3.66645900	-3.76481000
C	0.05822100	-3.32891900	1.96262000
H	0.82859600	-3.46175100	2.73307200
H	-0.17682100	-4.31891800	1.55228700
H	0.47145100	-2.70732300	1.16104600
C	-0.81917600	-1.29739400	3.15212600
H	-0.39593200	-0.64950200	2.37688200
H	-1.69091400	-0.79647700	3.59298600
H	-0.06116400	-1.40706000	3.93701600
C	-1.68145300	-3.55892800	3.73432700
H	-1.87961900	-4.58560900	3.40587600
H	-0.91420800	-3.61577000	4.51419000
H	-2.59551100	-3.16301700	4.19210600
C	-1.59247000	3.96725100	0.49497000
H	-2.29893900	4.52795500	-0.12924200
H	-0.80548000	4.66014600	0.81720000
H	-1.12855300	3.18740800	-0.12316800
C	-1.28759200	2.61718800	2.59697100
H	-1.76695400	2.19200300	3.48810800
H	-0.80852000	1.80932400	2.03198900
H	-0.49726800	3.30214700	2.92846100
C	-2.95303300	4.47806600	2.53081600
H	-2.18828500	5.17167500	2.89593600
H	-3.65757400	5.06187700	1.92677800
H	-3.48866800	4.08693200	3.40421500
C	1.32896100	2.32306100	-2.85724500
H	1.81470900	1.79713500	-3.68898600
H	0.82967400	1.58758800	-2.21580100
H	0.55501200	2.98045500	-3.27223500
C	1.62954300	3.87370400	-0.89737500
H	2.33688300	4.48478500	-0.32357700
H	0.85525500	4.54093200	-1.29560500
H	1.14684300	3.16637100	-0.21000200
C	3.01348800	4.16550800	-2.95969800
H	2.25962900	4.82911000	-3.39632000
H	3.72114700	4.79770500	-2.41057100
H	3.55027600	3.68526900	-3.78676400

Table S60: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 2.013 Å

Cu	-1.48254100	0.11496200	0.23718100
Cu	1.47989100	0.09194700	-0.23741500
O	-0.00591900	-0.84843200	0.02268700
O	0.00441000	1.16411500	-0.02478100
N	-4.27753500	0.67709400	0.13986800
N	-3.09390200	1.24799800	0.52518900
N	-3.73072500	-1.63412000	0.03646300
N	-2.57765700	-1.45638300	0.73664600
N	2.57183800	-1.50488600	-0.64567100
N	3.72971500	-1.63901000	0.05792800
N	3.08979900	1.20836700	-0.59845600
N	4.27625800	0.66186700	-0.18768300
C	-4.31265700	-0.51462000	-0.69257700
C	-3.42502500	2.36867700	1.19428000
C	-4.82261400	2.51308100	1.21537000
C	-5.32930100	1.42951700	0.53986900
C	-2.38265000	3.29736300	1.75909400
C	-2.40504800	-2.57029000	1.47916700
C	-3.45529300	-3.46628300	1.20882000
C	-4.28356400	-2.83794500	0.30975200
C	-1.31967800	-2.72989300	2.52157000
C	4.31484500	-0.47731100	0.71514700
C	5.32473800	1.39746700	-0.62657000
C	4.81274200	2.44270700	-1.35594400
C	3.41572600	2.29458700	-1.32456200
C	2.37034700	3.18907800	-1.93701700
C	4.29136700	-2.85005800	-0.16028300
C	3.46452200	-3.52804100	-1.02341700
C	2.40555500	-2.65479300	-1.33232900
C	1.31868700	-2.87613800	-2.36214000
H	-5.37086600	-0.75758600	-0.82794200
H	-5.38741300	3.31043500	1.67766200
H	-3.61174000	-4.43802600	1.65562000
H	5.37349400	-0.71230400	0.86034300
H	5.37294700	3.21784300	-1.85969700
H	3.62693900	-4.51930100	-1.42297900
C	-3.67391300	-0.26847300	-2.04000300
C	-4.41673600	-0.33946300	-3.21151700
N	-2.38058300	0.07224900	-1.99860300
C	-3.78193900	-0.02711000	-4.41223500
H	-5.46668600	-0.62505000	-3.19140400
C	-1.79064800	0.39292500	-3.15299100
C	-2.44724100	0.35698000	-4.38046900
H	-4.32804900	-0.07108200	-5.35156300
H	-0.74928000	0.70018100	-3.08231000
H	-1.91798600	0.63051700	-5.28944200
C	3.68312500	-0.14313900	2.04746000
C	4.43520300	-0.12393200	3.21495600
N	2.38722900	0.18625800	1.99233800
C	3.80728900	0.27055200	4.39490500
H	5.48693300	-0.40352300	3.20714400
C	1.80339500	0.58563600	3.12515500
C	2.46947700	0.64244200	4.34666400
H	4.36091800	0.29740600	5.33043700
H	0.75935200	0.88066000	3.04027800

H	1.94540400	0.97597100	5.23841600
H	-6.34427300	1.13357400	0.30580300
H	-5.22141100	-3.13726200	-0.14160400
H	5.23349900	-3.11918800	0.30114000
H	6.34107000	1.11743100	-0.37935700
C	0.03212100	-3.42244700	-1.72619400
H	-0.69015100	-3.66084200	-2.51741600
H	0.22284900	-4.34345100	-1.16196800
H	-0.42276700	-2.68692700	-1.05334100
C	1.02525000	-1.55762000	-3.08023800
H	0.62595200	-0.81450500	-2.38078700
H	1.92440100	-1.14356900	-3.55411900
H	0.27166500	-1.71518200	-3.86125100
C	1.82506600	-3.89884100	-3.38669800
H	1.97295800	-4.88802200	-2.93874700
H	1.08467300	-4.01673100	-4.18528000
H	2.76887000	-3.58587500	-3.84824600
C	-0.03507200	-3.31899400	1.92033100
H	0.69278500	-3.49610600	2.72230700
H	-0.22709200	-4.28050400	1.42871100
H	0.41383000	-2.63595400	1.19056500
C	-1.02368000	-1.37136900	3.15948900
H	-0.62324900	-0.66950000	2.41932000
H	-1.92250900	-0.92978400	3.60849100
H	-0.27098400	-1.48449900	3.94895500
C	-1.82825600	-3.68596200	3.60831300
H	-1.97361700	-4.70242800	3.22493900
H	-1.08995300	-3.75135600	4.41494600
H	-2.77356200	-3.34500700	4.04625900
C	-1.62376700	3.92889100	0.58453400
H	-2.29563400	4.51876600	-0.05075900
H	-0.83986900	4.59919100	0.95816200
H	-1.14526300	3.16207900	-0.03932200
C	-1.41721400	2.50818300	2.64747800
H	-1.93592600	2.04399900	3.49577700
H	-0.91717200	1.72311500	2.06801500
H	-0.63994300	3.17341900	3.04340600
C	-3.05471500	4.39471500	2.58411500
H	-2.29527200	5.06525700	2.99996200
H	-3.72899400	5.00809300	1.97501600
H	-3.62715200	3.98255200	3.42382000
C	1.40526300	2.34972900	-2.77812300
H	1.92244400	1.84618600	-3.60459000
H	0.91511800	1.59203100	-2.15555800
H	0.62090500	2.98886900	-3.20200200
C	1.61288100	3.88450500	-0.79812000
H	2.28541800	4.50991600	-0.19861100
H	0.82739300	4.53156900	-1.20761300
H	1.13570300	3.15444800	-0.13070000
C	3.03822000	4.24069400	-2.82299300
H	2.27601800	4.88540800	-3.27333700
H	3.71225200	4.88852300	-2.25046900
H	3.61002100	3.78422300	-3.63995900

Table S61: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 1.881 Å

Cu	-1.55461600	0.09730000	0.17129900
Cu	1.55461900	0.09731300	-0.17130900
O	-0.00001500	-0.78555300	-0.00004200
O	-0.00001800	1.09602300	-0.00000300
N	-4.33404600	0.74452800	-0.01713200
N	-3.15569300	1.25637400	0.45192100
N	-3.86583900	-1.58397700	-0.10153600
N	-2.69744700	-1.48364800	0.59367000
N	2.69742900	-1.48372300	-0.59324100
N	3.86580800	-1.58385100	0.10202900
N	3.15563100	1.25636900	-0.45209100
N	4.33395200	0.74465100	0.01717500
C	-4.35903100	-0.44164300	-0.85764800
C	-3.48481200	2.36203400	1.14572500
C	-4.87617200	2.55387900	1.10271100
C	-5.38199800	1.51347800	0.36116100
C	-2.43931000	3.23202100	1.79314100
C	-2.62701300	-2.58443300	1.37043100
C	-3.75269200	-3.39370900	1.13039700
C	-4.52395300	-2.72390400	0.21242500
C	-1.55423800	-2.81149900	2.41243600
C	4.35891700	-0.44134300	0.85794300
C	5.38194700	1.51337100	-0.36145500
C	4.87617200	2.55355000	-1.10336000
C	3.48480500	2.36177700	-1.14628000
C	2.43927200	3.23157200	-1.79390400
C	4.52416000	-2.72364100	-0.21194300
C	3.75302100	-3.39362500	-1.12988100
C	2.62723500	-2.58452800	-1.37000400
C	1.55446800	-2.81189000	-2.41194200
H	-5.41412800	-0.64702400	-1.06087100
H	-5.43816300	3.35277800	1.56593600
H	-3.98849900	-4.33683500	1.60330000
H	5.41400900	-0.64665200	1.06126900
H	5.43821600	3.35227600	-1.56682200
H	3.98898700	-4.33674100	-1.60272600
C	-3.62884400	-0.21548300	-2.16229400
C	-4.29183600	-0.27729100	-3.38079900
N	-2.33142400	0.09235700	-2.04094000
C	-3.56980000	0.00674400	-4.53837000
H	-5.34810300	-0.53476800	-3.42959600
C	-1.65543500	0.38450700	-3.15464900
C	-2.22956500	0.35384300	-4.42249800
H	-4.05346300	-0.03234400	-5.51152300
H	-0.61355800	0.66382800	-3.01230200
H	-1.63482800	0.60365600	-5.29700200
C	3.62867200	-0.21492800	2.16251000
C	4.29159400	-0.27652700	3.38106400
N	2.33127600	0.09293300	2.04100300
C	3.56951400	0.00783900	4.53853000
H	5.34784000	-0.53406100	3.42997200
C	1.65524800	0.38538200	3.15460700
C	2.22931100	0.35501800	4.42248800
H	4.05311600	-0.03105700	5.51172000
H	0.61339100	0.66470400	3.01215500

H	1.63455100	0.60514800	5.29688600
H	-6.39280900	1.25788500	0.06887400
H	-5.48265000	-2.95521000	-0.23506700
H	5.48288900	-2.95476600	0.23557200
H	6.39274600	1.25788400	-0.06903000
C	0.27132100	-3.37737500	-1.78950700
H	-0.44684600	-3.61334800	-2.58497400
H	0.46810900	-4.30168600	-1.23307300
H	-0.19562600	-2.65479800	-1.11079000
C	1.25075900	-1.48415600	-3.10851800
H	0.85346400	-0.75614400	-2.39153000
H	2.14607300	-1.05631000	-3.57706700
H	0.49421800	-1.63112500	-3.88880900
C	2.07769900	-3.81400700	-3.44611900
H	2.24022700	-4.80527800	-3.00759200
H	1.34139400	-3.93472600	-4.24798500
H	3.01738400	-3.48123800	-3.90225600
C	-0.27103000	-3.37701600	1.79015500
H	0.44710800	-3.61281800	2.58569900
H	-0.46773400	-4.30143000	1.23386000
H	0.19590700	-2.65452400	1.11134500
C	-1.25061500	-1.48357300	3.10869600
H	-0.85336700	-0.75574900	2.39148900
H	-2.14594200	-1.05564800	3.57714600
H	-0.49404800	-1.63029900	3.88900600
C	-2.07743500	-3.81342000	3.44680700
H	-2.23983200	-4.80480900	3.00850700
H	-1.34116900	-3.93387500	4.24875100
H	-3.01718500	-3.48064000	3.90280200
C	-1.61207600	3.88719500	0.67964500
H	-2.23667600	4.52424100	0.04187600
H	-0.82292200	4.51380700	1.11320500
H	-1.13179700	3.13158700	0.04337500
C	-1.53302100	2.37460100	2.68023800
H	-2.09524900	1.89300800	3.48994600
H	-1.04111100	1.59656700	2.08439600
H	-0.74756100	2.99503200	3.12898000
C	-3.11014900	4.31373500	2.63899700
H	-2.34843300	4.93945800	3.11625600
H	-3.73836200	4.97523900	2.03115700
H	-3.73090100	3.88386900	3.43433400
C	1.53290800	2.37389400	-2.68066700
H	2.09506400	1.89204400	-3.49027400
H	1.04100500	1.59605200	-2.08456300
H	0.74744200	2.99422700	-3.12953300
C	1.61211800	3.88711800	-0.68057500
H	2.23674100	4.52440000	-0.04306500
H	0.82291200	4.51356100	-1.11428200
H	1.13192800	3.13169500	-0.04401700
C	3.11010400	4.31297400	-2.64017000
H	2.34840200	4.93867500	-3.11748200
H	3.73849500	4.97455200	-2.03259200
H	3.73068600	3.88284200	-3.43549700

Table S62: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 1.749 Å

Cu	-1.63156800	0.09788500	0.14800900
Cu	1.63163500	0.09772500	-0.14762900
O	-0.00013600	-0.70858500	-0.00030300
O	-0.00003100	1.04124100	0.00145100
N	-4.39552100	0.76172200	-0.09991700
N	-3.22611600	1.26523600	0.39453800
N	-3.94625600	-1.57394900	-0.13223900
N	-2.77592200	-1.49024000	0.56289200
N	2.77584600	-1.49048700	-0.56222900
N	3.94674000	-1.57339400	0.13215100
N	3.22599900	1.26521100	-0.39520400
N	4.39543800	0.76239100	0.09991300
C	-4.40177400	-0.43870600	-0.92107200
C	-3.55872100	2.38050300	1.06810800
C	-4.94673800	2.58752600	0.98887900
C	-5.44535200	1.54452400	0.24469000
C	-2.50992500	3.23798700	1.72771700
C	-2.74518500	-2.56735400	1.37198300
C	-3.89732300	-3.34635200	1.15772800
C	-4.64418600	-2.68020200	0.21720400
C	-1.66936200	-2.79817700	2.40889300
C	4.40185100	-0.43808500	0.92106500
C	5.44502700	1.54565700	-0.24437700
C	4.94620700	2.58833100	-0.98889100
C	3.55831500	2.38061500	-1.06864300
C	2.50929800	3.23778100	-1.72830200
C	4.64578400	-2.67851200	-0.21868000
C	3.89915000	-3.34478500	-1.15927800
C	2.74597200	-2.56697400	-1.37220500
C	1.66966300	-2.79848100	-2.40841600
H	-5.45037100	-0.63857500	-1.15970000
H	-5.51286100	3.39678200	1.42886000
H	-4.16312700	-4.26761700	1.65712300
H	5.45047800	-0.63771000	1.15976800
H	5.51210900	3.39776500	-1.42882700
H	4.16566900	-4.26536700	-1.65953600
C	-3.62405700	-0.23993300	-2.20408500
C	-4.24482100	-0.32519000	-3.44322100
N	-2.32850200	0.06428400	-2.04846700
C	-3.48303100	-0.07034500	-4.58176600
H	-5.30030800	-0.57830700	-3.52264700
C	-1.61301100	0.32745300	-3.14487300
C	-2.14505500	0.27169900	-4.43002400
H	-3.93470700	-0.12846200	-5.56919800
H	-0.57422500	0.60342300	-2.97293300
H	-1.52056100	0.49885900	-5.28996100
C	3.62406500	-0.23951000	2.20406400
C	4.24465500	-0.32515900	3.44326200
N	2.32856800	0.06491900	2.04843100
C	3.48275100	-0.07042700	4.58176000
H	5.30009000	-0.57846000	3.52279000
C	1.61294200	0.32795900	3.14476600
C	2.14484800	0.27187600	4.42996100
H	3.93432000	-0.12879400	5.56922600
H	0.57422500	0.60413500	2.97267200

H	1.52032200	0.49897500	5.28989200
H	-6.45143400	1.29629400	-0.06963200
H	-5.60809800	-2.89455100	-0.22739900
H	5.61017700	-2.89208800	0.22524300
H	6.45110200	1.29793300	0.07037500
C	0.38678100	-3.34626600	-1.77097000
H	-0.33719000	-3.59270900	-2.55798300
H	0.58038700	-4.26017000	-1.19674500
H	-0.07590300	-2.60884500	-1.10510300
C	1.36853500	-1.47282000	-3.11140900
H	0.97770200	-0.73863200	-2.39590600
H	2.26350500	-1.05008200	-3.58493600
H	0.60788600	-1.62051300	-3.88764700
C	2.18071600	-3.81201200	-3.43598900
H	2.34876200	-4.79761100	-2.98657300
H	1.43700100	-3.94241400	-4.22938300
H	3.11573800	-3.48451900	-3.90549200
C	-0.38623900	-3.34666500	1.77253400
H	0.33725600	-3.59263600	2.56013000
H	-0.57971500	-4.26102200	1.19897800
H	0.07690000	-2.60989500	1.10629100
C	-1.36834700	-1.47209800	3.11113500
H	-0.97709600	-0.73837700	2.39538100
H	-2.26344600	-1.04892600	3.58403000
H	-0.60804600	-1.61942300	3.88778000
C	-2.18111300	-3.81091600	3.43693100
H	-2.34882800	-4.79686700	2.98817700
H	-1.43792000	-3.94070300	4.23091900
H	-3.11646400	-3.48307700	3.90552600
C	-1.64810600	3.86725900	0.62503500
H	-2.24775100	4.50654200	-0.03394400
H	-0.85837400	4.48591700	1.06874500
H	-1.16648100	3.09704400	0.00694300
C	-1.63416100	2.37116300	2.63725600
H	-2.21868400	1.90687300	3.44113800
H	-1.14773600	1.57660700	2.05772900
H	-0.84425200	2.97987600	3.09407000
C	-3.17695600	4.33885300	2.55089000
H	-2.41459800	4.95607600	3.03810700
H	-3.78185200	5.00465500	1.92424200
H	-3.82136300	3.92701800	3.33683800
C	1.63261600	2.37052100	-2.63651700
H	2.21634100	1.90564600	-3.44064600
H	1.14661200	1.57638300	-2.05606400
H	0.84236200	2.97904600	-3.09298800
C	1.64844500	3.86806700	-0.62541000
H	2.24877400	4.50759000	0.03271100
H	0.85858200	4.48668500	-1.06894600
H	1.16705200	3.09837800	-0.00648700
C	3.17599000	4.33785400	-2.55279800
H	2.41341500	4.95476800	-3.04006900
H	3.78133900	5.00411700	-1.92708200
H	3.81988100	3.92523300	-3.33875300

Table S63: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 1.618 Å

Cu	1.70746500	0.10134700	-0.13273600
Cu	-1.70740600	0.10124400	0.13251100
O	0.00006700	-0.62165500	-0.00028400
O	-0.00007100	0.99720700	0.00036600
N	4.45377400	0.76394200	0.15744300
N	3.29330000	1.26980400	-0.35175600
N	4.00585400	-1.57536200	0.14792300
N	2.83470500	-1.49780400	-0.54718200
N	-2.83475300	-1.49774500	0.54695700
N	-4.00576200	-1.57543700	-0.14838400
N	-3.29310700	1.26982900	0.35177900
N	-4.45364700	0.76390900	-0.15727100
C	4.43958000	-0.44898100	0.96112500
C	3.63061100	2.39655500	-1.00100400
C	5.01628000	2.60929200	-0.89252700
C	5.50656400	1.55695200	-0.15479600
C	2.58244300	3.25317300	-1.66409000
C	2.82354800	-2.55866000	-1.37589600
C	3.98841600	-3.32277300	-1.17754200
C	4.72321400	-2.66278100	-0.22294800
C	1.74500400	-2.78204500	-2.41079400
C	-4.43953900	-0.44880400	-0.96125600
C	-5.50642900	1.55686500	0.15514600
C	-5.01610300	2.60916500	0.89289800
C	-3.63040300	2.39651100	1.00115100
C	-2.58221100	3.25314500	1.66418700
C	-4.72326300	-2.66270900	0.22268600
C	-3.98863400	-3.32252900	1.17751900
C	-2.82375000	-2.55842100	1.37588300
C	-1.74534900	-2.78162400	2.41097300
H	5.48117600	-0.65137600	1.22639700
H	5.58757000	3.42788900	-1.30819200
H	4.26831400	-4.23091900	-1.69300900
H	-5.48115500	-0.65109900	-1.22651600
H	-5.58737000	3.42767700	1.30876000
H	-4.26860400	-4.23059400	1.69309100
C	3.62624400	-0.26800200	2.22598600
C	4.21313500	-0.36903700	3.48029700
N	2.33302600	0.03323000	2.04267700
C	3.41970100	-0.13513800	4.60161100
H	5.26724400	-0.61866100	3.58498800
C	1.58543400	0.27383400	3.12270800
C	2.08367000	0.20099400	4.42037900
H	3.84566600	-0.20556300	5.59960300
H	0.54926300	0.54316200	2.92402800
H	1.43527700	0.41020100	5.26721600
C	-3.62624500	-0.26763200	-2.22611100
C	-4.21318800	-0.36836300	-3.48041700
N	-2.33296800	0.03336100	-2.04278800
C	-3.41974200	-0.13446200	-4.60172200
H	-5.26734700	-0.61777700	-3.58510800
C	-1.58536500	0.27398700	-3.12280800
C	-2.08364300	0.20138800	-4.42047800
H	-3.84573700	-0.20468800	-5.59971500
H	-0.54913600	0.54309800	-2.92412700

H	-1.43521700	0.41054800	-5.26730100
H	6.50792300	1.30896100	0.17453500
H	5.68921300	-2.87085700	0.22004100
H	-5.68917600	-2.87088100	-0.22044800
H	-6.50781800	1.30885300	-0.17407800
C	-0.45375100	-3.30219500	1.76826700
H	0.27340100	-3.54714300	2.55289900
H	-0.63288700	-4.21233800	1.18360300
H	0.00094000	-2.55138200	1.11219600
C	-1.46622600	-1.45327700	3.11928900
H	-1.09583200	-0.70678100	2.40440500
H	-2.36699400	-1.05004800	3.59851300
H	-0.69879200	-1.58933500	3.89096200
C	-2.23992500	-3.80839200	3.43235100
H	-2.39905300	-4.79209000	2.97530600
H	-1.49249900	-3.93669700	4.22259100
H	-3.17701200	-3.49523400	3.90760500
C	0.45345600	-3.30240400	-1.76779900
H	-0.27380700	-3.54750500	-2.55227900
H	0.63261900	-4.21240300	-1.18292000
H	-0.00113100	-2.55139800	-1.11187500
C	1.46584900	-1.45386500	-3.11941600
H	1.09569800	-0.70713400	-2.40465300
H	2.36654000	-1.05087700	-3.59898300
H	0.69821200	-1.59006600	-3.89086300
C	2.23938600	-3.80909800	-3.43197500
H	2.39860700	-4.79266600	-2.97468200
H	1.49181600	-3.93762900	-4.22204200
H	3.17638300	-3.49607300	-3.90749500
C	1.70409700	3.87029500	-0.56645300
H	2.29303300	4.50630100	0.10507800
H	0.91898200	4.49045500	-1.01611900
H	1.21612500	3.09486600	0.04013300
C	1.71948000	2.38684200	-2.58723700
H	2.31362200	1.93275300	-3.38988500
H	1.23460500	1.58291400	-2.01863600
H	0.92836400	2.99280100	-3.04550800
C	3.25130800	4.36330900	-2.47277100
H	2.49121800	4.97956200	-2.96477100
H	3.84533700	5.02823000	-1.83476800
H	3.90753400	3.96043000	-3.25353400
C	-1.71946100	2.38688300	2.58760400
H	-2.31374400	1.93307500	3.39030600
H	-1.23469400	1.58274500	2.01921700
H	-0.92828200	2.99280800	3.04581300
C	-1.70366300	3.86996800	0.56654300
H	-2.29246900	4.50579000	-0.10527600
H	-0.91864200	4.49025500	1.01619600
H	-1.21555800	3.09437300	-0.03972500
C	-3.25104400	4.36350800	2.47257600
H	-2.49093500	4.97975000	2.96455800
H	-3.84491800	5.02838700	1.83438100
H	-3.90740700	3.96084300	3.25333300

Table S64: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 1.488 Å

Cu	1.76271100	0.10320300	-0.12283500
Cu	-1.76282700	0.10322500	0.12270500
O	-0.00011100	-0.53564500	0.00026900
O	-0.00001900	0.95267300	-0.00064000
N	4.50006100	0.74427500	0.18477800
N	3.34612500	1.26751400	-0.32084900
N	4.03752100	-1.59448000	0.13182900
N	2.86587900	-1.50410900	-0.56071900
N	-2.86612000	-1.50384000	0.56109900
N	-4.03798400	-1.59391300	-0.13112800
N	-3.34600200	1.26790900	0.32075500
N	-4.50008000	0.74490400	-0.18476600
C	4.46826100	-0.48296900	0.96701400
C	3.69163500	2.40747700	-0.94087700
C	5.07786800	2.61115300	-0.81801900
C	5.55867100	1.53989100	-0.10113700
C	2.64895400	3.28455800	-1.58672300
C	2.85558300	-2.54685900	-1.41094200
C	4.02167600	-3.31341700	-1.23142100
C	4.75664900	-2.67269500	-0.26340800
C	1.77276100	-2.73955000	-2.44699000
C	-4.46855700	-0.48258900	-0.96662600
C	-5.55850300	1.54075800	0.10116900
C	-5.07740800	2.61197900	0.81792100
C	-3.69121300	2.40800500	0.94070400
C	-2.64829900	3.28492100	1.58638200
C	-4.75717700	-2.67206300	0.26413500
C	-4.02209000	-3.31299800	1.23192200
C	-2.85579800	-2.54670000	1.41119700
C	-1.77273100	-2.73976900	2.44691900
H	5.50487500	-0.69612200	1.24294900
H	5.65626700	3.43641200	-1.21015100
H	4.30143600	-4.21085100	-1.76531700
H	-5.50522400	-0.69564900	-1.24242500
H	-5.65559900	3.43741000	1.20999900
H	-4.30189500	-4.21040300	1.76584500
C	3.63920200	-0.31755400	2.22465900
C	4.21124400	-0.43814400	3.48405300
N	2.34778000	-0.01120400	2.03252900
C	3.40575200	-0.22047300	4.59997200
H	5.26374900	-0.69091400	3.59674200
C	1.58773600	0.21219500	3.10775000
C	2.07171500	0.11866800	4.40933900
H	3.82093200	-0.30598900	5.60130600
H	0.55346400	0.48277000	2.90104000
H	1.41391400	0.31481000	5.25207900
C	-3.63956300	-0.31768300	-2.22439000
C	-4.21169900	-0.43849600	-3.48372000
N	-2.34808600	-0.01148000	-2.03242900
C	-3.40623200	-0.22120300	-4.59973200
H	-5.26424600	-0.69114400	-3.59629300
C	-1.58806400	0.21159400	-3.10772700
C	-2.07213900	0.11782500	-4.40926300
H	-3.82148300	-0.30690500	-5.60102100
H	-0.55376000	0.48212800	-2.90109300

H	-1.41437500	0.31370700	-5.25209300
H	6.55669800	1.27995700	0.22908700
H	5.72292900	-2.88953000	0.17478500
H	-5.72360900	-2.88867000	-0.17383100
H	-6.55661500	1.28100700	-0.22893900
C	-0.46892600	-3.23285300	1.80675900
H	0.27434300	-3.42573300	2.59108000
H	-0.62120800	-4.16788100	1.25478600
H	-0.04587300	-2.48926600	1.12243800
C	-1.52863400	-1.39682900	3.14156000
H	-1.17890000	-0.64836000	2.41757600
H	-2.44053400	-1.01172200	3.61433700
H	-0.75987700	-1.50403600	3.91636300
C	-2.24125100	-3.76802600	3.47824200
H	-2.38468600	-4.75783500	3.02915200
H	-1.48732000	-3.87671500	4.26532900
H	-3.18135100	-3.46921300	3.95691200
C	0.46875500	-3.23271000	-1.80728900
H	-0.27436300	-3.42524100	-2.59183900
H	0.62083200	-4.16796100	-1.25563600
H	0.04565400	-2.48933700	-1.12276600
C	1.52900300	-1.39638700	-3.14130900
H	1.17928600	-0.64801500	-2.41720500
H	2.44106100	-1.01130900	-3.61380600
H	0.76038300	-1.50324900	-3.91629500
C	2.24143200	-3.76754300	-3.47851400
H	2.38451500	-4.75754400	-3.02973500
H	1.48773700	-3.87580800	-4.26588500
H	3.18174800	-3.46874400	-3.95676700
C	1.78950700	3.90573000	-0.47524500
H	2.39494700	4.52571800	0.19644400
H	1.01290500	4.54408400	-0.91387500
H	1.29242400	3.13452900	0.12930200
C	1.76429400	2.43978400	-2.50939600
H	2.34364400	1.98711700	-3.32362400
H	1.27397000	1.63602900	-1.94530600
H	0.97635000	3.06120500	-2.95209600
C	3.32639600	4.39219600	-2.39166300
H	2.57110600	5.02141000	-2.87460600
H	3.93240800	5.04559900	-1.75301900
H	3.97291200	3.98661000	-3.17909200
C	-1.76345500	2.43996900	2.50870900
H	-2.34262800	1.98714900	3.32297800
H	-1.27325300	1.63634000	1.94433300
H	-0.97540300	3.06130500	2.95133900
C	-1.78909100	3.90612300	0.47473600
H	-2.39464500	4.52625900	-0.19671600
H	-1.01228800	4.54433800	0.91321700
H	-1.29228000	3.13492200	-0.13003600
C	-3.32543700	4.39252600	2.39162600
H	-2.56996900	5.02161000	2.87446400
H	-3.93153500	5.04606900	1.75320900
H	-3.97180600	3.98690600	3.17915800

Table S65: XYZ coordinates for optimised structure: Singlet minimum path, M06L/6-31g(d), O...O = 1.359 Å

Cu	-1.80296200	0.10144200	0.11482800
Cu	1.80301300	0.10124200	-0.11513200
O	-0.00002300	-0.45727400	0.00000200
O	0.00004400	0.90130100	-0.00142200
N	-4.53214500	0.74113200	-0.20592900
N	-3.38145100	1.26896600	0.30077500
N	-4.06931600	-1.59857200	-0.12413700
N	-2.89516200	-1.50880800	0.56453000
N	2.89516600	-1.50935800	-0.56324700
N	4.06918800	-1.59863300	0.12572700
N	3.38134300	1.26870900	-0.30179000
N	4.53201800	0.74117000	0.20531400
C	-4.49082500	-0.49499700	-0.97425700
C	-3.72827200	2.41677000	0.90386700
C	-5.11360400	2.62107500	0.77027000
C	-5.59178600	1.54165900	0.06339500
C	-2.68397600	3.29782000	1.54186700
C	-2.89390300	-2.53739800	1.43090700
C	-4.06858400	-3.29446000	1.26850100
C	-4.79934900	-2.66220500	0.29157500
C	-1.80438700	-2.72252500	2.46069400
C	4.49067500	-0.49423000	0.97479700
C	5.59162300	1.54168800	-0.06420000
C	5.11348000	2.62068200	-0.77174000
C	3.72818700	2.41621100	-0.90544200
C	2.68392200	3.29675000	-1.54418400
C	4.79935100	-2.66248200	-0.28920000
C	4.06874100	-3.29547500	-1.26576300
C	2.89406200	-2.53855100	-1.42889700
C	1.80473600	-2.72433900	-2.45877000
H	-5.52389400	-0.71154300	-1.26052700
H	-5.69330100	3.45214400	1.14804700
H	-4.35512400	-4.18112300	1.81655200
H	5.52374200	-0.71048400	1.26129000
H	5.69316700	3.45158500	-1.14989700
H	4.35539700	-4.18252500	-1.81313200
C	-3.64798500	-0.34147500	-2.22514500
C	-4.20999800	-0.47298400	-3.48798900
N	-2.35699000	-0.03386000	-2.02672200
C	-3.39656900	-0.26630800	-4.60010700
H	-5.26179800	-0.72610400	-3.60610000
C	-1.58905400	0.17871300	-3.09896900
C	-2.06364700	0.07342300	-4.40291900
H	-3.80480300	-0.36051100	-5.60350900
H	-0.55575300	0.45012700	-2.88826200
H	-1.39925900	0.26118100	-5.24240200
C	3.64778500	-0.33957100	2.22550700
C	4.20977100	-0.46984600	3.48849000
N	2.35677200	-0.03224900	2.02672400
C	3.39631400	-0.26213700	4.60039200
H	5.26158800	-0.72277600	3.60685700
C	1.58881600	0.18131500	3.09876300
C	2.06338600	0.07734400	4.40282800
H	3.80452300	-0.35533100	5.60389800
H	0.55549000	0.45243300	2.88783100

H	1.39896100	0.26589900	5.24210500
H	-6.58816000	1.27921900	-0.26982600
H	-5.76854100	-2.87670500	-0.14126600
H	5.76848600	-2.87667700	0.14392200
H	6.58797000	1.27949500	0.26929600
C	0.50306200	-3.20961400	-1.80861800
H	-0.24973200	-3.39333100	-2.58605100
H	0.65285400	-4.14802200	-1.26176300
H	0.09326700	-2.46547000	-1.11703100
C	1.56319200	-1.37687000	-3.14607000
H	1.22280500	-0.63010800	-2.41521300
H	2.47394800	-0.99369900	-3.62253100
H	0.78898300	-1.47591600	-3.91654800
C	2.25998000	-3.75166200	-3.49630400
H	2.40471100	-4.74270900	-3.05030800
H	1.49867800	-3.85656200	-4.27681700
H	3.19652100	-3.45487000	-3.98321300
C	-0.50280500	-3.20812600	1.81059600
H	0.25024600	-3.39101900	2.58797500
H	-0.65258600	-4.14704400	1.26461400
H	-0.09333300	-2.46454000	1.11822600
C	-1.56280100	-1.37464700	3.14716000
H	-1.22271300	-0.62826400	2.41578400
H	-2.47347700	-0.99132800	3.62365400
H	-0.78837000	-1.47317100	3.91748200
C	-2.25936600	-3.74926200	3.49892400
H	-2.40423800	-4.74055000	3.05350700
H	-1.49786700	-3.85374900	4.27930000
H	-3.19577400	-3.45219100	3.98591900
C	-1.81886200	3.90173800	0.42500400
H	-2.42086300	4.50914400	-0.26106700
H	-1.04638500	4.54889800	0.85787700
H	-1.31630500	3.12041400	-0.16211700
C	-1.80272900	2.45978400	2.47409200
H	-2.38367400	2.01641800	3.29227200
H	-1.31424900	1.64891800	1.91801400
H	-1.01284900	3.08291000	2.91089500
C	-3.35911400	4.41666900	2.33274200
H	-2.60306500	5.04844900	2.81112200
H	-3.96092500	5.06521700	1.68516400
H	-4.00967700	4.02222000	3.12250200
C	1.80349500	2.45811600	-2.47665000
H	2.38506800	2.01478000	-3.29439800
H	1.31505700	1.64719200	-1.92062600
H	1.01361400	3.08081200	-2.91405800
C	1.81801500	3.90062600	-0.42792200
H	2.41944200	4.50845100	0.25828400
H	1.04551400	4.54738100	-0.86136000
H	1.31544600	3.11928600	0.15916900
C	3.35905200	4.41566200	-2.33498800
H	2.60300200	5.04699900	-2.81394900
H	3.96024900	5.06463700	-1.68726600
H	4.01020100	4.02127000	-3.12429300

Table S66: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, Oxo (The calculation of the oxo runs always into the peroxy. Thus, the O...O distance was fixed.)

Cu	1.47080300	0.04422400	-0.20885000
Cu	-1.47072700	0.04452800	0.20879100
O	-0.00000200	-0.98834300	0.00043600
O	0.00008200	1.14165700	-0.00056100
N	4.21747500	0.81026400	-0.02524800
N	3.03222400	1.27970600	-0.52198000
N	3.82844000	-1.52919300	0.12396100
N	2.68781100	-1.48199300	-0.61681100
N	-2.68786500	-1.48121900	0.61821500
N	-3.82856500	-1.52900900	-0.12241700
N	-3.03201000	1.28044100	0.52081200
N	-4.21732800	0.81066000	0.02455600
C	4.31379100	-0.35475800	0.83967700
C	3.34555700	2.37961500	-1.24265300
C	4.73407900	2.59929600	-1.17967500
C	5.24995700	1.59238000	-0.40758000
C	2.34814200	3.26616800	-1.95474900
C	2.67060200	-2.60769500	-1.36463100
C	3.80754300	-3.37764200	-1.05149000
C	4.52240100	-2.66047400	-0.12714400
C	1.65021600	-2.93578600	-2.43695900
C	-4.31386700	-0.35521200	-0.83921300
C	-5.24970400	1.59325500	0.40620000
C	-4.73368700	2.60083900	1.17732900
C	-3.34519300	2.38104000	1.24049300
C	-2.34765300	3.26812000	1.95176700
C	-4.52262800	-2.65997200	0.12983200
C	-3.80777100	-3.37633700	1.05479900
C	-2.67072700	-2.60620800	1.36711000
C	-1.65032200	-2.93334400	2.43970700
H	5.37876900	-0.52044200	0.99088600
H	5.28593900	3.39352200	-1.65039600
H	4.08644700	-4.32434900	-1.48007800
H	-5.37889000	-0.52090800	-0.99008800
H	-5.28544300	3.39556400	1.64733100
H	-4.08674600	-4.32259700	1.48432700
C	3.65809200	-0.13126600	2.18401000
C	4.41325300	-0.15120700	3.34919900
N	2.34837600	0.11760500	2.15060800
C	3.76904700	0.11272700	4.55428100
H	5.47614900	-0.36153900	3.32141600
C	1.74221600	0.38126400	3.31074600
C	2.40984900	0.39108000	4.53163000
H	4.32133800	0.10770400	5.48614000
H	0.68474400	0.59864600	3.25932700
H	1.86888800	0.61506800	5.44236700
C	-3.65840700	-0.13321500	-2.18391400
C	-4.41386500	-0.15399500	-3.34889600
N	-2.34855500	0.11501000	-2.15110300
C	-3.76984000	0.10841600	-4.55440800
H	-5.47685000	-0.36381400	-3.32063400
C	-1.74255700	0.37717200	-3.31166400
C	-2.41049800	0.38610900	-4.53238600
H	-4.32237000	0.10271200	-5.48612200

H	-0.68495400	0.59402600	-3.26074100
H	-1.86965500	0.60889400	-5.44348700
H	6.25944500	1.37277400	-0.09757300
H	5.46777000	-2.85487500	0.35457700
H	-5.46806200	-2.85472800	-0.35161900
H	-6.25923000	1.37346600	0.09644600
C	-0.41230100	-3.62078200	1.83361600
H	0.26280500	-3.91796900	2.64029500
H	-0.69455200	-4.51936200	1.28069200
H	0.11888400	-2.94423400	1.16359500
C	-1.23658600	-1.65212800	3.17582400
H	-0.74891600	-0.95248200	2.49517300
H	-2.09946500	-1.16263300	3.63384100
H	-0.52610200	-1.90237000	3.96681300
C	-2.29252700	-3.89642100	3.45692500
H	-2.52378900	-4.86512900	3.00918100
H	-1.58553000	-4.07428700	4.26959900
H	-3.20674900	-3.48143200	3.88736400
C	0.41209200	-3.62248900	-1.83024700
H	-0.26297900	-3.92046300	-2.63666600
H	0.69422800	-4.52051500	-1.27636500
H	-0.11908800	-2.94519700	-1.16097300
C	1.23663900	-1.65527500	-3.17440000
H	0.74894600	-0.95490800	-2.49450600
H	2.09959500	-1.16630300	-3.63282900
H	0.52621600	-1.90626300	-3.96520600
C	2.29237900	-3.89995500	-3.45316700
H	2.52353400	-4.86822600	-3.00442400
H	1.58540100	-4.07858700	-4.26569000
H	3.20665800	-3.48548800	-3.88398700
C	1.61733800	4.10834900	-0.89088100
H	2.32217800	4.73282800	-0.33724100
H	0.88954800	4.76320200	-1.37595700
H	1.09292900	3.46409700	-0.18444200
C	1.33973900	2.43236800	-2.75609600
H	1.84652100	1.80191600	-3.49127800
H	0.73795700	1.81128700	-2.09047500
H	0.66332400	3.10361500	-3.29057600
C	3.08812100	4.20998000	-2.91794300
H	2.35606900	4.82537300	-3.44448900
H	3.76077600	4.88697900	-2.38712800
H	3.66358500	3.65774700	-3.66483500
C	-1.33933800	2.43494800	2.75388900
H	-1.84619800	1.80523900	3.48965400
H	-0.73760100	1.81318300	2.08886400
H	-0.66286100	3.10662000	3.28775700
C	-1.61676100	4.10922800	0.88711000
H	-2.32153100	4.73329400	0.33291500
H	-0.88887300	4.76443000	1.37156900
H	-1.09245500	3.46425800	0.18125000
C	-3.08750800	4.21292400	2.91408400
H	-2.35537000	4.82867900	3.44008800
H	-3.76003800	4.88954700	2.38263200
H	-3.66308000	3.66146300	3.66146300

Table S67: XYZ coordinates for Optimised structure: Singlet minimum path, TPSSh/def2tzvp, Peroxo

Cu	-1.82455100	0.03759000	0.04504400
Cu	1.82453300	0.03752400	-0.04501400
O	-0.00003800	-0.61537200	-0.00023000
O	0.00002500	0.80669600	-0.00000900
N	-4.47476300	0.98309600	-0.34848700
N	-3.32981000	1.37236200	0.27932600
N	-4.26632000	-1.39270600	-0.30939600
N	-3.12970300	-1.48136400	0.43501500
N	3.12968700	-1.48143000	-0.43478200
N	4.26627000	-1.39268500	0.30967600
N	3.32981900	1.37230700	-0.27950700
N	4.47477600	0.98312000	0.34834300
C	-4.53247900	-0.23197400	-1.14790100
C	-3.63928900	2.49158300	0.95888700
C	-4.99617600	2.80775700	0.74828900
C	-5.49326300	1.83108100	-0.07689300
C	-2.63695500	3.28073200	1.77276800
C	-3.28734000	-2.55865900	1.22779200
C	-4.53209000	-3.16055100	0.95769700
C	-5.12902000	-2.38992700	-0.00747900
C	-2.27851200	-2.98925000	2.27221100
C	4.53245700	-0.23180500	1.14797200
C	5.49329600	1.83102700	0.07657700
C	4.99621600	2.80757000	-0.74876600
C	3.63931300	2.49139700	-0.95927500
C	2.63699000	3.28041800	-1.77329500
C	5.12894500	-2.38999400	0.00797600
C	4.53204400	-3.16075100	-0.95711100
C	3.28732300	-2.55887000	-1.22736300
C	2.27854400	-2.98960700	-2.27177000
H	-5.56708200	-0.32847500	-1.47087500
H	-5.54202700	3.64089400	1.15543400
H	-4.94629300	-4.03736200	1.42380000
H	5.56705300	-0.32828100	1.47097200
H	5.54208300	3.64061700	-1.15607400
H	4.94624400	-4.03764900	-1.42305200
C	-3.64375500	-0.16106400	-2.37474300
C	-4.19317100	-0.20977400	-3.64864300
N	-2.33175800	-0.03547100	-2.14866300
C	-3.33803400	-0.11922500	-4.74278500
H	-5.26283500	-0.31307500	-3.78776200
C	-1.51680900	0.05660700	-3.20331500
C	-1.97581200	0.01949500	-4.51494000
H	-3.73214300	-0.15288200	-5.75121600
H	-0.46374400	0.16665700	-2.98215900
H	-1.27540200	0.09994300	-5.33646600
C	3.64372300	-0.16064700	2.37479400
C	4.19313700	-0.20904800	3.64870700
N	2.33172200	-0.03513700	2.14868100
C	3.33799700	-0.11826800	4.74282700
H	5.26280400	-0.31229100	3.78785000
C	1.51677100	0.05716600	3.20331300
C	1.97577200	0.02036600	4.51494700
H	3.73210500	-0.15168200	5.75126600
H	0.46370400	0.16714300	2.98213400

H	1.27535800	0.10098400	5.33645200
H	-6.47775600	1.67428700	-0.48877600
H	-6.08837200	-2.46758000	-0.49436600
H	6.08826900	-2.46759800	0.49492400
H	6.47779600	1.67427400	0.48846000
C	1.02761300	-3.57597500	-1.59348000
H	0.32870700	-3.92465600	-2.35803900
H	1.28764300	-4.42524900	-0.95794100
H	0.52346500	-2.82622900	-0.98471300
C	1.88899100	-1.77725300	-3.13423000
H	1.43911300	-0.99058800	-2.52309700
H	2.75929300	-1.36079000	-3.64622100
H	1.15995700	-2.08297200	-3.88837500
C	2.90159400	-4.06383400	-3.17763700
H	3.14731000	-4.96949800	-2.61838100
H	2.18385100	-4.34074400	-3.95231400
H	3.80615000	-3.70150700	-3.67168200
C	-1.02759200	-3.57566000	1.59394000
H	-0.32864500	-3.92423400	2.35851200
H	-1.28762200	-4.42501600	0.95850900
H	-0.52349300	-2.82596600	0.98506900
C	-1.88895400	-1.77678100	3.13450700
H	-1.43911700	-0.99018200	2.52325500
H	-2.75924600	-1.36026900	3.64647500
H	-1.15988400	-2.08238800	3.88866300
C	-2.90150200	-4.06337900	3.17823300
H	-3.14722800	-4.96911300	2.61909400
H	-2.18372000	-4.34018400	3.95291200
H	-3.80604200	-3.70100800	3.67227500
C	-1.73037400	4.06175400	0.80013300
H	-2.31641600	4.75644400	0.19409700
H	-0.99468800	4.64063600	1.36385900
H	-1.20000000	3.38372900	0.12960000
C	-1.78767900	2.34650600	2.64868500
H	-2.41510300	1.76037300	3.32417700
H	-1.18866900	1.66657500	2.03780800
H	-1.09971600	2.94312700	3.25264400
C	-3.37662300	4.27592600	2.68119500
H	-2.64835700	4.83141000	3.27548400
H	-3.94938300	5.00340000	2.10219900
H	-4.05469200	3.76496900	3.36894900
C	1.78768400	2.34604300	-2.64902500
H	2.41509100	1.75975500	-3.32439900
H	1.18865400	1.66625700	-2.03801000
H	1.09974200	2.94256600	-3.25310600
C	1.73043400	4.06164800	-0.80080700
H	2.31649400	4.75642900	-0.19489400
H	0.99476800	4.64045000	-1.36464300
H	1.20003600	3.38375700	-0.13015800
C	3.37667800	4.27541400	-2.68192200
H	2.64842400	4.83079900	-3.27631800
H	3.94946300	5.00298600	-2.10307300
H	4.05473300	3.76430600	-3.36958100

Table S68: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 2.277 Å

Cu	1.41244800	0.03309900	-0.24429200
Cu	-1.40277000	0.04162800	0.22001200
O	0.00987400	-1.07349400	0.03916500
O	-0.00288500	1.20033000	-0.08503100
N	4.15783000	0.83096500	-0.09357100
N	2.96644500	1.26546000	-0.60576400
N	3.78373300	-1.49953900	0.16589400
N	2.65228900	-1.48323300	-0.58900500
N	-2.62251500	-1.45549500	0.69889600
N	-3.75073700	-1.54690900	-0.05589700
N	-2.97391300	1.28145400	0.51193500
N	-4.15889300	0.79090800	0.03382100
C	4.27358000	-0.29226300	0.82230800
C	3.26226600	2.34340700	-1.36696400
C	4.64672000	2.58680600	-1.30976400
C	5.17752900	1.61622000	-0.50212700
C	2.25513700	3.17817800	-2.12570300
C	2.62959800	-2.64642200	-1.27710100
C	3.75865900	-3.40602200	-0.91409100
C	4.47039200	-2.64757300	-0.02082600
C	1.62044900	-3.02549500	-2.34323500
C	-4.26053000	-0.39759500	-0.79676500
C	-5.19458100	1.57470000	0.40281200
C	-4.68252400	2.60297400	1.14715800
C	-3.29155800	2.39605900	1.21007400
C	-2.31202300	3.31881400	1.90277000
C	-4.41909200	-2.68896000	0.21343600
C	-3.69852200	-3.36726100	1.16226700
C	-2.58349200	-2.56437800	1.47159000
C	-1.57606200	-2.84696900	2.56915800
H	5.34208500	-0.44562900	0.96196900
H	5.18648300	3.37178100	-1.80905400
H	4.03525400	-4.37428600	-1.29311900
H	-5.32731700	-0.57579900	-0.91898000
H	-5.23848300	3.40310500	1.60263600
H	-3.96232300	-4.30908800	1.61076400
C	3.64171500	-0.01155700	2.16769800
C	4.42356300	0.02431400	3.31503900
N	2.33027100	0.22964800	2.15180800
C	3.80620500	0.33974200	4.52170800
H	5.48674800	-0.18230100	3.27222500
C	1.75062300	0.54311500	3.31339600
C	2.44562000	0.61112400	4.51726600
H	4.37960400	0.37915100	5.43990300
H	0.69109200	0.75378700	3.27813500
H	1.92394000	0.87382800	5.42893500
C	-3.64070800	-0.21056400	-2.16301200
C	-4.43298600	-0.26180300	-3.30262300
N	-2.33002100	0.03482900	-2.17651300
C	-3.82783100	-0.03610800	-4.53505300
H	-5.49499200	-0.46768900	-3.23444000
C	-1.76206300	0.26157800	-3.36389900
C	-2.46786500	0.23710800	-4.56322400
H	-4.40944600	-0.06697900	-5.44839300
H	-0.70280100	0.47600300	-3.35495700

H	-1.95470000	0.43081400	-5.49673300
H	6.18976600	1.42403600	-0.18303100
H	5.41110300	-2.82271200	0.47714300
H	-5.35533000	-2.91580800	-0.27194600
H	-6.20407500	1.33984400	0.10420600
C	-0.35574600	-3.60746300	2.01535900
H	0.30346100	-3.87787800	2.84431100
H	-0.66215300	-4.52801900	1.51383400
H	0.20011600	-2.98768100	1.31169400
C	-1.12725500	-1.53685000	3.22796000
H	-0.60527900	-0.90152400	2.51124500
H	-1.97731400	-0.99015700	3.64338500
H	-0.43569400	-1.76128700	4.04311300
C	-2.25221300	-3.72668600	3.63956200
H	-2.50852000	-4.71435200	3.25140100
H	-1.55511600	-3.87362200	4.46683600
H	-3.15701800	-3.26016400	4.03574900
C	0.43013900	-3.78448800	-1.72556500
H	-0.23432000	-4.11957500	-2.52607100
H	0.76968800	-4.66566600	-1.17683600
H	-0.13140200	-3.13981700	-1.04951600
C	1.12442300	-1.77431700	-3.07801900
H	0.58111900	-1.11535800	-2.39923900
H	1.95338900	-1.22466200	-3.53046400
H	0.43853500	-2.07272300	-3.87390500
C	2.31136700	-3.95066300	-3.36539300
H	2.59812900	-4.90627500	-2.92188600
H	1.61156000	-4.16554900	-4.17535100
H	3.19960500	-3.48482900	-3.79819800
C	1.43922800	3.99600900	-1.10748100
H	2.08855400	4.65501800	-0.52641800
H	0.70924600	4.61504100	-1.63476700
H	0.90878700	3.33333000	-0.42233300
C	1.32535400	2.28471100	-2.95841700
H	1.89257600	1.67858500	-3.66941800
H	0.73824800	1.63454100	-2.30838400
H	0.63162200	2.91272100	-3.52241700
C	2.98954900	4.14487000	-3.06998700
H	2.25168500	4.72518600	-3.62728800
H	3.61470900	4.85247500	-2.52120000
H	3.61292200	3.61146600	-3.79178800
C	-1.21967300	2.53520500	2.63951000
H	-1.65603700	1.85800900	3.37887000
H	-0.60340200	1.97107300	1.93795200
H	-0.56988500	3.23852600	3.16599900
C	-1.68645200	4.23225300	0.82875400
H	-2.45342100	4.83860100	0.34144700
H	-0.96469300	4.90714900	1.29498200
H	-1.17501900	3.64210700	0.06890200
C	-3.06156300	4.19461600	2.92276300
H	-2.34107200	4.83418800	3.43627700
H	-3.79004700	4.84932100	2.44051600
H	-3.57442800	3.59114400	3.67549100

Table S69: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 2.145 Å

Cu	1.45733200	0.03987300	-0.19986800
Cu	-1.45735300	0.03978600	0.19986400
O	0.00000500	-1.00167700	-0.00012000
O	-0.00002700	1.14329400	0.00012500
N	4.21016400	0.81564100	-0.00090100
N	3.02799300	1.27952200	-0.50813800
N	3.82813200	-1.52385300	0.14302800
N	2.69410000	-1.47872100	-0.60694500
N	-2.69406400	-1.47894500	0.60657100
N	-3.82808600	-1.52392900	-0.14342600
N	-3.02806400	1.27930600	0.50844900
N	-4.21021300	0.81550600	0.00109100
C	4.30273300	-0.34887900	0.86462300
C	3.34223000	2.38023100	-1.22713100
C	4.72936400	2.60576700	-1.15230700
C	5.24276500	1.60156600	-0.37501800
C	2.34819600	3.26226700	-1.94975900
C	2.68484200	-2.60381600	-1.35605800
C	3.82309800	-3.36949100	-1.03701700
C	4.52825600	-2.65180200	-0.10555300
C	1.67495100	-2.93395700	-2.43787000
C	-4.30271400	-0.34879100	-0.86473700
C	-5.24285200	1.60128800	0.37540400
C	-4.72949700	2.60531200	1.15295100
C	-3.34235100	2.37982300	1.22771500
C	-2.34836500	3.26173800	1.95055500
C	-4.52817500	-2.65196100	0.10486900
C	-3.82300400	-3.36985700	1.03616400
C	-2.68477500	-2.60422500	1.35540500
C	-1.67487000	-2.93461600	2.43713100
H	5.36683900	-0.51078500	1.02579800
H	5.28208100	3.40162700	-1.61926600
H	4.10924500	-4.31376600	-1.46620300
H	-5.36680600	-0.51070300	-1.02599700
H	-5.28225000	3.40103000	1.62010900
H	-4.10912400	-4.31424900	1.46511100
C	3.63287300	-0.12890000	2.20268500
C	4.37769000	-0.14472900	3.37460400
N	2.32189800	0.11242700	2.15797900
C	3.72164700	0.11556500	4.57407500
H	5.44195700	-0.34904500	3.35611900
C	1.70438700	0.37268300	3.31297900
C	2.36121500	0.38636200	4.53964800
H	4.26586800	0.11360400	5.51068500
H	0.64616700	0.58412100	3.25265500
H	1.81110200	0.60728900	5.44564000
C	-3.63279600	-0.12841000	-2.20270200
C	-4.37753300	-0.14404600	-3.37467500
N	-2.32186600	0.11313600	-2.15784200
C	-3.72144900	0.11666900	-4.57403300
H	-5.44176900	-0.34853200	-3.35631600
C	-1.70432100	0.37380500	-3.31272900
C	-2.36106500	0.38768800	-4.53944000
H	-4.26560500	0.11486600	-5.51068100
H	-0.64614300	0.58542400	-3.25227400

H	-1.81092800	0.60894900	-5.44533600
H	6.25048600	1.38599100	-0.05654500
H	5.47110900	-2.84329000	0.38222900
H	-5.47101600	-2.84336200	-0.38297200
H	-6.25056200	1.38575100	0.05686900
C	-0.43781700	-3.63553200	1.84457200
H	0.22810400	-3.93435600	2.65826500
H	-0.72332200	-4.53457900	1.29408400
H	0.10463900	-2.96734600	1.17539300
C	-1.25690400	-1.65369400	3.17143300
H	-0.75785400	-0.96066600	2.49230300
H	-2.11953200	-1.15524500	3.62012200
H	-0.55505700	-1.90634300	3.96932900
C	-2.33285300	-3.88786500	3.45351100
H	-2.56819600	-4.85673300	3.00826000
H	-1.63384800	-4.06763800	4.27265800
H	-3.24718500	-3.46370800	3.87469000
C	0.43791800	-3.63506800	-1.84550100
H	-0.22800000	-3.93367800	-2.65927500
H	0.72344700	-4.53426200	-1.29526700
H	-0.10455000	-2.96708400	-1.17613100
C	1.25695300	-1.65285100	-3.17183100
H	0.75789900	-0.96001200	-2.49251100
H	2.11956700	-1.15426600	-3.62039700
H	0.55510100	-1.90530200	-3.96978600
C	2.33296600	-3.88691400	-3.45450300
H	2.56833600	-4.85589500	-3.00951200
H	1.63397000	-4.06648800	-4.27370200
H	3.24728800	-3.46261700	-3.87556500
C	1.60017900	4.09938000	-0.89387100
H	2.29508000	4.72689500	-0.33117400
H	0.87487000	4.75102400	-1.38693700
H	1.07067900	3.45169800	-0.19445400
C	1.35436700	2.42460200	-2.76516800
H	1.87370900	1.79778400	-3.49467200
H	0.74703900	1.79961700	-2.10851500
H	0.68148700	3.09322700	-3.30734300
C	3.09461800	4.21136700	-2.90272000
H	2.36569800	4.82356700	-3.43728700
H	3.75713200	4.89122000	-2.36288400
H	3.68208100	3.66328800	-3.64331300
C	-1.35441800	2.42393000	2.76566700
H	-1.87366400	1.79684600	3.49501000
H	-0.74706200	1.79920000	2.10879700
H	-0.68157700	3.09246100	3.30800600
C	-1.60048000	4.09923100	0.89487400
H	-2.29546700	4.72685000	0.33239900
H	-0.87520300	4.75079600	1.38809300
H	-1.07095700	3.45180500	0.19523600
C	-3.09483000	4.21048800	2.90383200
H	-2.36594100	4.82260200	3.43854000
H	-3.75743700	4.89043600	2.36423100
H	-3.68220200	3.66213600	3.64429400

Table S70: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 2.013 Å

Cu	-1.51898800	0.04343600	0.15573600
Cu	1.51899700	0.04342800	-0.15577500
O	0.00000900	-0.92736600	0.00003800
O	0.00000500	1.08557000	-0.00007300
N	-4.26510300	0.84058600	-0.09374900
N	-3.09266300	1.29328900	0.44228700
N	-3.90774600	-1.50617600	-0.19945700
N	-2.77378800	-1.48274700	0.55193800
N	2.77380100	-1.48278500	-0.55183200
N	3.90771900	-1.50618300	0.19962000
N	3.09267200	1.29325500	-0.44237500
N	4.26510900	0.84056100	0.09367300
C	-4.33997500	-0.33323500	-0.94866900
C	-3.41438000	2.39533600	1.15364900
C	-4.79763900	2.63307600	1.04794700
C	-5.30100800	1.63319000	0.25770700
C	-2.42284700	3.26015900	1.89999700
C	-2.80164300	-2.59683000	1.31596300
C	-3.96146000	-3.33369500	1.00679700
C	-4.64274300	-2.60886300	0.06300300
C	-1.79798600	-2.93801000	2.39997900
C	4.33996000	-0.33317000	0.94871700
C	5.30102800	1.63311500	-0.25785800
C	4.79767100	2.63295100	-1.04817100
C	3.41440500	2.39523800	-1.15382900
C	2.42287300	3.26002700	-1.90021900
C	4.64267600	-2.60893500	-0.06267600
C	3.96140600	-3.33384100	-1.00642500
C	2.80164000	-2.59695500	-1.31573100
C	1.79803200	-2.93818600	-2.39977600
H	-5.39832100	-0.48415500	-1.15209200
H	-5.35472900	3.43322800	1.50240200
H	-4.27439700	-4.26434100	1.44682600
H	5.39830200	-0.48408100	1.15216900
H	5.35477400	3.43305500	-1.50269400
H	4.27432300	-4.26454700	-1.44634000
C	-3.61053500	-0.13645400	-2.25927600
C	-4.30081000	-0.15175500	-3.46376100
N	-2.29813600	0.08258800	-2.15990600
C	-3.58605200	0.08317900	-4.63461700
H	-5.36836000	-0.33665900	-3.49182300
C	-1.62279500	0.31684200	-3.28762000
C	-2.22337700	0.32833900	-4.54251600
H	-4.08769800	0.08081600	-5.59469900
H	-0.56456200	0.50789100	-3.17921000
H	-1.62929600	0.52778900	-5.42539500
C	3.61049600	-0.13625100	2.25928900
C	4.30075000	-0.15140600	3.46378800
N	2.29809300	0.08274700	2.15987000
C	3.58596400	0.08363300	4.63460600
H	5.36830400	-0.33628000	3.49189000
C	1.62272600	0.31710200	3.28754700
C	2.22328400	0.32874500	4.54245400
H	4.08759100	0.08138400	5.59469800
H	0.56448900	0.50811200	3.17909900

H	1.62918100	0.52827000	5.42530100
H	-6.30296200	1.42507200	-0.08313900
H	-5.58820000	-2.78049600	-0.42708800
H	5.58810200	-2.78055700	0.42747800
H	6.30298100	1.42500100	0.08299200
C	0.52903600	-3.57400500	-1.80273400
H	-0.13514600	-3.87967800	-2.61533200
H	0.77442500	-4.46093000	-1.21461300
H	-0.00179200	-2.86411000	-1.16752000
C	1.43490200	-1.66784400	-3.18237200
H	0.96066700	-0.93145000	-2.53101100
H	2.31975800	-1.21767500	-3.63838800
H	0.72962300	-1.91929500	-3.97770900
C	2.43556200	-3.94748500	-3.37252600
H	2.63974100	-4.90445000	-2.88748700
H	1.73876300	-4.13889300	-4.19087000
H	3.36478400	-3.56598200	-3.80194100
C	-0.52903200	-3.57388300	1.80290600
H	0.13518800	-3.87952100	2.61548600
H	-0.77446600	-4.46083600	1.21484700
H	0.00177500	-2.86403100	1.16762500
C	-1.43479700	-1.66762700	3.18248400
H	-0.96058200	-0.93127900	2.53105700
H	-2.31962400	-1.21742100	3.63851900
H	-0.72948300	-1.91904600	3.97780000
C	-2.43548000	-3.94724300	3.37282000
H	-2.63969700	-4.90423300	2.88784600
H	-1.73864100	-4.13861400	4.19113900
H	-3.36467300	-3.56570200	3.80226200
C	-1.62135400	4.07364100	0.86566800
H	-2.28229600	4.71506700	0.27833500
H	-0.89620600	4.70984800	1.37884900
H	-1.08500300	3.41166400	0.18476200
C	-1.47547000	2.40102800	2.74898800
H	-2.03116800	1.79465600	3.46866800
H	-0.87029900	1.75059800	2.11491600
H	-0.79651700	3.05309700	3.30351400
C	-3.17494700	4.23022300	2.82639500
H	-2.44940600	4.83295000	3.37612400
H	-3.81096400	4.91765500	2.26468900
H	-3.79156600	3.69787600	3.55467600
C	1.47556300	2.40085300	-2.74924300
H	2.03131200	1.79449800	-3.46889900
H	0.87039700	1.75040200	-2.11518800
H	0.79660300	3.05289000	-3.30379900
C	1.62130600	4.07348100	-0.86592800
H	2.28219800	4.71493200	-0.27856500
H	0.89615900	4.70966400	-1.37914400
H	1.08494700	3.41148700	-0.18504600
C	3.17497500	4.23011300	-2.82659000
H	2.44943600	4.83282400	-3.37633900
H	3.81095800	4.91755700	-2.26486000
H	3.79162900	3.69778500	-3.55485400

Table S71: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 1.881 Å

Cu	-1.59373900	0.04297600	0.11415500
Cu	1.59374000	0.04297700	-0.11415200
O	0.00000400	-0.85842000	0.00004000
O	-0.00000100	1.02276300	-0.00001900
N	-4.31802000	0.88548000	-0.19431000
N	-3.15606800	1.31625500	0.37816600
N	-4.00647900	-1.47154400	-0.25718500
N	-2.87496700	-1.48399100	0.49870700
N	2.87497800	-1.48400300	-0.49862200
N	4.00649800	-1.47150100	0.25725700
N	3.15605300	1.31625500	-0.37823500
N	4.31801500	0.88552200	0.19425100
C	-4.38213200	-0.29896400	-1.03556600
C	-3.47879600	2.42269000	1.07967300
C	-4.85429800	2.68541400	0.93392100
C	-5.35140400	1.69454500	0.12773700
C	-2.48864800	3.26390600	1.85468500
C	-2.95209700	-2.58811700	1.27229200
C	-4.13912400	-3.28236200	0.96803400
C	-4.78676600	-2.54128200	0.01296300
C	-1.95822900	-2.95425600	2.35668000
C	4.38214500	-0.29887500	1.03557200
C	5.35138900	1.69457600	-0.12785700
C	4.85426800	2.68538300	-0.93411100
C	3.47876100	2.42265400	-1.07980600
C	2.48858700	3.26381000	-1.85484900
C	4.78679800	-2.54124100	-0.01284200
C	4.13918300	-3.28235200	-0.96790600
C	2.95211500	-2.58817100	-1.27215000
C	1.95824600	-2.95437800	-2.35651300
H	-5.43333400	-0.43076900	-1.28395000
H	-5.41102200	3.49488000	1.37226500
H	-4.48824200	-4.19705300	1.41412800
H	5.43335000	-0.43065600	1.28395400
H	5.41098400	3.49481700	-1.37252400
H	4.48832900	-4.19704000	-1.41398500
C	-3.59117500	-0.13918900	-2.31612300
C	-4.22719500	-0.15705900	-3.54989100
N	-2.27714600	0.04180800	-2.16549000
C	-3.45452000	0.02957800	-4.69224300
H	-5.29790400	-0.30842700	-3.62203900
C	-1.54423500	0.22686700	-3.26618300
C	-2.08907000	0.22951500	-4.54610700
H	-3.91400900	0.02332200	-5.67318700
H	-0.48562300	0.38302200	-3.11298800
H	-1.45086800	0.38743000	-5.40626900
C	3.59119600	-0.13903600	2.31612700
C	4.22722800	-0.15682900	3.54989000
N	2.27716500	0.04194400	2.16549400
C	3.45456200	0.02987400	4.69223700
H	5.29793800	-0.30818400	3.62203800
C	1.54426300	0.22707100	3.26618200
C	2.08911000	0.22979800	4.54610200
H	3.91406000	0.02368000	5.67317800
H	0.48565100	0.38321600	3.11298700

H	1.45091600	0.38776500	5.40625900
H	-6.34666400	1.50294700	-0.24125900
H	-5.73442700	-2.68213000	-0.48260400
H	5.73446600	-2.68204800	0.48272400
H	6.34665400	1.50300700	0.24113600
C	0.65984700	-3.51788400	-1.75193200
H	-0.00149400	-3.84342900	-2.55914000
H	0.86655500	-4.38011400	-1.11439400
H	0.13968800	-2.76063500	-1.16386700
C	1.65038600	-1.70825600	-3.20195800
H	1.20531000	-0.92205500	-2.58854400
H	2.55570800	-1.31411200	-3.66914200
H	0.94111000	-1.96711600	-3.99140500
C	2.57622400	-4.02813200	-3.26939900
H	2.75441500	-4.96214100	-2.73177600
H	1.88118100	-4.24599300	-4.08256200
H	3.51708600	-3.69237600	-3.71164000
C	-0.65975700	-3.51761900	1.75212300
H	0.00157900	-3.84314700	2.55934300
H	-0.86636300	-4.37983500	1.11453200
H	-0.13963900	-2.76029400	1.16412100
C	-1.65051200	-1.70812800	3.20216600
H	-1.20547600	-0.92187600	2.58878900
H	-2.55588800	-1.31407300	3.66932100
H	-0.94124700	-1.96694600	3.99163600
C	-2.57613500	-4.02808900	3.26952100
H	-2.75420200	-4.96210900	2.73187800
H	-1.88110700	-4.24588800	4.08271400
H	-3.51705400	-3.69244000	3.71172300
C	-1.64956400	4.07260900	0.84648300
H	-2.28527100	4.73136700	0.25053700
H	-0.92476100	4.69115700	1.38143700
H	-1.10937600	3.40915100	0.16968900
C	-1.57453000	2.38047600	2.71592400
H	-2.15565500	1.77799600	3.41840700
H	-0.96737600	1.72251100	2.09096700
H	-0.89529600	3.01477200	3.29037900
C	-3.24396700	4.23816500	2.77380800
H	-2.52127800	4.82599300	3.34312000
H	-3.85872600	4.93887600	2.20494100
H	-3.88301600	3.70886500	3.48473700
C	1.57440400	2.38030000	-2.71593900
H	2.15547700	1.77773900	-3.41839500
H	0.96728500	1.72240600	-2.09087200
H	0.89514000	3.01454200	-3.29041600
C	1.64957200	4.07263100	-0.84668500
H	2.28532400	4.73144400	-0.25084600
H	0.92474700	4.69113100	-1.38166200
H	1.10941400	3.40925300	-0.16978800
C	3.24386800	4.23796100	-2.77411900
H	2.52115400	4.82574200	-3.34344800
H	3.85867500	4.93871900	-2.20536200
H	3.88286300	3.70857400	-3.48503300

Table S72: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 1.749 Å

Cu	-1.67966800	0.04269900	0.08397700
Cu	1.67967400	0.04270500	-0.08397600
O	0.00000600	-0.78821000	0.00002300
O	0.00000100	0.96164000	-0.00001200
N	-4.37711700	0.92521900	-0.27109200
N	-3.22426300	1.33930800	0.32852700
N	-4.10632700	-1.44018400	-0.28783600
N	-2.97518000	-1.48209800	0.46781700
N	2.97519200	-1.48209500	-0.46778300
N	4.10634300	-1.44015500	0.28786400
N	3.22425800	1.33931500	-0.32855900
N	4.37711800	0.92524700	0.27106100
C	-4.43476600	-0.27270200	-1.09420200
C	-3.54487200	2.45147100	1.01887100
C	-4.91276800	2.73575400	0.84081800
C	-5.40640100	1.74994900	0.02560200
C	-2.55330000	3.27299400	1.81338500
C	-3.08771200	-2.57630900	1.24868800
C	-4.29671100	-3.23559400	0.95273800
C	-4.92071500	-2.48246900	-0.00887700
C	-2.09393500	-2.96415900	2.32508300
C	4.43477800	-0.27265300	1.09420100
C	5.40639700	1.74997000	-0.02567000
C	4.91275700	2.73573800	-0.84092900
C	3.54485200	2.45146400	-1.01892900
C	2.55325800	3.27295900	-1.81344400
C	4.92073800	-2.48244100	0.00892400
C	4.29674100	-3.23558300	-0.95268300
C	3.08772900	-2.57632200	-1.24863100
C	2.09394700	-2.96420500	-2.32501000
H	-5.47892300	-0.39011600	-1.37707800
H	-5.46735000	3.55505300	1.26354600
H	-4.67319500	-4.13637700	1.40480200
H	5.47893600	-0.39005500	1.37707700
H	5.46733600	3.55501500	-1.26370200
H	4.67323600	-4.13636600	-1.40473800
C	-3.59757400	-0.15104800	-2.35055400
C	-4.19192800	-0.18150500	-3.60467000
N	-2.28436700	0.00388400	-2.16270500
C	-3.37797200	-0.03875500	-4.72442500
H	-5.26287400	-0.31000100	-3.70945500
C	-1.51042300	0.14597900	-3.24165600
C	-2.01316600	0.13142200	-4.53828500
H	-3.80539200	-0.05645400	-5.71961700
H	-0.45376400	0.27957000	-3.05507700
H	-1.34380500	0.25333700	-5.38039900
C	3.59758700	-0.15097400	2.35055300
C	4.19194400	-0.18139900	3.60466800
N	2.28437800	0.00394700	2.16270300
C	3.37799000	-0.03862600	4.72442100
H	5.26289100	-0.30988900	3.70945300
C	1.51043700	0.14606600	3.24165300
C	2.01318300	0.13154200	4.53828100
H	3.80541200	-0.05629900	5.71961300
H	0.45377700	0.27965100	3.05507300

H	1.34382400	0.25347600	5.38039300
H	-6.39602700	1.57189400	-0.36473800
H	-5.87118600	-2.59894400	-0.50536300
H	5.87121100	-2.59889700	0.50540800
H	6.39602800	1.57192800	0.36466300
C	0.79292700	-3.50208300	-1.70374700
H	0.12619700	-3.84294500	-2.50011000
H	0.99423900	-4.34872400	-1.04400400
H	0.27824600	-2.72681300	-1.13512600
C	1.79236700	-1.73560500	-3.19931000
H	1.36011600	-0.92895600	-2.60268200
H	2.69860900	-1.36135600	-3.68073400
H	1.07629900	-2.00658200	-3.97855500
C	2.70420700	-4.06332700	-3.21119200
H	2.88621000	-4.98125000	-2.64761300
H	2.00454500	-4.30421800	-4.01384400
H	3.64230300	-3.74073800	-3.66885100
C	-0.79289200	-3.50200700	1.70384000
H	-0.12616200	-3.84284100	2.50021400
H	-0.99417300	-4.34866100	1.04410400
H	-0.27822700	-2.72672900	1.13521500
C	-1.79240000	-1.73554500	3.19937800
H	-1.36017500	-0.92888400	2.60274800
H	-2.69865700	-1.36132500	3.68079700
H	-1.07632500	-2.00649400	3.97862700
C	-2.70417700	-4.06329100	3.21126500
H	-2.88614700	-4.98122300	2.64769100
H	-2.00452000	-4.30415600	4.01392900
H	-3.64228900	-3.74072400	3.66890800
C	-1.68502000	4.07386000	0.82319900
H	-2.30020900	4.74678700	0.22155700
H	-0.95849800	4.67740100	1.37278000
H	-1.14493500	3.40712200	0.14925000
C	-1.66630700	2.37039800	2.68391300
H	-2.26760900	1.77385400	3.37416400
H	-1.05934300	1.70369400	2.06744600
H	-0.98593300	2.99068600	3.27221800
C	-3.30747000	4.25381000	2.72619000
H	-2.58548200	4.82969400	3.30848300
H	-3.90497100	4.96468300	2.15161600
H	-3.96373800	3.72981500	3.42522100
C	1.66616700	2.37031500	-2.68382300
H	2.26739400	1.77368900	-3.37406900
H	1.05923300	1.70368400	-2.06724700
H	0.98576500	2.99057200	-3.27212800
C	1.68507800	4.07394300	-0.82326500
H	2.30033500	4.74690100	-0.22172800
H	0.95853700	4.67746100	-1.37284700
H	1.14501800	3.40728500	-0.14921700
C	3.30739600	4.25366800	-2.72639000
H	2.58538600	4.82953200	-3.30867400
H	3.90497200	4.96456500	-2.15192300
H	3.96358600	3.72958600	-3.42543000

Table S73: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 1.618 Å

Cu	1.75141500	0.04170500	-0.06482300
Cu	-1.75141200	0.04170300	0.06482100
O	0.00000200	-0.71663200	0.00000200
O	0.00000000	0.90217900	-0.00000900
N	4.42759700	0.94804600	0.31233000
N	3.27960500	1.35343800	-0.30076300
N	4.18136100	-1.42210500	0.29957600
N	3.04840300	-1.48264600	-0.45262000
N	-3.04839800	-1.48264500	0.45264100
N	-4.18135600	-1.42211700	-0.29955700
N	-3.27960600	1.35343700	0.30074000
N	-4.42759500	0.94803300	-0.31235100
C	4.48161400	-0.25902600	1.12313000
C	3.59703200	2.46989600	-0.98345100
C	4.96026900	2.76674100	-0.78827700
C	5.45342700	1.78288000	0.03019100
C	2.60188300	3.27945400	-1.78598400
C	3.18139600	-2.56815700	-1.24059400
C	4.40595900	-3.20356700	-0.95580100
C	5.01720700	-2.44481800	0.00968700
C	2.18185400	-2.97189700	-2.30529700
C	-4.48161000	-0.25905200	-1.12313000
C	-5.45342600	1.78287300	-0.03023300
C	-4.96027000	2.76675400	0.78821200
C	-3.59703900	2.46990300	0.98341400
C	-2.60190000	3.27947300	1.78594700
C	-5.01720000	-2.44482700	-0.00965100
C	-4.40595200	-3.20355900	0.95584900
C	-3.18138900	-2.56814200	1.24063300
C	-2.18184800	-2.97186100	2.30534400
H	5.52087200	-0.36883500	1.42634400
H	5.51242300	3.59259300	-1.20152500
H	4.79928600	-4.09339900	-1.41520600
H	-5.52086700	-0.36886800	-1.42634300
H	-5.51242400	3.59261800	1.20143600
H	-4.79927700	-4.09338400	1.41526900
C	3.61796900	-0.16042000	2.36460200
C	4.18841400	-0.20160900	3.62947700
N	2.30597800	-0.01584700	2.15615900
C	3.35257600	-0.08173700	4.73571400
H	5.25839900	-0.32108700	3.75268900
C	1.51032300	0.10479700	3.22214100
C	1.98959400	0.07770300	4.52715100
H	3.76199400	-0.10856700	5.73824300
H	0.45600600	0.23077700	3.01676800
H	1.30395900	0.18186700	5.35846300
C	-3.61796400	-0.16046500	-2.36460300
C	-4.18840900	-0.20167600	-3.62947800
N	-2.30597500	-0.01588500	-2.15616200
C	-3.35257100	-0.08181900	-4.73571600
H	-5.25839400	-0.32115800	-3.75268900
C	-1.51031900	0.10474300	-3.22214600
C	-1.98959000	0.07762800	-4.52715600
H	-3.76198900	-0.10866600	-5.73824500
H	-0.45600300	0.23072900	-3.01677400

H	-1.30395500	0.18177900	-5.35846800
H	6.44013000	1.61265800	0.43129500
H	5.97103600	-2.54581300	0.50311000
H	-5.97102900	-2.54583100	-0.50307300
H	-6.44012700	1.61264400	-0.43134000
C	-0.89891800	-3.52751300	1.66228200
H	-0.22113400	-3.87365300	2.44687400
H	-1.12239600	-4.37356300	1.00889700
H	-0.38602800	-2.76091600	1.08160700
C	-1.84669600	-1.74863100	3.17521700
H	-1.40655700	-0.95024900	2.57280600
H	-2.73964900	-1.35716800	3.66757500
H	-1.12613300	-2.03286700	3.94561200
C	-2.79704900	-4.06170500	3.19870600
H	-3.00342800	-4.97515900	2.63622400
H	-2.09024100	-4.31641400	3.99080600
H	-3.72277000	-3.72396300	3.67044500
C	0.89892500	-3.52753900	-1.66222400
H	0.22114100	-3.87369600	-2.44680800
H	1.12240500	-4.37357400	-1.00882100
H	0.38603400	-2.76093100	-1.08156400
C	1.84669900	-1.74868400	-3.17519300
H	1.40655300	-0.95029300	-2.57279800
H	2.73965200	-1.35722600	-3.66755500
H	1.12614100	-2.03293800	-3.94558600
C	2.79705600	-4.06175700	-3.19863900
H	3.00343500	-4.97520000	-2.63613900
H	2.09024800	-4.31648100	-3.99073400
H	3.72277600	-3.72402300	-3.67038400
C	1.71474400	4.06920600	-0.80298100
H	2.31613600	4.75035800	-0.19662800
H	0.98515300	4.66336200	-1.35868100
H	1.17751000	3.39625800	-0.13284900
C	1.73308800	2.36540900	-2.66362300
H	2.34738700	1.77603800	-3.34843100
H	1.12866700	1.69014600	-2.05353800
H	1.05018500	2.97718900	-3.25795600
C	3.35149100	4.26924800	-2.69251000
H	2.62785000	4.83829900	-3.27949400
H	3.93754000	4.98546200	-2.11277300
H	4.01828900	3.75275600	-3.38713000
C	-1.73315200	2.36545000	2.66365700
H	-2.34748700	1.77612000	3.34846700
H	-1.12871900	1.69015100	2.05362400
H	-1.05026100	2.97724500	3.25798900
C	-1.71471300	4.06916800	0.80294100
H	-2.31607100	4.75030500	0.19653900
H	-0.98513000	4.66333400	1.35864100
H	-1.17746900	3.39618000	0.13285600
C	-3.35152100	4.26931900	2.69240600
H	-2.62789000	4.83837900	3.27939300
H	-3.93753500	4.98552100	2.11261900
H	-4.01835400	3.75286800	3.38702300

Table S74: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 1.488 Å

Cu	-1.80213900	0.03908000	0.05140900
Cu	1.80214400	0.03906900	-0.05142000
O	-0.00000100	-0.64900300	0.00007400
O	0.00000900	0.83918500	0.00003200
N	-4.46034200	0.97296800	-0.33769900
N	-3.31448800	1.36627100	0.28621100
N	-4.24060100	-1.40111800	-0.30775000
N	-3.10525300	-1.48147200	0.43939200
N	3.10525600	-1.48148100	-0.43936800
N	4.24061200	-1.40110700	0.30776000
N	3.31448000	1.36626500	-0.28624700
N	4.46033700	0.97298100	0.33767300
C	-4.51711000	-0.23922000	-1.14126200
C	-3.62610900	2.48430100	0.96751800
C	-4.98479700	2.79523500	0.76142400
C	-5.48087000	1.81711100	-0.06253800
C	-2.62591000	3.27873200	1.77886400
C	-3.25565400	-2.56174200	1.23018700
C	-4.49428500	-3.17378400	0.95490800
C	-5.09524000	-2.40639900	-0.01029600
C	-2.24993000	-2.98518600	2.28075300
C	4.51711800	-0.23919400	1.14125400
C	5.48085100	1.81714400	0.06252100
C	4.98477200	2.79525100	-0.76145600
C	3.62608800	2.48430200	-0.96754800
C	2.62587800	3.27871800	-1.77889700
C	5.09526700	-2.40636900	0.01029000
C	4.49431400	-3.17376400	-0.95490800
C	3.25566700	-2.56174600	-1.23016700
C	2.24993300	-2.98520400	-2.28071800
H	-5.55322300	-0.33949400	-1.45819200
H	-5.53237700	3.62609100	1.17084700
H	-4.90235100	-4.05477200	1.41851900
H	5.55323500	-0.33945700	1.45817700
H	5.53234400	3.62611100	-1.17088400
H	4.90238900	-4.05474500	-1.41852400
C	-3.63587400	-0.15931300	-2.37250000
C	-4.19135900	-0.20499600	-3.64388000
N	-2.32394300	-0.02813300	-2.15128100
C	-3.34161000	-0.10492100	-4.74142300
H	-5.26113800	-0.31310200	-3.77854900
C	-1.51441400	0.07333300	-3.20906400
C	-1.97915500	0.04000400	-4.51892100
H	-3.74001100	-0.13593200	-5.74825700
H	-0.46103200	0.18819100	-2.99219000
H	-1.28292800	0.12816000	-5.34322500
C	3.63589000	-0.15927600	2.37249700
C	4.19138100	-0.20495400	3.64387500
N	2.32395900	-0.02809000	2.15128300
C	3.34163600	-0.10486700	4.74142000
H	5.26115900	-0.31306600	3.77854100
C	1.51443500	0.07338800	3.20906700
C	1.97918100	0.04006600	4.51892300
H	3.74004100	-0.13587300	5.74825300
H	0.46105300	0.18825200	2.99219500

H	1.28295800	0.12823300	5.34323000
H	-6.46602600	1.65689200	-0.47150100
H	-6.05279800	-2.49101500	-0.49955400
H	6.05283200	-2.49097000	0.49953700
H	6.46600700	1.65694100	0.47149100
C	0.99143400	-3.56716900	-1.61278100
H	0.29907800	-3.91545000	-2.38348600
H	1.24337200	-4.41605500	-0.97349000
H	0.48301500	-2.81497500	-1.01051400
C	1.87240300	-1.76920000	-3.14326900
H	1.42275200	-0.98167300	-2.53329900
H	2.74811500	-1.35639400	-3.64897300
H	1.14658100	-2.06959600	-3.90259200
C	2.87306100	-4.06090900	-3.18507100
H	3.10944700	-4.96954700	-2.62661400
H	2.15883800	-4.33141700	-3.96523400
H	3.78304500	-3.70273900	-3.67213600
C	-0.99144800	-3.56720900	1.61283400
H	-0.29909700	-3.91547700	2.38355000
H	-1.24341000	-4.41611500	0.97357800
H	-0.48301200	-2.81505300	1.01053400
C	-1.87236700	-1.76916400	3.14326300
H	-1.42269200	-0.98166900	2.53326900
H	-2.74806800	-1.35631800	3.64895400
H	-1.14655400	-2.06955500	3.90259700
C	-2.87308500	-4.06084300	3.18514500
H	-3.10948600	-4.96949900	2.62672300
H	-2.15887000	-4.33133700	3.96532000
H	-3.78306300	-3.70263700	3.67219200
C	-1.72419800	4.06227000	0.80385100
H	-2.31414000	4.75367900	0.19784000
H	-0.99009500	4.64493900	1.36573700
H	-1.19204200	3.38570300	0.13329900
C	-1.77175500	2.34970800	2.65545100
H	-2.39597100	1.76268800	3.33318300
H	-1.17117900	1.67105200	2.04492000
H	-1.08530300	2.95030600	3.25715500
C	-3.36855300	4.27237600	2.68665800
H	-2.64165700	4.83142300	3.27926000
H	-3.94473100	4.99693600	2.10739400
H	-4.04378600	3.75983400	3.37603200
C	1.77167100	2.34967100	-2.65540800
H	2.39584800	1.76260800	-3.33313900
H	1.17110600	1.67105400	-2.04482200
H	1.08520600	2.95025500	-3.25711100
C	1.72421700	4.06231800	-0.80388800
H	2.31419500	4.75374200	-0.19792900
H	0.99010600	4.64497800	-1.36577400
H	1.19207100	3.38579300	-0.13328600
C	3.36851000	4.27230400	-2.68676400
H	2.64160500	4.83133500	-3.27936900
H	3.94471900	4.99688300	-2.10755400
H	4.04371200	3.75971700	-3.37613400

Table S75: XYZ coordinates for optimised structure: Singlet minimum path, TPSSh/def2tzvp, O...O = 1.359 Å

Cu	1.84623500	0.03608100	-0.03923900
Cu	-1.84623700	0.03609300	0.03923100
O	-0.00000600	-0.58296800	-0.00003000
O	0.00001000	0.77558400	-0.00001900
N	4.48918200	0.99083300	0.35785800
N	3.34527400	1.37808900	-0.27284000
N	4.28952000	-1.38662300	0.30946300
N	3.15168900	-1.48217800	-0.43226000
N	-3.15167900	-1.48217800	0.43230300
N	-4.28952000	-1.38664200	-0.30941000
N	-3.34528100	1.37808800	0.27281000
N	-4.48918400	0.99081300	-0.35788700
C	4.54683200	-0.22735800	1.15285500
C	3.65353500	2.49907900	-0.94931000
C	5.00906300	2.81875700	-0.73442100
C	5.50646300	1.84195000	0.09056500
C	2.64968300	3.28528400	-1.76423300
C	3.31510000	-2.55673100	-1.22695800
C	4.56514700	-3.14996500	-0.96201900
C	5.15893600	-2.37693000	0.00329900
C	2.30309600	-2.99251000	-2.26594400
C	-4.54683300	-0.22740600	-1.15284200
C	-5.50646700	1.84193900	-0.09062700
C	-5.00907300	2.81877000	0.73433300
C	-3.65354700	2.49909900	0.94924200
C	-2.64970200	3.28533300	1.76414500
C	-5.15893900	-2.37693100	-0.00320000
C	-4.56514200	-3.14993900	0.96213400
C	-3.31508900	-2.55670200	1.22703900
C	-2.30307200	-2.99245400	2.26602500
H	5.57988800	-0.32125400	1.48148400
H	5.55395000	3.65405200	-1.13849200
H	4.98442000	-4.02306000	-1.43060200
H	-5.57988900	-0.32131400	-1.48146600
H	-5.55396400	3.65407800	1.13837400
H	-4.98441300	-4.02301800	1.43074900
C	3.65126800	-0.16449000	2.37568300
C	4.19527900	-0.21685900	3.65178300
N	2.33922000	-0.04281600	2.14548900
C	3.33557800	-0.13463100	4.74296900
H	5.26474500	-0.31671900	3.79476600
C	1.51965600	0.04100800	3.19746100
C	1.97366500	-0.00034400	4.51056500
H	3.72596800	-0.17135100	5.75273800
H	0.46691300	0.14762800	2.97277800
H	1.26971800	0.07341800	5.32967700
C	-3.65127000	-0.16458000	-2.37567300
C	-4.19528100	-0.21700000	-3.65177000
N	-2.33922300	-0.04289000	-2.14548400
C	-3.33558100	-0.13480900	-4.74295900
H	-5.26474600	-0.31687200	-3.79475000
C	-1.51965900	0.04089900	-3.19745900
C	-1.97366800	-0.00050600	-4.51056200
H	-3.72597100	-0.17156900	-5.75272800
H	-0.46691600	0.14753200	-2.97277900

H	-1.26972200	0.07322900	-5.32967700
H	6.49029900	1.68703900	0.50473000
H	6.11991000	-2.44887300	0.48785300
H	-6.11991900	-2.44888500	-0.48774100
H	-6.49030000	1.68701400	-0.50479500
C	-1.05600500	-3.57682800	1.57890100
H	-0.35134600	-3.92566300	2.33808700
H	-1.31948800	-4.42559100	0.94408300
H	-0.55709700	-2.82588800	0.96726400
C	-1.90807700	-1.78332900	3.13078600
H	-1.46085400	-0.99454100	2.52015400
H	-2.77542400	-1.36781600	3.64852200
H	-1.17549000	-2.09217000	3.88024600
C	-2.92311000	-4.06921200	3.17065200
H	-3.17396600	-4.97178800	2.60867500
H	-2.20185500	-4.35112400	3.94025700
H	-3.82420400	-3.70712600	3.67116600
C	1.05602400	-3.57687400	-1.57882200
H	0.35137500	-3.92573000	-2.33800800
H	1.31950400	-4.42562100	-0.94398200
H	0.55710400	-2.82592400	-0.96720700
C	1.90810400	-1.78340600	-3.13073700
H	1.46087100	-0.99460600	-2.52012800
H	2.77545500	-1.36790000	-3.64847400
H	1.17552600	-2.09226700	-3.88019700
C	2.92314800	-4.06928500	-3.17054100
H	3.17400100	-4.97184800	-2.60854200
H	2.20190300	-4.35121700	-3.94014800
H	3.82424600	-3.70720700	-3.67105300
C	1.74097200	4.06546600	-0.79274500
H	2.32530900	4.76168200	-0.18681900
H	1.00465800	4.64264900	-1.35741100
H	1.21119600	3.38704500	-0.12204300
C	1.80233800	2.34802500	-2.63890800
H	2.43094000	1.76195600	-3.31334800
H	1.20435500	1.66760700	-2.02731200
H	1.11322500	2.94231100	-3.24388100
C	3.38742300	4.28083100	-2.67379200
H	2.65829700	4.83427900	-3.26895100
H	3.95871800	5.01001200	-2.09549000
H	4.06671400	3.77032300	-3.36067300
C	-1.80232700	2.34810600	2.63882300
H	-2.43090800	1.76203700	3.31328200
H	-1.20433800	1.66768800	2.02723200
H	-1.11321700	2.94241500	3.24377600
C	-1.74101800	4.06552100	0.79263400
H	-2.32537800	4.76171800	0.18670600
H	-1.00470800	4.64272600	1.35728300
H	-1.21123800	3.38710200	0.12193400
C	-3.38745200	4.28087900	2.67369900
H	-2.65833100	4.83434600	3.26884500
H	-3.95876400	5.01004200	2.09539400
H	-4.06672800	3.77036600	3.36059100

Table S76: XYZ coordinates for optimised structure: Broken Symmetry minimum path, Oxo

Cu	1.43040500	0.04850200	-0.25649600
Cu	-1.41979700	0.05135600	0.22515500
O	0.01255400	-0.98310600	0.03370700
O	-0.00423600	1.14999700	-0.08354400
N	4.18931700	0.75494500	-0.20373000
N	2.98033700	1.23711100	-0.64139200
N	3.74679800	-1.56527300	0.06210100
N	2.58499100	-1.48679400	-0.65065800
N	-2.55357300	-1.46930800	0.72693000
N	-3.70635400	-1.60965000	0.00887800
N	-2.98732900	1.24207100	0.57031500
N	-4.18990300	0.71190800	0.16945400
C	4.29975900	-0.37642200	0.70701700
C	3.27274800	2.33124100	-1.38954000
C	4.66849300	2.53537800	-1.40022500
C	5.21412500	1.52564800	-0.64364800
C	2.23861700	3.21230600	-2.06028000
C	2.49337500	-2.63900400	-1.36251100
C	3.60594700	-3.45284400	-1.05271400
C	4.38419900	-2.73849500	-0.17168300
C	1.43160900	-2.95592400	-2.40469900
C	-4.28459600	-0.46147900	-0.68744100
C	-5.22991000	1.46429800	0.60494700
C	-4.70186100	2.51350000	1.31783500
C	-3.30000500	2.35188500	1.28770400
C	-2.29275800	3.30899700	1.89490500
C	-4.32050900	-2.78327000	0.29663000
C	-3.53517600	-3.43523200	1.21892100
C	-2.44387300	-2.58228000	1.49691800
C	-1.39188000	-2.81703400	2.57020900
H	5.36791800	-0.56654100	0.81477000
H	5.20435700	3.32108000	-1.90823800
H	3.82902400	-4.42735300	-1.45740400
H	-5.34972300	-0.67505500	-0.77996900
H	-5.25315200	3.29889100	1.80938800
H	-3.74091400	-4.39259000	1.67075900
C	3.70964000	-0.07129500	2.06942100
C	4.51457800	-0.06431900	3.20744100
N	2.40322400	0.22913900	2.07086100
C	3.92892000	0.28685100	4.42695500
H	5.56880900	-0.31870900	3.14857400
C	1.85716900	0.57823800	3.24512900
C	2.57671100	0.62233100	4.44238700
H	4.51985900	0.30560400	5.33704900
H	0.80657400	0.83798900	3.22172000
H	2.08153800	0.91671100	5.36157600
C	-3.70739600	-0.21035200	-2.06538000
C	-4.52070900	-0.25427200	-3.19646400
N	-2.40273900	0.09656900	-2.08857500
C	-3.94567500	0.04841100	-4.43380900
H	-5.57315100	-0.51099600	-3.11903200
C	-1.86706500	0.39942100	-3.28035900
C	-2.59528700	0.38926400	-4.47311800
H	-4.54308400	0.02613200	-5.33958900
H	-0.81832600	0.66678200	-3.27508300
H	-2.10801800	0.64671700	-5.40747500
H	6.23647700	1.29532600	-0.37987500
H	5.33470200	-2.95995800	0.29247200
H	-5.26204600	-3.04825700	-0.16294500
H	-6.24940400	1.19518800	0.36818600
C	-0.13649500	-3.50082600	1.98375200
H	0.55813200	-3.73530700	2.79851300
H	-0.39655600	-4.43845000	1.48108900

H	0.36423500	-2.84157200	1.27029900
C	-1.00663300	-1.48047800	3.22693600
H	-0.54540300	-0.81393500	2.49409700
H	-1.87987000	-0.98451100	3.66539400
H	-0.27851700	-1.66186900	4.02465600
C	-1.99214600	-3.74206200	3.65391700
H	-2.19203400	-4.74709800	3.26809700
H	-1.27064000	-3.84611600	4.47062300
H	-2.91986200	-3.33451700	4.06978200
C	0.21501900	-3.65693800	-1.75957100
H	-0.49040700	-3.94707200	-2.54662000
H	0.51978800	-4.56388600	-1.22664000
H	-0.29077600	-2.98656200	-1.06054200
C	0.98259100	-1.66669000	-3.11335300
H	0.49636100	-0.99026800	-2.40610700
H	1.82918900	-1.15225900	-3.58189800
H	0.25696800	-1.91481900	-3.89518800
C	2.04566900	-3.90693900	-3.45783600
H	2.29231400	-4.88473400	-3.03140500
H	1.31308200	-4.07601600	-4.25356900
H	2.94853400	-3.48389800	-3.91114900
C	1.47645300	3.98128400	-0.95840600
H	2.16036600	4.60817100	-0.37594600
H	0.72308100	4.63157100	-1.41629100
H	0.97320900	3.28560300	-0.28036200
C	1.26475700	2.35408300	-2.88731100
H	1.79274000	1.80451200	-3.67495100
H	0.74233100	1.64769200	-2.23644700
H	0.51652000	3.00078300	-3.35865600
C	2.93381400	4.22340200	-2.99361200
H	2.17249000	4.83666500	-3.48590700
H	3.59305900	4.90152100	-2.44120700
H	3.51795400	3.72226800	-3.77354600
C	-1.16786400	2.54577800	2.61455100
H	-1.57329900	1.91585100	3.41546900
H	-0.60703700	1.92861200	1.90703800
H	-0.47183300	3.26308400	3.06329700
C	-1.71551200	4.16988300	0.74684100
H	-2.50509400	4.76076900	0.27013800
H	-0.96430300	4.86181900	1.14339500
H	-1.24543000	3.54007500	-0.01280600
C	-2.99500900	4.23303000	2.91122200
H	-2.25169400	4.89958900	3.35997200
H	-3.75182800	4.86482500	2.43470100
H	-3.46865800	3.66301600	3.71813600

Table S77: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, Peroxo

Cu	1.77840100	0.03932000	0.00912400
Cu	-1.79811000	0.06379500	0.05536900
O	-0.00771400	-0.59407300	0.25586500
O	-0.01753500	0.86326300	0.03930900
N	4.45814900	0.90126700	0.25164300
N	3.31033900	1.25239100	-0.40613500
N	4.13128500	-1.44389200	0.53832700
N	3.00479000	-1.53888600	-0.23290200
N	-3.07899100	-1.37491900	0.59480400
N	-4.21135700	-1.41103600	-0.17080300
N	-3.28701300	1.39098600	0.04020600
N	-4.42160500	0.93162300	-0.56939800
C	4.46128200	-0.19292900	1.21506000
C	3.65262800	2.26936300	-1.22731100
C	5.02813000	2.55585800	-1.07858500
C	5.50683800	1.66950500	-0.14072600
C	2.65341300	3.00526600	-2.09878600
C	3.11745600	-2.70988200	-0.90336600
C	4.31365100	-3.35820500	-0.52351900
C	4.93866000	-2.52210000	0.37312700
C	2.14246300	-3.17055700	-1.97466400
C	-4.45054400	-0.38988100	-1.18379000
C	-5.44157700	1.81937800	-0.45027200
C	-4.95488800	2.89866700	0.25279300
C	-3.60723500	2.60038500	0.55227000
C	-2.61285100	3.47439100	1.29170900
C	-5.07220300	-2.36727200	0.26218100
C	-4.47597300	-2.98675000	1.33688900
C	-3.23633800	-2.33711900	1.53217100
C	-2.21840800	-2.62613900	2.62113500
H	5.49184000	-0.29765100	1.55379900
H	5.59655600	3.31221400	-1.59656000
H	4.67879300	-4.30999600	-0.87517000
H	-5.47224000	-0.54153000	-1.53157900
H	-5.50121000	3.78826100	0.52394900
H	-4.88654900	-3.79615200	1.91980000
C	3.57096200	0.10420100	2.40963300
C	4.09241200	0.20133000	3.69739300
N	2.27319100	0.29558200	2.12162200
C	3.21949800	0.52215800	4.74148700
H	5.14898700	0.03656500	3.88527200
C	1.44391900	0.61218900	3.12679700
C	1.87345000	0.73756400	4.44887900
H	3.58876400	0.60838600	5.75836400
H	0.41125700	0.77623200	2.84673300
H	1.16519000	1.00095400	5.22698300
C	-3.49914800	-0.49249800	-2.36483800
C	-3.97221900	-0.72809900	-3.65365600
N	-2.19732500	-0.32595600	-2.07524100
C	-3.04598800	-0.79054000	-4.69880100
H	-5.03351800	-0.85775000	-3.84230300
C	-1.31585100	-0.38579200	-3.08441800
C	-1.69396500	-0.61391700	-4.40840900
H	-3.37798600	-0.97068100	-5.71621400
H	-0.27806500	-0.24314000	-2.81003700
H	-0.94239800	-0.64912900	-5.18969900
H	6.49293900	1.52618000	0.27747000
H	5.87820600	-2.60442700	0.90072400
H	-6.02424200	-2.52605200	-0.22394200
H	-6.41468200	1.61458800	-0.87328800
C	-1.00863400	-3.37558300	2.01959900
H	-0.30411900	-3.63347600	2.81860400
H	-1.32455200	-4.30408600	1.53211600

H	-0.48693100	-2.75402700	1.28755700
C	-1.75095100	-1.30170100	3.25518700
H	-1.28498500	-0.66053500	2.50029700
H	-2.58750600	-0.76051300	3.71034400
H	-1.00774500	-1.50697500	4.03335500
C	-2.86325900	-3.50686600	3.70969300
H	-3.14713400	-4.49008700	3.31927300
H	-2.14039000	-3.67112100	4.51517700
H	-3.75018600	-3.03231300	4.14363600
C	0.72993100	-3.37725200	-1.39297700
H	0.06073100	-3.73861400	-2.18230300
H	0.74452600	-4.12632100	-0.59440500
H	0.31916000	-2.44717000	-0.99168200
C	2.11437000	-2.10789700	-3.09654600
H	1.81204400	-1.12816100	-2.70975700
H	3.10150200	-1.99651600	-3.55787300
H	1.40564400	-2.40968700	-3.87595400
C	2.62630900	-4.50543600	-2.57590000
H	2.65773600	-5.29923400	-1.82155200
H	1.93052600	-4.82041700	-3.36006800
H	3.61862600	-4.41186000	-3.03037500
C	1.89744200	4.01707200	-1.20442700
H	2.58863000	4.74607000	-0.76841000
H	1.15948600	4.56284600	-1.80284200
H	1.37543300	3.50663800	-0.38888000
C	1.65888200	2.01550300	-2.73091900
H	2.17503900	1.30626500	-3.38794500
H	1.11966700	1.46076300	-1.95569000
H	0.91976800	2.56156800	-3.32680300
C	3.38978600	3.76630400	-3.21861900
H	2.65657600	4.26997900	-3.85669600
H	4.05582100	4.53728700	-2.81707900
H	3.97813700	3.08867600	-3.84699900
C	-1.87362500	2.64390700	2.35951100
H	-2.57211800	2.23568400	3.09815100
H	-1.32711200	1.81756300	1.89342500
H	-1.14850800	3.27728900	2.88212600
C	-1.60288800	4.04233200	0.26851900
H	-2.11204800	4.64981900	-0.48732100
H	-0.87368300	4.67861600	0.78213300
H	-1.06406100	3.23713100	-0.23996200
C	-3.34854000	4.64026700	1.97952800
H	-2.62487100	5.25110900	2.52847700
H	-3.84352300	5.29274700	1.25215300
H	-4.09728200	4.28097900	2.69415200

Table S78: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 2.277 Å

Cu	0	1.38897900	0.01495700	-0.26787200
Cu	0	-1.38180600	0.06498200	0.18486100
O	-1	0.01124800	-1.05443900	0.13206900
O	-1	-0.00472400	1.19503900	-0.22213400
N	0	4.14152300	0.73323000	-0.28176400
N	0	2.93567600	1.15551600	-0.78786200
N	0	3.69683500	-1.52785100	0.29196500
N	0	2.56019900	-1.53796300	-0.46385600
N	0	-2.52951300	-1.38008600	0.82850900
N	0	-3.65059800	-1.62298900	0.08884500
N	0	-2.95020300	1.27832600	0.32738100
N	0	-4.14597600	0.69723100	-0.01958900
C	0	4.25019000	-0.26317100	0.77384300
C	0	3.23883200	2.12640400	-1.68944700
C	0	4.63696600	2.31244600	-1.72660300
C	0	5.17298100	1.42072000	-0.82936100
C	0	2.22708600	2.93551300	-2.47681800
C	0	2.47531700	-2.77565300	-1.01565300
C	0	3.56833900	-3.54770900	-0.56327800
C	0	4.32702400	-2.72680200	0.23851300
C	0	1.44434200	-3.22336300	-2.03967800
C	0	-4.23045500	-0.56552700	-0.73884500
C	0	-5.19245400	1.49440700	0.30559400
C	0	-4.67643500	2.62569600	0.89062200
C	0	-3.27447700	2.46821400	0.89848300
C	0	-2.27666100	3.49719400	1.39103900
C	0	-4.25240100	-2.77204600	0.48233400
C	0	-3.49018800	-3.30184200	1.49775300
C	0	-2.42580800	-2.39985200	1.71909900
C	0	-1.41133300	-2.49373500	2.84796500
H	0	5.31857700	-0.43655300	0.90514900
H	0	5.18035500	3.01073700	-2.34255800
H	0	3.79214500	-4.56905700	-0.82754500
H	0	-5.29461300	-0.79238200	-0.80879800
H	0	-5.23516700	3.46435100	1.27384000
H	0	-3.69490500	-4.20746800	2.04617600
C	0	3.66340700	0.22053700	2.08415700
C	0	4.47819100	0.39984300	3.20108800
N	0	2.35229500	0.49701300	2.05604200
C	0	3.89728100	0.90821900	4.36604700
H	0	5.53626600	0.15693500	3.16632700
C	0	1.81098000	0.99735100	3.17682300
C	0	2.53946900	1.21976200	4.34864700
H	0	4.49534200	1.06349500	5.25824100
H	0	0.75592900	1.23460400	3.13061300
H	0	2.04615500	1.63038800	5.22317000
C	0	-3.65336700	-0.47569200	-2.13658600
C	0	-4.47575900	-0.64018800	-3.25022500
N	0	-2.34500600	-0.19166400	-2.20106600
C	0	-3.90657700	-0.49368800	-4.51790500
H	0	-5.53089100	-0.87169400	-3.13671700
C	0	-1.81513000	-0.04055300	-3.42429500
C	0	-2.55171600	-0.18088000	-4.60397600
H	0	-4.51078500	-0.61409400	-5.41133900
H	0	-0.76212300	0.20744600	-3.45904000
H	0	-2.06673800	-0.04413800	-5.56466000
H	0	6.19302900	1.22331600	-0.53208400
H	0	5.26087300	-2.88989400	0.75736300
H	0	-5.17228900	-3.10544500	0.02344800
H	0	-6.20792500	1.19554200	0.08806500
C	0	-0.15800100	-3.28269100	2.40428400
H	0	0.51091100	-3.40394200	3.26390900
H	0	-0.42787700	-4.28082000	2.04292500

H	0	0.37367900	-2.74924600	1.61262500
C	0	-1.00934500	-1.08651700	3.31929800
H	0	-0.50544300	-0.54416300	2.51595300
H	0	-1.88085200	-0.51239300	3.65374800
H	0	-0.31109000	-1.17001100	4.15874500
C	0	-2.06565500	-3.23903400	4.03507400
H	0	-2.27727100	-4.28651000	3.79640400
H	0	-1.37164600	-3.23387800	4.88169000
H	0	-2.99589300	-2.75723800	4.35440300
C	0	0.22825100	-3.87881000	-1.34606200
H	0	-0.46137600	-4.25294200	-2.11120600
H	0	0.53798100	-4.72689500	-0.72596500
H	0	-0.29540400	-3.15295800	-0.71959500
C	0	0.98716700	-2.02868900	-2.89259000
H	0	0.48233400	-1.28500200	-2.27144800
H	0	1.83334200	-1.55923800	-3.40715000
H	0	0.27500300	-2.37383200	-3.64948900
C	0	2.10002600	-4.26836100	-2.97291600
H	0	2.35467800	-5.19101700	-2.44111600
H	0	1.38898800	-4.53461700	-3.76156500
H	0	3.00537300	-3.87697100	-3.44910300
C	0	1.56725700	3.93625200	-1.50072100
H	0	2.31258500	4.62448100	-1.08744500
H	0	0.81346100	4.52830400	-2.03155100
H	0	1.08282400	3.40767400	-0.67575600
C	0	1.16628100	2.02088700	-3.11312400
H	0	1.62938800	1.29996600	-3.79734900
H	0	0.60690700	1.48984600	-2.33838000
H	0	0.45763600	2.62967600	-3.68546000
C	0	2.94044100	3.72083000	-3.59619600
H	0	2.19315600	4.27638400	-4.17122700
H	0	3.65149000	4.45124600	-3.19589600
H	0	3.47002400	3.05467600	-4.28644800
C	0	-1.20915900	2.84273700	2.28570600
H	0	-1.66693300	2.37014900	3.16296600
H	0	-0.64111500	2.10030900	1.71864800
H	0	-0.50880300	3.60883900	2.63637900
C	0	-1.62202000	4.14226700	0.14845100
H	0	-2.37307200	4.65145600	-0.46527800
H	0	-0.87986200	4.88366400	0.46465100
H	0	-1.12515000	3.38369600	-0.46212500
C	0	-3.00367300	4.58934300	2.20148600
H	0	-2.26560800	5.30945300	2.56801600
H	0	-3.72254500	5.14349600	1.58860800
H	0	-3.52687800	4.17246600	3.06933200

Table S79: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 2.145 Å

Cu	0	1.42959400	0.01214300	-0.25992800
Cu	0	-1.42322800	0.06112100	0.17221400
O	-1	0.01124800	-0.98744500	0.13207000
O	-1	-0.00472400	1.12804200	-0.22213500
N	0	4.18326100	0.73826900	-0.29359800
N	0	2.97648000	1.14588000	-0.80716800
N	0	3.75190800	-1.52105400	0.30195000
N	0	2.60195300	-1.55344500	-0.43306900
N	0	-2.56710500	-1.38068000	0.85672700
N	0	-3.70492100	-1.62678700	0.14412500
N	0	-2.99374100	1.27962700	0.29514500
N	0	-4.19030700	0.69214100	-0.03522700
C	0	4.28938000	-0.24646000	0.77365200
C	0	3.27511300	2.10287500	-1.72354100
C	0	4.67251200	2.29451500	-1.76540700
C	0	5.21253400	1.41963200	-0.85344400
C	0	2.25321900	2.89110600	-2.51885000
C	0	2.53051800	-2.79572300	-0.97648300
C	0	3.64336900	-3.54761200	-0.53872400
C	0	4.40163900	-2.70944600	0.24534400
C	0	1.48885700	-3.26459600	-1.98034200
C	0	-4.27116100	-0.59107200	-0.71812900
C	0	-5.23554900	1.49993900	0.26824200
C	0	-4.71656000	2.64662800	0.82071600
C	0	-3.31497900	2.48549700	0.83095600
C	0	-2.30784000	3.52079500	1.29008700
C	0	-4.32293100	-2.75028700	0.58364800
C	0	-3.55517800	-3.26093200	1.60476700
C	0	-2.47066700	-2.37265900	1.77885700
C	0	-1.43635600	-2.44782700	2.89115800
H	0	5.35728800	-0.40943400	0.92054800
H	0	5.21304700	2.98467600	-2.39304300
H	0	3.87866300	-4.56710900	-0.79987500
H	0	-5.33475000	-0.81743000	-0.79669800
H	0	-5.27309400	3.49724800	1.18028000
H	0	-3.76709600	-4.14443400	2.18555200
C	0	3.67991000	0.24745000	2.06999300
C	0	4.47293700	0.44256800	3.19954500
N	0	2.36771300	0.51622700	2.01678800
C	0	3.86773600	0.95883600	4.34864300
H	0	5.53277500	0.20558500	3.18626600
C	0	1.80252300	1.02455600	3.12192900
C	0	2.50858000	1.26240800	4.30420500
H	0	4.44873200	1.12643100	5.24983800
H	0	0.74739800	1.25548900	3.05256300
H	0	1.99776300	1.67911400	5.16569700
C	0	-3.67219000	-0.54024000	-2.10890800
C	0	-4.47312400	-0.74122600	-3.23187200
N	0	-2.36394300	-0.25112200	-2.15968100
C	0	-3.88179800	-0.62745000	-4.49283000
H	0	-5.52895000	-0.97498200	-3.13068800
C	0	-1.81231100	-0.13117100	-3.37662000
C	0	-2.52732000	-0.30891400	-4.56435900
H	0	-4.46941100	-0.77642100	-5.39300300
H	0	-0.76042000	0.12305200	-3.39861700
H	0	-2.02668100	-0.19584100	-5.52005800
H	0	6.23355700	1.23037300	-0.55422900
H	0	5.34561200	-2.85433600	0.75109400
H	0	-5.25477400	-3.08184900	0.14817500
H	0	-6.25186300	1.19670000	0.06090800
C	0	-0.17176100	-3.20584700	2.42721800
H	0	0.51363200	-3.31160500	3.27593000
H	0	-0.42353100	-4.20966700	2.06879800

H	0	0.33562700	-2.65944500	1.62830200
C	0	-1.06072200	-1.02995600	3.35403900
H	0	-0.59205600	-0.47372800	2.53859300
H	0	-1.93911600	-0.47854100	3.70757200
H	0	-0.34031600	-1.09347200	4.17636900
C	0	-2.05106300	-3.20847200	4.08870900
H	0	-2.24401200	-4.25997600	3.85133500
H	0	-1.34161300	-3.18951100	4.92218100
H	0	-2.98548400	-2.74800500	4.42700200
C	0	0.25506000	-3.85852300	-1.26366500
H	0	-0.43808600	-4.25559400	-2.01404300
H	0	0.54281600	-4.68078600	-0.59986100
H	0	-0.25796600	-3.09186600	-0.67800400
C	0	1.06278400	-2.09342000	-2.88172200
H	0	0.58162000	-1.31108000	-2.28972000
H	0	1.92013400	-1.66759500	-3.41488600
H	0	0.33879800	-2.44784100	-3.62312200
C	0	2.11607600	-4.36431000	-2.86805700
H	0	2.34729400	-5.26953800	-2.29688500
H	0	1.39761300	-4.64568400	-3.64456400
H	0	3.03058700	-4.01710700	-3.36082100
C	0	1.58983800	3.90315600	-1.55679900
H	0	2.33204200	4.60155000	-1.15521600
H	0	0.83171700	4.48316700	-2.09468800
H	0	1.10923200	3.38598200	-0.72209300
C	0	1.19556200	1.95648500	-3.13143600
H	0	1.65972400	1.22666900	-3.80528400
H	0	0.64575600	1.43340200	-2.34416100
H	0	0.47732800	2.54841100	-3.70939400
C	0	2.95396600	3.66178600	-3.65608800
H	0	2.20032500	4.20378800	-4.23578200
H	0	3.66386300	4.40241000	-3.27279400
H	0	3.48300500	2.98690900	-4.33820000
C	0	-1.25556300	2.88586400	2.21678100
H	0	-1.72530300	2.45200400	3.10734400
H	0	-0.69458700	2.11410900	1.68245300
H	0	-0.54601000	3.65417900	2.54330000
C	0	-1.63393400	4.10860400	0.02963900
H	0	-2.37260700	4.60206300	-0.61138200
H	0	-0.88576400	4.85289900	0.32384400
H	0	-1.13987400	3.32139200	-0.54669500
C	0	-3.02613900	4.65236100	2.05211300
H	0	-2.28246100	5.37934500	2.39288600
H	0	-3.73677300	5.18741700	1.41320700
H	0	-3.55754000	4.27589800	2.93326400

Table S80: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 2.013 Å

Cu	0	1.47758800	0.00686600	-0.25714300
Cu	0	-1.47116900	0.05831400	0.17175200
O	-1	0.01124800	-0.92043300	0.13206800
O	-1	-0.00472400	1.06103000	-0.22213300
N	0	4.23405600	0.72906400	-0.31648600
N	0	3.02573500	1.13513300	-0.82490500
N	0	3.81006400	-1.53556300	0.27057600
N	0	2.64224300	-1.57623600	-0.43544700
N	0	-2.60891200	-1.38495200	0.89183000
N	0	-3.76580100	-1.62323800	0.20754900
N	0	-3.04202600	1.28300500	0.30223200
N	0	-4.24118800	0.69556700	-0.01467500
C	0	4.33705400	-0.25976000	0.74809800
C	0	3.31879700	2.09431800	-1.73891900
C	0	4.71572100	2.28877900	-1.78757400
C	0	5.26091400	1.41246900	-0.87920300
C	0	2.28348900	2.87662500	-2.52238400
C	0	2.57620900	-2.81477100	-0.98737600
C	0	3.70873900	-3.55629600	-0.58363100
C	0	4.47477100	-2.71438400	0.18885400
C	0	1.51354000	-3.28557500	-1.96809900
C	0	-4.32103300	-0.59988100	-0.67504400
C	0	-5.28332200	1.50933300	0.28530900
C	0	-4.75769100	2.66186400	0.82018300
C	0	-3.35644700	2.49568500	0.82310700
C	0	-2.33600800	3.52732400	1.26083500
C	0	-4.40059100	-2.72217800	0.68435800
C	0	-3.62490200	-3.22570500	1.70303300
C	0	-2.51899400	-2.35668400	1.83530000
C	0	-1.46279500	-2.42433000	2.92736900
H	0	5.40406000	-0.41722000	0.90645800
H	0	5.25273000	2.98109600	-2.41602700
H	0	3.94971000	-4.57113000	-0.85740400
H	0	-5.38417500	-0.82494600	-0.76197300
H	0	-5.30970800	3.51853800	1.17251100
H	0	-3.84303700	-4.09185700	2.30723200
C	0	3.70852000	0.22801700	2.03823700
C	0	4.48108200	0.41759300	3.18251800
N	0	2.39683500	0.49676000	1.96577900
C	0	3.85526800	0.92746500	4.32354400
H	0	5.54107400	0.18128300	3.18663500
C	0	1.81135600	0.99969100	3.06260200
C	0	2.49691500	1.23150200	4.25780000
H	0	4.42060500	1.09055000	5.23546800
H	0	0.75788600	1.23136400	2.97358500
H	0	1.97182700	1.64424100	5.11257800
C	0	-3.70383300	-0.57076000	-2.05887900
C	0	-4.48572800	-0.78891000	-3.19170900
N	0	-2.39517200	-0.27962300	-2.09487100
C	0	-3.87412400	-0.69060200	-4.44441800
H	0	-5.54252000	-1.02361500	-3.10454100
C	0	-1.82340900	-0.17404900	-3.30366400
C	0	-2.51934700	-0.36935700	-4.49966000
H	0	-4.44715700	-0.85287900	-5.35166600
H	0	-0.77221200	0.08407300	-3.31014000
H	0	-2.00466100	-0.26720600	-5.44907900
H	0	6.28348800	1.22320100	-0.58536700
H	0	5.43166300	-2.85112500	0.67209300
H	0	-5.34623900	-3.04443900	0.27229000
H	0	-6.30171800	1.20564100	0.08913300
C	0	-0.18934100	-3.14628600	2.43293400
H	0	0.51406200	-3.24470400	3.26774000
H	0	-0.42359400	-4.15161900	2.06730500

H	0	0.29193300	-2.57938400	1.63187900
C	0	-1.11311100	-1.00111100	3.39675200
H	0	-0.68129900	-0.42268400	2.57585300
H	0	-1.99717100	-0.47658900	3.77560000
H	0	-0.37127600	-1.05246600	4.20076000
C	0	-2.03542300	-3.21148900	4.12777400
H	0	-2.21393400	-4.26313900	3.87942600
H	0	-1.30835000	-3.19027000	4.94583100
H	0	-2.97052600	-2.77384600	4.49367400
C	0	0.27083000	-3.82637800	-1.22613100
H	0	-0.43751600	-4.23005300	-1.95866700
H	0	0.54354400	-4.63359600	-0.53812400
H	0	-0.22128900	-3.02996900	-0.66211700
C	0	1.11110400	-2.12465300	-2.89435100
H	0	0.66598600	-1.31092200	-2.31597200
H	0	1.97355800	-1.73939900	-3.44937500
H	0	0.36479300	-2.47316900	-3.61625100
C	0	2.10132800	-4.42378600	-2.83266300
H	0	2.31657500	-5.31855100	-2.23907200
H	0	1.36673100	-4.70760300	-3.59294500
H	0	3.01806200	-4.11335100	-3.34548800
C	0	1.60688400	3.86887300	-1.54897700
H	0	2.33980900	4.57108000	-1.13714400
H	0	0.84224100	4.44632400	-2.08034900
H	0	1.13092800	3.33667400	-0.72051600
C	0	1.23711200	1.93032500	-3.13743900
H	0	1.70784500	1.21427500	-3.82106200
H	0	0.70292000	1.38882500	-2.35152700
H	0	0.50368800	2.51493000	-3.70361300
C	0	2.96817400	3.66770600	-3.65491500
H	0	2.20550900	4.20593000	-4.22634600
H	0	3.67066500	4.41286000	-3.26675300
H	0	3.50278000	3.00615400	-4.34564300
C	0	-1.28625100	2.89277800	2.19092500
H	0	-1.75550700	2.47958800	3.09126200
H	0	-0.74065000	2.10297400	1.66667800
H	0	-0.56252900	3.65523900	2.49950200
C	0	-1.65962100	4.08861500	-0.01062100
H	0	-2.39493000	4.57777100	-0.65874900
H	0	-0.90414200	4.83087300	0.26953800
H	0	-1.17283300	3.28858700	-0.57608600
C	0	-3.03789800	4.67753600	2.00932800
H	0	-2.28596200	5.40337700	2.33414000
H	0	-3.74822900	5.20816900	1.36636800
H	0	-3.56723100	4.31918400	2.89914700

Table S81: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.881 Å

Cu	0	1.53918300	-0.00386200	-0.25729100
Cu	0	-1.53180000	0.05632100	0.17726900
O	-1	0.01124900	-0.85351300	0.13208300
O	-1	-0.00472500	0.99411500	-0.22214800
N	0	4.29818600	0.70964100	-0.36554600
N	0	3.09049400	1.10066100	-0.88446600
N	0	3.87592700	-1.54461700	0.26963400
N	0	2.69357800	-1.61121800	-0.41083800
N	0	-2.66440600	-1.36664400	0.97512000
N	0	-3.84926100	-1.59900400	0.33711100
N	0	-3.09554700	1.29757900	0.28016900
N	0	-4.29861900	0.71124700	-0.01737700
C	0	4.39203300	-0.25548500	0.72152000
C	0	3.38258700	2.02940400	-1.82705300
C	0	4.78001400	2.22013300	-1.88720300
C	0	5.32619400	1.37140700	-0.95293300
C	0	2.33790400	2.78334600	-2.62582600
C	0	2.63684400	-2.85798700	-0.94271800
C	0	3.78880600	-3.57811400	-0.55510900
C	0	4.55802400	-2.71406300	0.18923900
C	0	1.55540600	-3.35381800	-1.88986700
C	0	-4.38153500	-0.61909100	-0.60505300
C	0	-5.33286200	1.55324800	0.22967900
C	0	-4.79552500	2.72514200	0.70962200
C	0	-3.39707200	2.53803900	0.73468400
C	0	-2.35564700	3.56141700	1.14029200
C	0	-4.51510800	-2.63940300	0.89649900
C	0	-3.73212800	-3.11214600	1.92435900
C	0	-2.58917600	-2.28304600	1.97243400
C	0	-1.49798100	-2.32988500	3.03054500
H	0	5.45690200	-0.40488300	0.90005600
H	0	5.31690800	2.89136100	-2.53840800
H	0	4.03786400	-4.59395300	-0.81761200
H	0	-5.44483700	-0.84026400	-0.69837200
H	0	-5.33861800	3.60662300	1.01143100
H	0	-3.96666400	-3.93252100	2.58391200
C	0	3.74003000	0.26039800	1.98948200
C	0	4.48875400	0.48192000	3.14344200
N	0	2.42857300	0.52375600	1.88731800
C	0	3.83935300	1.01922700	4.25845700
H	0	5.54905000	0.24937700	3.17436000
C	0	1.81981100	1.05397800	2.95812200
C	0	2.48181000	1.31851000	4.15949000
H	0	4.38676500	1.20736700	5.17648300
H	0	0.76852900	1.28170900	2.83886000
H	0	1.94022500	1.75278500	4.99303700
C	0	-3.73914800	-0.66851800	-1.97759200
C	0	-4.49540700	-0.95200200	-3.11296600
N	0	-2.43025500	-0.37542100	-2.00523100
C	0	-3.85723600	-0.92042000	-4.35601300
H	0	-5.55316900	-1.18536100	-3.03554600
C	0	-1.83236300	-0.33256100	-3.20486600
C	0	-2.50265200	-0.59607100	-4.40201400
H	0	-4.41083000	-1.13487000	-5.26451600
H	0	-0.78253800	-0.06898300	-3.20029100
H	0	-1.96955000	-0.54297000	-5.34523400
H	0	6.34931600	1.18813600	-0.65716400
H	0	5.52586000	-2.83044000	0.65579100
H	0	-5.48243700	-2.94851400	0.52686600
H	0	-6.35371000	1.25312000	0.04090000
C	0	-0.23654800	-3.04697500	2.50179600
H	0	0.49698700	-3.12975700	3.31207100
H	0	-0.47430200	-4.05821500	2.15529700

H	0	0.21381000	-2.48578100	1.67886000
C	0	-1.14488900	-0.89527700	3.46361300
H	0	-0.75238500	-0.32585500	2.61655400
H	0	-2.01961400	-0.37246700	3.86551200
H	0	-0.37258600	-0.92476300	4.23967500
C	0	-2.02183300	-3.10358200	4.26024400
H	0	-2.20862400	-4.15765400	4.02862200
H	0	-1.26423400	-3.07311600	5.04982400
H	0	-2.94259200	-2.66292700	4.65771800
C	0	0.29894000	-3.80831800	-1.11549800
H	0	-0.42449400	-4.23484400	-1.81978900
H	0	0.54887800	-4.57873700	-0.37850500
H	0	-0.16938500	-2.96442200	-0.60193800
C	0	1.19013200	-2.23215400	-2.87927000
H	0	0.78917000	-1.36601200	-2.34560800
H	0	2.06199300	-1.91536400	-3.46205200
H	0	0.42200300	-2.58895800	-3.57381000
C	0	2.09935000	-4.55844800	-2.68907500
H	0	2.29041500	-5.42250500	-2.04373700
H	0	1.35084400	-4.86304000	-3.42744600
H	0	3.02139700	-4.30880000	-3.22508800
C	0	1.67330700	3.81173600	-1.68189300
H	0	2.41181400	4.52610500	-1.30254700
H	0	0.90399600	4.37210800	-2.22470800
H	0	1.20467500	3.31165000	-0.82918300
C	0	1.28279000	1.81380400	-3.18840100
H	0	1.74311100	1.07334800	-3.85265200
H	0	0.76395600	1.29796500	-2.37503900
H	0	0.53723800	2.37504600	-3.76202200
C	0	3.00761900	3.52979200	-3.79654400
H	0	2.23942200	4.04895800	-4.37816300
H	0	3.71742300	4.28646000	-3.44546500
H	0	3.53231400	2.84153700	-4.46847600
C	0	-1.36699000	2.94354600	2.14632900
H	0	-1.88143500	2.61705000	3.05711000
H	0	-0.85438100	2.08902100	1.69473200
H	0	-0.61067000	3.68612700	2.42318100
C	0	-1.60805400	4.01411400	-0.13379400
H	0	-2.29870400	4.47114100	-0.85071100
H	0	-0.84660000	4.75681500	0.12828600
H	0	-1.11527600	3.16499600	-0.61803000
C	0	-3.03835900	4.78149100	1.78814000
H	0	-2.27224400	5.50229100	2.09064100
H	0	-3.70958000	5.29040500	1.08805100
H	0	-3.60816800	4.50074800	2.68078800

Table S82: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.749 Å

Cu	0	1.62104400	-0.01156200	-0.24103300
Cu	0	-1.61347100	0.05003400	0.17133500
O	-1	0.01124800	-0.78644600	0.13207100
O	-1	-0.00472400	0.92704800	-0.22213600
N	0	4.36521200	0.73497600	-0.34004500
N	0	3.15752900	1.10993600	-0.86600700
N	0	3.97197200	-1.54243000	0.24033400
N	0	2.77511900	-1.62875400	-0.41347400
N	0	-2.74347200	-1.37486400	0.99643300
N	0	-3.93988000	-1.58169800	0.36988200
N	0	-3.16784100	1.30733400	0.29866600
N	0	-4.36901100	0.72995700	-0.01811900
C	0	4.45404300	-0.25336800	0.72705400
C	0	3.43993800	2.05443000	-1.79323700
C	0	4.83415700	2.27179900	-1.83977800
C	0	5.38760100	1.42170100	-0.90970800
C	0	2.37679800	2.78361900	-2.59044100
C	0	2.74500300	-2.86380500	-0.97115000
C	0	3.92824800	-3.55736800	-0.63226300
C	0	4.68887100	-2.68747600	0.11420400
C	0	1.64310900	-3.36974500	-1.88818900
C	0	-4.44180700	-0.60688600	-0.59348000
C	0	-5.40359400	1.57244900	0.22951400
C	0	-4.86539200	2.73806600	0.72501300
C	0	-3.46744000	2.54382900	0.76022900
C	0	-2.41798000	3.55588600	1.17570500
C	0	-4.63993500	-2.58456100	0.95694700
C	0	-3.86808600	-3.06083100	1.99151100
C	0	-2.69665800	-2.27100900	2.01248600
C	0	-1.59636100	-2.32850400	3.05998500
H	0	5.51678900	-0.38711900	0.92846500
H	0	5.36468300	2.96048700	-2.47806200
H	0	4.19921100	-4.56004500	-0.92238700
H	0	-5.50259100	-0.82548500	-0.71632600
H	0	-5.40805700	3.61867200	1.03047300
H	0	-4.12483300	-3.85972800	2.66892000
C	0	3.76133500	0.22304700	1.99035600
C	0	4.47493300	0.42965000	3.16882900
N	0	2.44686900	0.46433700	1.86430900
C	0	3.78657100	0.92450100	4.28025500
H	0	5.53854700	0.21745500	3.22151300
C	0	1.79913700	0.95246400	2.93229100
C	0	2.42555000	1.19817700	4.15609000
H	0	4.30727500	1.09955000	5.21623200
H	0	0.74624700	1.15936700	2.79009900
H	0	1.85487000	1.59821400	4.98730600
C	0	-3.75906100	-0.67391700	-1.94664200
C	0	-4.47873400	-0.97263400	-3.10152200
N	0	-2.44819900	-0.38475400	-1.94071100
C	0	-3.80101000	-0.96223000	-4.32395700
H	0	-5.53903000	-1.20209600	-3.05460600
C	0	-1.81088600	-0.36271600	-3.12055800
C	0	-2.44415900	-0.64338500	-4.33328700
H	0	-4.32664800	-1.18900700	-5.24596400
H	0	-0.76111300	-0.10104500	-3.08380100
H	0	-1.88187600	-0.60751500	-5.26019900
H	0	6.41122600	1.25241500	-0.60751500
H	0	5.66973800	-2.78562500	0.55704800
H	0	-5.61850600	-2.86938500	0.59755500
H	0	-6.42410600	1.27755400	0.03079000
C	0	-0.32683000	-3.00736500	2.50269400
H	0	0.41519400	-3.09970100	3.30412200
H	0	-0.54918900	-4.01225900	2.12876100

H	0	0.11015400	-2.41657500	1.69324800
C	0	-1.26908100	-0.89629100	3.52381800
H	0	-0.91044200	-0.29328800	2.68414700
H	0	-2.14939300	-0.40629800	3.95354400
H	0	-0.48247500	-0.92515400	4.28554500
C	0	-2.09371200	-3.14109900	4.27453300
H	0	-2.27286500	-4.19025200	4.01545800
H	0	-1.32635500	-3.12368100	5.05504700
H	0	-3.01351700	-2.72179000	4.69667200
C	0	0.39568300	-3.78792600	-1.07994400
H	0	-0.34476700	-4.22756000	-1.75796900
H	0	0.65036000	-4.53805400	-0.32390100
H	0	-0.05867800	-2.92592000	-0.58403200
C	0	1.27502800	-2.26358600	-2.89528200
H	0	0.90724200	-1.37529000	-2.37307600
H	0	2.13877500	-1.97761700	-3.50529900
H	0	0.48320100	-2.61949700	-3.56332300
C	0	2.15597700	-4.59888800	-2.66834400
H	0	2.35662400	-5.44666600	-2.00437100
H	0	1.38750500	-4.91644100	-3.38028300
H	0	3.06624600	-4.37169200	-3.23377300
C	0	1.65124700	3.76052200	-1.63680200
H	0	2.35147300	4.49423600	-1.22310900
H	0	0.87140700	4.30334700	-2.18234100
H	0	1.18486800	3.22156500	-0.80603800
C	0	1.37374100	1.77766400	-3.18485000
H	0	1.87266900	1.07587300	-3.86244300
H	0	0.88056100	1.21548000	-2.38575400
H	0	0.60236300	2.31324700	-3.74879000
C	0	3.02989200	3.58187600	-3.73538500
H	0	2.24976600	4.08499600	-4.31530500
H	0	3.70652600	4.35580700	-3.35741700
H	0	3.58803800	2.92937800	-4.41589100
C	0	-1.40635200	2.90975400	2.14066300
H	0	-1.89890800	2.56637600	3.05727900
H	0	-0.91013000	2.06077000	1.66030800
H	0	-0.63808500	3.64125500	2.41407500
C	0	-1.69742500	4.04922400	-0.10003600
H	0	-2.40314000	4.53047500	-0.78568300
H	0	-0.92871400	4.78215400	0.16851600
H	0	-1.21728800	3.21778400	-0.62567900
C	0	-3.08727100	4.75466800	1.87481800
H	0	-2.31583700	5.46561600	2.18705300
H	0	-3.77015100	5.28585900	1.20316400
H	0	-3.64214600	4.44465400	2.76709900

Table S83: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.685 Å

Cu	-1	1.66053800	-0.01780200	-0.26154600
Cu	-1	-1.65290000	0.04817700	0.19572200
O	-1	0.01124900	-0.75301100	0.13208500
O	-1	-0.00472500	0.89361300	-0.22215000
N	0	4.39179900	0.74707900	-0.40724600
N	0	3.17609800	1.10788400	-0.92276100
N	0	4.02323900	-1.53465600	0.17826100
N	0	2.81237800	-1.63833600	-0.44731900
N	0	-2.77331400	-1.36162800	1.06391200
N	0	-3.98611600	-1.55470300	0.46430700
N	0	-3.18951800	1.32303700	0.33270900
N	0	-4.39755100	0.75342100	0.03113300
C	0	4.49560000	-0.24015600	0.65980500
C	0	3.43989500	2.04501700	-1.86198500
C	0	4.83188200	2.27311000	-1.92660900
C	0	5.40290700	1.43461900	-0.99623500
C	0	2.35835800	2.75545000	-2.65189600
C	0	2.78793300	-2.87356300	-1.00371000
C	0	3.98918000	-3.54987700	-0.69453800
C	0	4.75418000	-2.66898300	0.03456800
C	0	1.66833400	-3.39321100	-1.89078400
C	0	-4.48198200	-0.59443800	-0.51638100
C	0	-5.42372400	1.60489700	0.28404000
C	0	-4.87135700	2.76967300	0.76612200
C	0	-3.47457100	2.56425400	0.78934500
C	0	-2.41167200	3.56768800	1.19198100
C	0	-4.69542300	-2.53213400	1.08285100
C	0	-3.91307800	-3.00658300	2.11034000
C	0	-2.72498300	-2.24181100	2.09275800
C	0	-1.59786200	-2.30938900	3.11035400
H	0	5.56045500	-0.36353700	0.85645800
H	0	5.34971300	2.96089100	-2.57632500
H	0	4.26785700	-4.54844400	-0.99152400
H	0	-5.54443600	-0.80720200	-0.63428400
H	0	-5.40410100	3.65682700	1.07018600
H	0	-4.17206900	-3.78940700	2.80552100
C	0	3.80408700	0.22989800	1.92655700
C	0	4.52056000	0.44392900	3.10184100
N	0	2.48598800	0.45708900	1.80794800
C	0	3.83196200	0.92983500	4.21704100
H	0	5.58670900	0.24373700	3.14920500
C	0	1.83746900	0.93658700	2.87949500
C	0	2.46721600	1.18803500	4.10019900
H	0	4.35531500	1.10978100	5.15060500
H	0	0.78163800	1.13094800	2.74171300
H	0	1.89630000	1.58028300	4.93494600
C	0	-3.80051900	-0.69549400	-1.86847500
C	0	-4.52374600	-1.00785200	-3.01737700
N	0	-2.48557800	-0.42332900	-1.86959900
C	0	-3.84639200	-1.03042600	-4.23982500
H	0	-5.58681100	-1.22290600	-2.96586000
C	0	-1.84775300	-0.43427600	-3.04937800
C	0	-2.48528600	-0.73030600	-4.25595600
H	0	-4.37548000	-1.26843900	-5.15700700
H	0	-0.79411600	-0.18786900	-3.01654900
H	0	-1.92305800	-0.72085300	-5.18352500
H	0	6.43138500	1.27505100	-0.70544500
H	0	5.74641500	-2.75287300	0.45447900
H	0	-5.68605500	-2.80361700	0.74698000
H	0	-6.44842400	1.31633600	0.09814000
C	0	-0.35284600	-3.00161400	2.51590000
H	0	0.41101700	-3.10529800	3.29510800
H	0	-0.59722900	-4.00256000	2.14517100

H	0	0.06875600	-2.41406400	1.69621200
C	0	-1.24157200	-0.87935800	3.55969400
H	0	-0.90712000	-0.28187800	2.70598000
H	0	-2.10220500	-0.38012200	4.01768100
H	0	-0.42979600	-0.91352800	4.29438500
C	0	-2.06901300	-3.11456800	4.33969100
H	0	-2.26875600	-4.16143400	4.08659400
H	0	-1.27940000	-3.10616200	5.09781800
H	0	-2.97099400	-2.68347000	4.78756300
C	0	0.43137300	-3.78118800	-1.05241400
H	0	-0.32395100	-4.23084000	-1.70710300
H	0	0.69248900	-4.51472500	-0.28246500
H	0	-0.00918500	-2.90456300	-0.57025400
C	0	1.29318600	-2.30607500	-2.91639500
H	0	0.95128200	-1.39913600	-2.40818400
H	0	2.14746000	-2.04725700	-3.55135300
H	0	0.48209900	-2.66604800	-3.55877700
C	0	2.15771100	-4.64395200	-2.65061100
H	0	2.36927300	-5.47542900	-1.96957800
H	0	1.37262000	-4.97555000	-3.33760000
H	0	3.05641600	-4.43589000	-3.24138300
C	0	1.62792900	3.72781900	-1.69713100
H	0	2.32206500	4.47173500	-1.29156700
H	0	0.83752700	4.25879500	-2.23909900
H	0	1.17406600	3.18752400	-0.86023200
C	0	1.36363100	1.73144900	-3.22978300
H	0	1.86443800	1.03712800	-3.91359200
H	0	0.89307200	1.16079700	-2.42301000
H	0	0.57441000	2.25263000	-3.78245800
C	0	2.98839100	3.55543400	-3.80823300
H	0	2.19598800	4.04495200	-4.38325000
H	0	3.65898800	4.34009700	-3.44180500
H	0	3.54828100	2.90616200	-4.49044200
C	0	-1.39425300	2.91126600	2.14400400
H	0	-1.87792800	2.57664700	3.06850000
H	0	-0.91653400	2.05350600	1.66043500
H	0	-0.61251600	3.63335900	2.40399000
C	0	-1.70163500	4.05816900	-0.09091700
H	0	-2.41076500	4.54898800	-0.76608000
H	0	-0.92210800	4.78226800	0.17051900
H	0	-1.23641200	3.22447300	-0.62622700
C	0	-3.06249700	4.77038500	1.90160400
H	0	-2.28202400	5.47441400	2.20716300
H	0	-3.74867500	5.30906100	1.23933500
H	0	-3.60993900	4.46229700	2.79910300

Table S84: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.618 Å

Cu	0	1.72836100	-0.05294500	-0.33334500
Cu	0	-1.73810900	0.04205200	0.09207600
O	-1	0.01124800	-0.71941900	0.13206500
O	-1	-0.00472400	0.86002100	-0.22213000
N	0	4.45067900	0.71760800	-0.42430600
N	0	3.24258300	1.09932400	-0.94331200
N	0	4.09058300	-1.60529200	-0.02891900
N	0	2.88721600	-1.67042300	-0.67591700
N	0	-2.96611300	-1.35602000	0.82554100
N	0	-4.17769400	-1.41381500	0.19429300
N	0	-3.21880000	1.38338600	0.21855300
N	0	-4.42457900	0.91883500	-0.22958400
C	0	4.54073800	-0.34958500	0.56421300
C	0	3.51636600	2.09258600	-1.81917400
C	0	4.90802700	2.33263500	-1.84327800
C	0	5.46774700	1.44431100	-0.95335500
C	0	2.44537800	2.85269000	-2.57702600
C	0	2.87983700	-2.86375000	-1.31682100
C	0	4.08041500	-3.55475900	-1.03966200
C	0	4.83035300	-2.72291300	-0.24011100
C	0	1.78714900	-3.30553700	-2.27690400
C	0	-4.54182400	-0.41523800	-0.80443800
C	0	-5.41576700	1.81918000	-0.00686900
C	0	-4.83787300	2.91143800	0.60012400
C	0	-3.46505800	2.60837600	0.73500700
C	0	-2.38235900	3.49520000	1.31888700
C	0	-4.97865900	-2.36108700	0.74476400
C	0	-4.26226300	-2.95173900	1.76048000
C	0	-3.01291900	-2.29389500	1.80045900
C	0	-1.88814000	-2.54415100	2.78959100
H	0	5.60189100	-0.47956800	0.77593400
H	0	5.43307800	3.06121600	-2.44059800
H	0	4.36768500	-4.53024000	-1.39873700
H	0	-5.60109800	-0.56623100	-1.01167900
H	0	-5.33970600	3.81278700	0.91499500
H	0	-4.60092500	-3.74590500	2.40666200
C	0	3.81371800	0.00827700	1.84836600
C	0	4.49152400	0.12307500	3.05940500
N	0	2.49621800	0.23095600	1.71409000
C	0	3.76186400	0.49544800	4.19230100
H	0	5.55853600	-0.06787000	3.12176500
C	0	1.80508700	0.59662000	2.80350800
C	0	2.39615800	0.74205200	4.05985400
H	0	4.25498200	0.59659900	5.15378400
H	0	0.75017900	0.78253800	2.64817400
H	0	1.79530500	1.04482800	4.91063400
C	0	-3.75241900	-0.54980800	-2.09585900
C	0	-4.38595300	-0.80747000	-3.30925000
N	0	-2.42529500	-0.38027300	-1.97641500
C	0	-3.59960000	-0.88802500	-4.46239300
H	0	-5.46257700	-0.93862300	-3.35928500
C	0	-1.67930500	-0.45447900	-3.08825000
C	0	-2.22223400	-0.70449600	-4.34956500
H	0	-4.05780600	-1.08531400	-5.42622900
H	0	-0.61644500	-0.30218300	-2.94990000
H	0	-1.57647400	-0.75054900	-5.21985000
H	0	6.49190100	1.27344300	-0.65388900
H	0	5.81636700	-2.83183000	0.18864700
H	0	-5.97874600	-2.53357000	0.37343100
H	0	-6.43574300	1.61237900	-0.29791500
C	0	-0.73031900	-3.29779300	2.09879200
H	0	0.04689800	-3.52574700	2.83705400
H	0	-1.07795600	-4.24263900	1.66761800

H	0	-0.28465200	-2.69154400	1.30566700
C	0	-1.38337400	-1.19743200	3.34298600
H	0	-1.00784600	-0.56715400	2.53115300
H	0	-2.18018600	-0.65894800	3.86731800
H	0	-0.56236900	-1.37139100	4.04703300
C	0	-2.41192400	-3.40076500	3.96044000
H	0	-2.71658800	-4.39937700	3.62879000
H	0	-1.61262200	-3.53084700	4.69705100
H	0	-3.26015300	-2.92454700	4.46434800
C	0	0.44189600	-3.49978600	-1.54874900
H	0	-0.31166300	-3.84514400	-2.26614400
H	0	0.53097500	-4.25656800	-0.76220100
H	0	0.08967800	-2.56796100	-1.09829300
C	0	1.65278400	-2.23491200	-3.38261000
H	0	1.41273600	-1.25389900	-2.95784000
H	0	2.58448700	-2.13629700	-3.94986900
H	0	0.85641200	-2.51901800	-4.07944400
C	0	2.18579700	-4.64199300	-2.93476700
H	0	2.27788700	-5.44486900	-2.19520100
H	0	1.40946800	-4.93693000	-3.64790300
H	0	3.12945300	-4.56014700	-3.48501400
C	0	1.77465200	3.83802100	-1.59107500
H	0	2.50506100	4.55088000	-1.19395500
H	0	0.99102300	4.40419000	-2.10677400
H	0	1.32261700	3.30321600	-0.75001300
C	0	1.39761100	1.87933600	-3.14677500
H	0	1.85224200	1.18879700	-3.86598000
H	0	0.93048400	1.30379700	-2.34112400
H	0	0.60937700	2.44159600	-3.65868200
C	0	3.08061600	3.64570600	-3.73585200
H	0	2.29407400	4.16420800	-4.29328500
H	0	3.77953800	4.40726400	-3.37376200
H	0	3.61098900	2.98707300	-4.43247900
C	0	-1.49934400	2.68314400	2.28562800
H	0	-2.09006600	2.27618700	3.11361500
H	0	-1.01052600	1.85864800	1.75661200
H	0	-0.71811600	3.32850500	2.70207600
C	0	-1.52681400	4.04965900	0.15704800
H	0	-2.13819300	4.64441500	-0.53001900
H	0	-0.73510900	4.69430400	0.55464600
H	0	-1.06170900	3.23653700	-0.40883300
C	0	-3.02213600	4.66996600	2.08397700
H	0	-2.23311700	5.28681500	2.52548400
H	0	-3.60854100	5.31444500	1.42019700
H	0	-3.67041200	4.31997300	2.89482800

Table S85: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.488 Å

Cu	0	1.76889100	-0.05795100	-0.31253500
Cu	0	-1.77193700	0.04338600	0.16207600
O	-1	0.01124700	-0.65235200	0.13204800
O	-1	-0.00472300	0.79295400	-0.22211300
N	0	4.46763500	0.77021800	-0.49579200
N	0	3.25159700	1.05935700	-1.05245100
N	0	4.15859000	-1.50537300	0.14865200
N	0	2.94831700	-1.67452000	-0.46689700
N	0	-2.95710400	-1.29191400	1.07428600
N	0	-4.17931900	-1.43145800	0.47830200
N	0	-3.26009100	1.37338000	0.17994500
N	0	-4.46768900	0.84198500	-0.18188500
C	0	4.57747000	-0.18251900	0.60210800
C	0	3.49857900	1.95565500	-2.03276400
C	0	4.88348400	2.22951400	-2.08608300
C	0	5.46622100	1.46019000	-1.10426400
C	0	2.40363800	2.58630100	-2.87104600
C	0	2.97095600	-2.92534400	-0.98486100
C	0	4.19903200	-3.54568300	-0.66436200
C	0	4.93252600	-2.61439000	0.03434700
C	0	1.86788400	-3.50448200	-1.85572800
C	0	-4.57291000	-0.54663600	-0.61212300
C	0	-5.46886100	1.74778600	-0.04118700
C	0	-4.89649600	2.91151500	0.42121800
C	0	-3.51586400	2.64636600	0.55571600
C	0	-2.43306500	3.61141900	0.99797400
C	0	-4.95696900	-2.32255000	1.14455500
C	0	-4.21237200	-2.79189200	2.20288400
C	0	-2.97134700	-2.11881600	2.14432700
C	0	-1.82045000	-2.24123600	3.12741800
H	0	5.64022900	-0.26509900	0.82886100
H	0	5.38978300	2.90058000	-2.76192100
H	0	4.51297700	-4.54312900	-0.92772900
H	0	-5.63268600	-0.73243700	-0.78580300
H	0	-5.40698400	3.83578100	0.64148900
H	0	-4.52724900	-3.51542000	2.93813700
C	0	3.83891700	0.29828700	1.83929400
C	0	4.51475400	0.56481300	3.02742100
N	0	2.51652200	0.47826700	1.68464100
C	0	3.77945900	1.05176100	4.11215600
H	0	5.58537400	0.40327600	3.10812400
C	0	1.82019700	0.95554300	2.72685400
C	0	2.40946300	1.25687300	3.95598300
H	0	4.27161000	1.27243200	5.05391400
H	0	0.76228900	1.10528800	2.55315500
H	0	1.80383300	1.64600600	4.76730200
C	0	-3.80095400	-0.80647100	-1.89540600
C	0	-4.44743700	-1.21094800	-3.06095100
N	0	-2.47534600	-0.60095400	-1.82021500
C	0	-3.67712900	-1.40810200	-4.21097600
H	0	-5.52176500	-1.36685000	-3.07705500
C	0	-1.74430800	-0.78889600	-2.92855900
C	0	-2.30179300	-1.18982900	-4.14365700
H	0	-4.14610900	-1.72151800	-5.13814200
H	0	-0.68247400	-0.60525000	-2.82432700
H	0	-1.66876900	-1.32368800	-5.01419300
H	0	6.49440000	1.35088200	-0.79017500
H	0	5.92788100	-2.64856000	0.45381300
H	0	-5.96197600	-2.54556700	0.81577700
H	0	-6.49133500	1.49409400	-0.28215600
C	0	-0.66848700	-3.05524700	2.49774400
H	0	0.12714100	-3.19396400	3.23875900
H	0	-1.01328200	-4.04523800	2.18063500

H	0	-0.24746900	-2.53508700	1.63377200
C	0	-1.32012600	-0.83370600	3.50517800
H	0	-0.96554200	-0.30323000	2.61561500
H	0	-2.11326200	-0.24103100	3.97376200
H	0	-0.48531200	-0.91442500	4.20991100
C	0	-2.30527600	-2.96246400	4.40115400
H	0	-2.60489200	-3.99510800	4.19199400
H	0	-1.48739000	-2.99943900	5.12779800
H	0	-3.14790600	-2.44052600	4.86773000
C	0	0.56462400	-3.69283800	-1.05246100
H	0	-0.19048100	-4.16519800	-1.69136500
H	0	0.72896400	-4.34333700	-0.18699200
H	0	0.16943600	-2.73562900	-0.70320300
C	0	1.62979600	-2.54976400	-3.04599100
H	0	1.34393800	-1.55076500	-2.69888700
H	0	2.53240300	-2.44993100	-3.65839900
H	0	0.82668000	-2.94026500	-3.68094200
C	0	2.31108700	-4.87529200	-2.40532600
H	0	2.47114700	-5.60079600	-1.60030700
H	0	1.52608700	-5.27237500	-3.05663500
H	0	3.22938200	-4.79823500	-2.99764900
C	0	1.70066100	3.66272200	-2.01044600
H	0	2.40750700	4.44108500	-1.70415600
H	0	0.90111100	4.13718300	-2.59022100
H	0	1.26190700	3.22086000	-1.11034600
C	0	1.38679100	1.51752300	-3.31251900
H	0	1.86336400	0.75581200	-3.93983000
H	0	0.93523700	1.03199900	-2.44083200
H	0	0.58288300	1.98708300	-3.88978700
C	0	3.01268900	3.25233100	-4.11994800
H	0	2.21001300	3.67636600	-4.73166000
H	0	3.68850800	4.07181200	-3.85327500
H	0	3.56247500	2.53128300	-4.73471200
C	0	-1.51431500	2.93590700	2.03437300
H	0	-2.07348600	2.64830000	2.93155400
H	0	-1.04502800	2.04385200	1.60669500
H	0	-0.71868300	3.62865300	2.32986800
C	0	-1.61408000	4.02733500	-0.24584600
H	0	-2.25279500	4.51865400	-0.98759000
H	0	-0.82802600	4.73221300	0.04696000
H	0	-1.14401800	3.15802300	-0.71567300
C	0	-3.07017600	4.86495400	1.62752400
H	0	-2.27864200	5.54108400	1.96600600
H	0	-3.68333100	5.41412200	0.90489300
H	0	-3.69165600	4.61151900	2.49337100

Table S86: XYZ coordinates for optimised structure: Broken-Symmetry minimum path, O...O = 1.359 Å

Cu	0	1.79162200	-0.09867000	-0.37926900
Cu	0	-1.80834100	0.04324200	0.12246100
O	-1	0.01124800	-0.58543300	0.13206800
O	-1	-0.00472400	0.72603500	-0.22213300
N	0	4.47760500	0.72218900	-0.62616300
N	0	3.25911000	0.98610800	-1.18939100
N	0	4.17437100	-1.53227200	0.09671900
N	0	2.95448000	-1.73082900	-0.49143200
N	0	-3.00877700	-1.24499800	1.07335700
N	0	-4.23422800	-1.37425900	0.48193700
N	0	-3.26688300	1.39664000	0.06904600
N	0	-4.47503800	0.86963200	-0.29578900
C	0	4.59069400	-0.19312100	0.50281400
C	0	3.49995700	1.84146300	-2.20621500
C	0	4.88459300	2.11497700	-2.27704600
C	0	5.47306200	1.38734300	-1.26746500
C	0	2.40064600	2.43884500	-3.06319300
C	0	2.97573700	-3.00081600	-0.95947000
C	0	4.21243300	-3.60266300	-0.63643100
C	0	4.95233300	-2.64135900	0.01320300
C	0	1.86125800	-3.61665800	-1.78948900
C	0	-4.59202800	-0.53797900	-0.65777600
C	0	-5.46347900	1.79701600	-0.21679500
C	0	-4.88048500	2.97053700	0.20625100
C	0	-3.50776400	2.68870100	0.38336100
C	0	-2.41763800	3.64982500	0.81633900
C	0	-5.04064800	-2.20703300	1.18903300
C	0	-4.31173700	-2.64784900	2.27052900
C	0	-3.04935600	-2.01900400	2.18078700
C	0	-1.89422000	-2.13969000	3.15864500
H	0	5.65395300	-0.26612200	0.73054300
H	0	5.38768100	2.75802600	-2.98193100
H	0	4.52677900	-4.60869900	-0.86455400
H	0	-5.65062000	-0.71724500	-0.84503100
H	0	-5.37974000	3.91173000	0.37446600
H	0	-4.64965100	-3.32555900	3.03854900
C	0	3.85487200	0.32658000	1.72674500
C	0	4.53420300	0.63114800	2.90365600
N	0	2.53126000	0.49975300	1.57214600
C	0	3.80178500	1.14926500	3.97576000
H	0	5.60548700	0.47481000	2.98529100
C	0	1.83708600	1.00631100	2.60221300
C	0	2.43045000	1.34586100	3.81906700
H	0	4.29708800	1.39971200	4.90836800
H	0	0.77836700	1.14856700	2.42693700
H	0	1.82703400	1.75752700	4.62083100
C	0	-3.79882300	-0.87419800	-1.91100200
C	0	-4.43213700	-1.32727700	-3.06598100
N	0	-2.47015900	-0.68952400	-1.82277500
C	0	-3.64682700	-1.59955800	-4.18998100
H	0	-5.50888500	-1.46349300	-3.09330500
C	0	-1.72448600	-0.95172700	-2.90651600
C	0	-2.26853600	-1.40570800	-4.10863600
H	0	-4.10611800	-1.95234200	-5.10780300
H	0	-0.66031400	-0.78614600	-2.79354600
H	0	-1.62291200	-1.59892100	-4.95851600
H	0	6.50295400	1.29144600	-0.95462000
H	0	5.95393700	-2.65486600	0.41872600
H	0	-6.05159800	-2.41468600	0.86856600
H	0	-6.48509100	1.54958700	-0.46770400
C	0	-0.77604300	-3.01053500	2.54314500
H	0	0.02580700	-3.14840700	3.27753600
H	0	-1.15541900	-3.99959000	2.26491200

H	0	-0.35159700	-2.53417300	1.65567700
C	0	-1.34468300	-0.73592900	3.47766800
H	0	-0.98534100	-0.25076400	2.56426500
H	0	-2.11233600	-0.10123300	3.93336100
H	0	-0.50301800	-0.81702900	4.17407700
C	0	-2.38609900	-2.79898400	4.46225200
H	0	-2.72261600	-3.82762000	4.29328200
H	0	-1.56103900	-2.83789800	5.18062400
H	0	-3.20514900	-2.23274300	4.91897300
C	0	0.54462900	-3.68406800	-0.99028500
H	0	-0.22678700	-4.16909800	-1.59951400
H	0	0.67303700	-4.27351700	-0.07661300
H	0	0.19045700	-2.68700600	-0.71707900
C	0	1.67253200	-2.76282600	-3.06373900
H	0	1.42068400	-1.72606200	-2.81319100
H	0	2.58537900	-2.74995900	-3.66885200
H	0	0.86388400	-3.18038300	-3.67416100
C	0	2.25752800	-5.04647000	-2.20838100
H	0	2.39388400	-5.69784800	-1.33811400
H	0	1.45948200	-5.47608800	-2.82214100
H	0	3.17729100	-5.05714300	-2.80321800
C	0	1.77191500	3.61781500	-2.28243100
H	0	2.51992200	4.38893700	-2.07015700
H	0	0.97280200	4.07284200	-2.87816400
H	0	1.34711300	3.27845200	-1.33239300
C	0	1.32659900	1.38032800	-3.37103600
H	0	1.74773700	0.54997500	-3.94920800
H	0	0.89327900	0.98852600	-2.44413200
H	0	0.51692300	1.83159100	-3.95450000
C	0	2.98968000	2.96272300	-4.38770900
H	0	2.18193700	3.36035900	-5.01065200
H	0	3.70327800	3.77649400	-4.22125000
H	0	3.49149700	2.16699400	-4.94904500
C	0	-1.54642300	2.99973200	1.90896100
H	0	-2.13896000	2.76297900	2.79947200
H	0	-1.08569900	2.07932000	1.53527300
H	0	-0.74436200	3.68699300	2.19984400
C	0	-1.55178100	3.99790100	-0.41650000
H	0	-2.15769100	4.46928400	-1.19779800
H	0	-0.76251700	4.70081300	-0.12785200
H	0	-1.08309400	3.10221200	-0.83508200
C	0	-3.04632800	4.94107800	1.37381600
H	0	-2.25143300	5.61489700	1.70919300
H	0	-3.62582000	5.47170000	0.61062000
H	0	-3.69850500	4.73590400	2.22987500

Table S87: XYZ coordinates for optimised structure: Triplet minimum path, Oxo

Cu	1.44873900	-0.00625200	-0.15163900
Cu	-1.51413400	-0.01603100	-0.08497900
O	0.06570800	-1.11794700	-0.21948800
O	-0.02650600	1.07077500	-0.03212900
N	4.16799500	0.90047500	0.02164200
N	2.99254700	1.21620200	-0.60645400
N	3.77150300	-1.33698900	0.72445600
N	2.75920000	-1.47760000	-0.18665300
N	-2.72076600	-1.37678100	0.95116600
N	-3.95732100	-1.54122000	0.39360000
N	-3.17059000	1.35601900	0.05198000
N	-4.36230300	0.73141600	-0.21040700
C	4.19831500	-0.00404600	1.16028300
C	3.32150000	2.10586700	-1.57392600
C	4.71267100	2.34994500	-1.53562500
C	5.21510000	1.57239000	-0.51884600
C	2.32274000	2.78752400	-2.49015300
C	2.85738200	-2.74213500	-0.67283800
C	3.92513200	-3.39899200	-0.02186800
C	4.49147600	-2.48101800	0.83104900
C	2.06409300	-3.30421500	-1.84460200
C	-4.40978200	-0.64729400	-0.65794300
C	-5.42477100	1.54609000	0.01349800
C	-4.91796400	2.75290100	0.43054400
C	-3.51180100	2.60855300	0.44433100
C	-2.51666900	3.70422800	0.77678200
C	-4.67551300	-2.50030600	1.03163400
C	-3.87539700	-2.99205500	2.03554700
C	-2.66235600	-2.26769800	1.96972300
C	-1.47876900	-2.43255400	2.90405000
H	5.24727700	-0.10237100	1.44035400
H	5.27527400	3.00895400	-2.17745400
H	4.26276500	-4.40911000	-0.19099900
H	-5.45956700	-0.88157000	-0.83332700
H	-5.48437700	3.63304200	0.68979200
H	-4.13432800	-3.76427900	2.74260700
C	3.41846700	0.55695000	2.33040800
C	4.06870600	0.94406400	3.50061600
N	2.10399200	0.71232200	2.11547200
C	3.31044500	1.54551500	4.50875700
H	5.13672800	0.78978100	3.62289000
C	1.39027400	1.30655000	3.08374400
C	1.94844600	1.73981600	4.28909400
H	3.77778400	1.86146300	5.43589000
H	0.33596700	1.44151300	2.88126500
H	1.32142300	2.21708200	5.03450100
C	-3.63075800	-0.84763300	-1.94190100
C	-4.24859000	-1.21396300	-3.13382200
N	-2.30383800	-0.65111200	-1.84738900
C	-3.45702100	-1.37745900	-4.27427400
H	-5.32217800	-1.36835900	-3.17208100
C	-1.54105100	-0.81563000	-2.94013200
C	-2.08135300	-1.17472000	-4.17370400
H	-3.90951700	-1.66012400	-5.21927700
H	-0.48069600	-0.66416400	-2.79758000
H	-1.43008300	-1.29198700	-5.03270000
H	6.21739800	1.44733900	-0.13478000
H	5.35028800	-2.54075900	1.48448800
H	-5.68352900	-2.74338700	0.72681300
H	-6.43732600	1.20336000	-0.14580100
C	-0.44000300	-3.38321800	2.26512000
H	0.37494900	-3.55996300	2.97690400
H	-0.88971000	-4.35116800	2.01853700

H	-0.02492900	-2.93839100	1.35727600
C	-0.82988700	-1.06640800	3.16989700
H	-0.44495400	-0.64245700	2.23826900
H	-1.54356800	-0.36605400	3.61953800
H	0.01328800	-1.18843100	3.85812200
C	-1.96054300	-3.03433700	4.24077900
H	-2.34399300	-4.05240500	4.11520900
H	-1.11490900	-3.08912900	4.93404000
H	-2.74118300	-2.42135200	4.70442800
C	0.69051200	-3.85713400	-1.40603700
H	0.19588200	-4.31404600	-2.27111600
H	0.80731800	-4.62930600	-0.63829500
H	0.05692500	-3.05912500	-1.00948900
C	1.89750500	-2.19885000	-2.90517600
H	1.38620400	-1.33242300	-2.47775300
H	2.86918000	-1.87115600	-3.29046500
H	1.30635400	-2.57811100	-3.74599600
C	2.86619000	-4.46400400	-2.47811700
H	2.94425900	-5.32242700	-1.80253100
H	2.34341600	-4.80500800	-3.37741300
H	3.87471000	-4.15236900	-2.77065700
C	1.64175600	3.91555900	-1.67990600
H	2.38102000	4.64624600	-1.33492300
H	0.91550700	4.43845000	-2.31196400
H	1.12107800	3.50675500	-0.80979700
C	1.26875500	1.79419200	-3.01154200
H	1.73905000	0.98136300	-3.57696000
H	0.68579700	1.37398500	-2.18495300
H	0.57279900	2.31564200	-3.67751500
C	3.05746300	3.40527100	-3.69785500
H	2.32437800	3.87191800	-4.36341100
H	3.75986300	4.18730100	-3.39089200
H	3.60392500	2.64870500	-4.27169600
C	-1.51580300	3.21895700	1.84076200
H	-2.03331900	2.92618100	2.76194900
H	-0.93973100	2.37022200	1.46155200
H	-0.81463600	4.02586200	2.08165800
C	-1.77675300	4.09366400	-0.52229300
H	-2.48273000	4.45111600	-1.27987200
H	-1.06400400	4.89900500	-0.31428000
H	-1.22729800	3.23980100	-0.92859100
C	-3.25872300	4.94178700	1.31964500
H	-2.52625900	5.71508400	1.57190600
H	-3.94148100	5.36738800	0.57619100
H	-3.82713100	4.70940700	2.22711900

Table S88: XYZ coordinates for optimised structure: Triplet minimum path, Peroxo

Cu	1.75880000	0.04363700	0.02982800
Cu	-1.75219100	0.06479300	0.04513400
O	-0.00970500	-0.50448400	0.69123100
O	0.01743700	0.93563200	0.48396200
N	4.47206100	0.88158100	0.16141800
N	3.28182600	1.29936900	-0.36807600
N	4.15477500	-1.47974500	0.22054700
N	2.96530800	-1.51015600	-0.45481000
N	-3.03335500	-1.44000400	0.48608000
N	-4.12972300	-1.44712600	-0.33151000
N	-3.28852900	1.35731500	0.13277000
N	-4.39566000	0.91651200	-0.53702000
C	4.54208300	-0.30795600	0.99977400
C	3.56527200	2.41977300	-1.06774200
C	4.94534000	2.70520200	-0.97077900
C	5.48831700	1.71101700	-0.18914000
C	2.50836600	3.25297000	-1.76525400
C	3.00709500	-2.63113100	-1.21200900
C	4.22072100	-3.31528500	-0.98457100
C	4.92913800	-2.55052600	-0.08546200
C	1.94339500	-2.98799600	-2.23466300
C	-4.36176600	-0.34723900	-1.25879400
C	-5.45273900	1.74895800	-0.35418100
C	-5.01726400	2.77565600	0.45289500
C	-3.66237000	2.50221900	0.74741200
C	-2.72024900	3.33699700	1.59366800
C	-4.99324800	-2.44160500	-0.00039900
C	-4.43402200	-3.11918600	1.05826200
C	-3.21677300	-2.46294700	1.35336500
C	-2.26026700	-2.80083200	2.48461700
H	5.59525700	-0.44567500	1.24403000
H	5.47505300	3.52994900	-1.42124600
H	4.54137400	-4.24265800	-1.43245100
H	-5.36425400	-0.49655400	-1.65948800
H	-5.60074100	3.61621200	0.79402000
H	-4.85400600	-3.97127700	1.56885200
C	3.74740600	-0.14929300	2.28502100
C	4.36376400	-0.19554900	3.53279100
N	2.43168000	0.05543300	2.11739200
C	3.56765400	-0.01445800	4.66788700
H	5.43244000	-0.36510400	3.62273800
C	1.67322900	0.23069800	3.21012500
C	2.20094500	0.20563800	4.50255700
H	4.01079200	-0.04171700	5.65821300
H	0.61889800	0.39724600	3.02602600
H	1.55034000	0.35793400	5.35693400
C	-3.37252600	-0.31482000	-2.41254800
C	-3.81592500	-0.43664600	-3.72769700
N	-2.07776700	-0.13816500	-2.08395800
C	-2.87769700	-0.36507700	-4.76058500
H	-4.86998500	-0.58016500	-3.94414600
C	-1.18561900	-0.06924400	-3.08571800
C	-1.53710900	-0.17394100	-4.43135200
H	-3.19126500	-0.45303800	-5.79578800
H	-0.15488800	0.07827000	-2.79036600
H	-0.77279900	-0.10449500	-5.19767900
H	6.49993400	1.52855500	0.14423000
H	5.90697500	-2.67917500	0.35635400
H	-5.91990600	-2.58259800	-0.53829100
H	-6.41123400	1.54742000	-0.81080900
C	-0.96309700	-3.41948900	1.91843700
H	-0.30039000	-3.69868400	2.74543600
H	-1.18165200	-4.32367200	1.33959000

H	-0.43263900	-2.71117400	1.27791800
C	-1.93664200	-1.52343400	3.28674200
H	-1.45132700	-0.77633600	2.65255200
H	-2.84486200	-1.08563800	3.71472200
H	-1.25520700	-1.76938800	4.10879900
C	-2.92180500	-3.82462000	3.42969000
H	-3.12007900	-4.77612700	2.92407400
H	-2.24475600	-4.03161900	4.26449400
H	-3.86150100	-3.44529400	3.84598600
C	0.54318800	-2.99220400	-1.59569000
H	-0.21377000	-3.19677200	-2.36112400
H	0.47011500	-3.76948500	-0.82861700
H	0.30851100	-2.03284900	-1.12468200
C	2.02067200	-1.94592400	-3.37580600
H	1.86833500	-0.92821000	-2.99686700
H	2.99956800	-1.97444100	-3.86555900
H	1.25579300	-2.16016100	-4.13089500
C	2.22415100	-4.38503300	-2.82155400
H	2.21918800	-5.15617600	-2.04355400
H	1.44453800	-4.63640700	-3.54789100
H	3.18563200	-4.42040100	-3.34467000
C	1.87245800	4.19361100	-0.71278900
H	2.62565000	4.86037400	-0.28036300
H	1.10171000	4.81192800	-1.18619700
H	1.41193800	3.62218400	0.09937500
C	1.43012700	2.34389300	-2.37714200
H	1.85518400	1.70610100	-3.16135100
H	0.98155800	1.71054400	-1.60391500
H	0.63204700	2.95055500	-2.81788900
C	3.15128800	4.09819700	-2.88259200
H	2.37200100	4.66389500	-3.40360100
H	3.86705100	4.82381500	-2.48254200
H	3.66581000	3.46992600	-3.61783600
C	-2.05126000	2.45185800	2.66573400
H	-2.79881700	1.99245100	3.32137000
H	-1.45196600	1.66311000	2.20062500
H	-1.38331600	3.06373500	3.28204400
C	-1.64682300	3.96184500	0.67435900
H	-2.10648800	4.60894400	-0.08068500
H	-0.95803800	4.56978100	1.27115800
H	-1.06862900	3.18634900	0.16348400
C	-3.50532700	4.46441500	2.29119800
H	-2.81998600	5.05091200	2.91110500
H	-3.96240400	5.14862500	1.56785200
H	-4.29113500	4.06665200	2.94285000

Table S89: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 2.277 Å

Cu	1.42476400	-0.00577400	-0.17254500
Cu	-1.48700000	-0.01941000	-0.08348200
O	0.07377700	-1.15787200	-0.21524400
O	-0.02494300	1.11160100	-0.05458500
N	4.13704400	0.90280500	0.02028200
N	2.96226500	1.21994500	-0.60900200
N	3.73572800	-1.33294200	0.72323600
N	2.73815200	-1.46801000	-0.20465400
N	-2.68656800	-1.38957700	0.95300600
N	-3.92328500	-1.55876600	0.39703900
N	-3.15569200	1.34847300	0.07203200
N	-4.34563300	0.71699900	-0.18144300
C	4.16918800	-0.00138600	1.15882300
C	3.29161700	2.11552000	-1.57171200
C	4.68193200	2.36279700	-1.52700300
C	5.18333300	1.58121700	-0.51308000
C	2.29792300	2.80091600	-2.49074500
C	2.83152300	-2.73534300	-0.68542900
C	3.88232800	-3.39889000	-0.01442200
C	4.44273600	-2.48330600	0.84523300
C	2.05623700	-3.29353000	-1.87098500
C	-4.38802900	-0.65710500	-0.64201400
C	-5.41186300	1.52251200	0.05701900
C	-4.90969000	2.73070400	0.47515400
C	-3.50229900	2.59700200	0.47351600
C	-2.51455700	3.70210600	0.79746500
C	-4.63183300	-2.53069900	1.02622700
C	-3.82513500	-3.02651600	2.02259200
C	-2.61841800	-2.29117500	1.96189100
C	-1.43345100	-2.45770000	2.89403100
H	5.21945100	-0.10320000	1.43294600
H	5.24476200	3.02645800	-2.16374300
H	4.21481900	-4.41193100	-0.17623100
H	-5.43762000	-0.89595600	-0.81237200
H	-5.47981500	3.60529200	0.74477400
H	-4.07587100	-3.80824000	2.72211400
C	3.39791300	0.56082300	2.33387700
C	4.05687900	0.94241700	3.50113000
N	2.08302300	0.72057000	2.12673400
C	3.30662700	1.54312900	4.51567700
H	5.12512600	0.78419500	3.61654400
C	1.37710600	1.31304700	3.10163900
C	1.94379500	1.74128200	4.30498000
H	3.78046200	1.85489900	5.44092300
H	0.32138000	1.44980000	2.90755700
H	1.32243800	2.21733500	5.05589500
C	-3.61791000	-0.83988500	-1.93379900
C	-4.24486000	-1.19355600	-3.12487700
N	-2.29077700	-0.64071000	-1.84785200
C	-3.46303400	-1.34126500	-4.27403400
H	-5.31837700	-1.35013000	-3.15561900
C	-1.53759000	-0.79022100	-2.94939400
C	-2.08714500	-1.13607600	-4.18258600
H	-3.92295000	-1.61362100	-5.21847700
H	-0.47651600	-0.63666100	-2.81589800
H	-1.44267000	-1.24115100	-5.04826000
H	6.18469900	1.45729500	-0.12623800
H	5.29111300	-2.54833200	1.51166800
H	-5.63870600	-2.77845600	0.72138900
H	-6.42338500	1.17305000	-0.09396700
C	-0.39703100	-3.40915800	2.25231600
H	0.42061500	-3.58517200	2.96123500
H	-0.84798900	-4.37735300	2.00887300

H	0.01363700	-2.96496000	1.34220100
C	-0.78352000	-1.09279300	3.16180000
H	-0.39819700	-0.66749400	2.23103000
H	-1.49690900	-0.39318400	3.61315400
H	0.05953400	-1.21657500	3.84985500
C	-1.91404300	-3.06102900	4.23073400
H	-2.29779200	-4.07889400	4.10467100
H	-1.06756300	-3.11679300	4.92291000
H	-2.69406500	-2.44844400	4.69594400
C	0.68417100	-3.86657900	-1.45315900
H	0.20477700	-4.31999600	-2.32857900
H	0.80186400	-4.64564100	-0.69253500
H	0.03803900	-3.08006500	-1.05444000
C	1.88994100	-2.18041800	-2.92301400
H	1.36981800	-1.32156900	-2.49129600
H	2.86209300	-1.84265100	-3.29831600
H	1.30708200	-2.55596300	-3.77117100
C	2.87823000	-4.43842200	-2.50700900
H	2.95497000	-5.30427300	-1.84086800
H	2.37081800	-4.77334000	-3.41734600
H	3.88770000	-4.11401200	-2.78178900
C	1.61767800	3.93011700	-1.68138200
H	2.35802800	4.65842400	-1.33369800
H	0.89500200	4.45551400	-2.31544400
H	1.09333900	3.52148700	-0.81359100
C	1.24292100	1.81248800	-3.01875800
H	1.71293900	0.99627800	-3.57964600
H	0.65126800	1.39822500	-2.19531200
H	0.55504000	2.33684200	-3.69078500
C	3.03961100	3.41829400	-3.69462800
H	2.31021800	3.88727500	-4.36255100
H	3.74222400	4.19868800	-3.38407800
H	3.58678900	2.66122700	-4.26713300
C	-1.49297200	3.22515300	1.84495900
H	-1.99437100	2.91852800	2.77065000
H	-0.90895100	2.38827700	1.45174100
H	-0.80104300	4.04094100	2.08277100
C	-1.79818700	4.10507100	-0.51073000
H	-2.51915600	4.45758100	-1.25642000
H	-1.09133700	4.91748700	-0.31012900
H	-1.24575500	3.25856100	-0.92812700
C	-3.26269600	4.92922200	1.35594200
H	-2.53514000	5.70933700	1.60130400
H	-3.96022700	5.35067800	0.62394600
H	-3.81578500	4.68680200	2.27024000

Table S90: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 2.145 Å

Cu	1.46607400	-0.00381400	-0.14264900
Cu	-1.53087400	-0.01660100	-0.08779900
O	0.06743700	-1.09517100	-0.19512500
O	-0.03111000	1.04650800	-0.04304900
N	4.18596200	0.89892000	0.03261800
N	3.01250500	1.21517900	-0.59910300
N	3.79359600	-1.34376900	0.72187600
N	2.77354700	-1.48282500	-0.18027300
N	-2.75020500	-1.36930100	0.93707900
N	-3.98472100	-1.52391500	0.37182900
N	-3.17612900	1.36391000	0.03984500
N	-4.36966500	0.75048600	-0.23929900
C	4.21431800	-0.01227100	1.16619700
C	3.34489000	2.10556300	-1.56449000
C	4.73605200	2.34884100	-1.52253200
C	5.23513500	1.57010000	-0.50495600
C	2.34732700	2.78829100	-2.48114700
C	2.87259500	-2.74429000	-0.67373200
C	3.94855700	-3.40099700	-0.03621400
C	4.51911600	-2.48538100	0.81647400
C	2.06872000	-3.30269400	-1.83998200
C	-4.42228000	-0.62879100	-0.68539100
C	-5.42786300	1.57246500	-0.02131900
C	-4.91569100	2.77269300	0.40840600
C	-3.51104300	2.61639600	0.43682100
C	-2.50881800	3.69904500	0.78971200
C	-4.71631500	-2.47297600	1.00974900
C	-3.92749700	-2.96808900	2.02101700
C	-2.70697300	-2.25604800	1.95979400
C	-1.52935400	-2.42784300	2.90037400
H	5.26238800	-0.10911300	1.45002400
H	5.30079600	3.00824000	-2.16208700
H	4.28788400	-4.40922500	-0.21310100
H	-5.47199000	-0.85652800	-0.86958600
H	-5.47765500	3.65591200	0.66701100
H	-4.19832300	-3.73488400	2.72948600
C	3.42838500	0.53836500	2.33734100
C	4.07198600	0.90964900	3.51626500
N	2.11523000	0.69863700	2.11679600
C	3.30863700	1.49915900	4.52762100
H	5.13904200	0.75229600	3.64287300
C	1.39662300	1.28145800	3.08843600
C	1.94821600	1.69822400	4.30257200
H	3.77102100	1.80254700	5.46140800
H	0.34394300	1.42136400	2.88106400
H	1.31749400	2.16682500	5.05034800
C	-3.63292600	-0.83629200	-1.96199200
C	-4.24209600	-1.19570300	-3.16040500
N	-2.30526100	-0.65204300	-1.85431600
C	-3.44045300	-1.36533600	-4.29295200
H	-5.31663700	-1.33998100	-3.20982900
C	-1.53277200	-0.82246900	-2.93924800
C	-2.06397300	-1.17558400	-4.17848600
H	-3.88603700	-1.64272600	-5.24279100
H	-0.47264100	-0.68053500	-2.78515900
H	-1.40537100	-1.29814000	-5.03112800
H	6.23634700	1.44381500	-0.11846100
H	5.38321500	-2.54556200	1.46284500
H	-5.72456200	-2.70786800	0.69933200
H	-6.44148500	1.23899000	-0.19301800
C	-0.48769600	-3.37584100	2.26219000
H	0.32146900	-3.55946500	2.97878200
H	-0.93739800	-4.34101600	2.00497800

H	-0.06409500	-2.92525200	1.36104600
C	-0.88058200	-1.06340900	3.17716300
H	-0.49084200	-0.63516200	2.24948400
H	-1.59573000	-0.36467800	3.62690100
H	-0.04072300	-1.19002600	3.86864300
C	-2.01955400	-3.03669800	4.23072400
H	-2.40369900	-4.05349000	4.09684800
H	-1.17804300	-3.09671600	4.92850300
H	-2.80195300	-2.42531800	4.69355900
C	0.69225700	-3.84103700	-1.39281500
H	0.18788200	-4.29446800	-2.25411600
H	0.80565500	-4.61300500	-0.62437200
H	0.06867000	-3.03623000	-0.99419400
C	1.90670900	-2.19764900	-2.90181700
H	1.40498300	-1.32555700	-2.47413000
H	2.87937400	-1.87851600	-3.29169900
H	1.30897400	-2.57318900	-3.73969800
C	2.85624300	-4.47118100	-2.47505000
H	2.93186500	-5.32768500	-1.79674800
H	2.32435100	-4.81102500	-3.36943200
H	3.86525200	-4.16919800	-2.77591700
C	1.65803700	3.90866600	-1.66744100
H	2.39244400	4.64098200	-1.31558000
H	0.93142200	4.43153100	-2.29908800
H	1.13619300	3.49282600	-0.80134300
C	1.29994600	1.79272100	-3.01190300
H	1.77607000	0.98703400	-3.58252900
H	0.71827400	1.36225900	-2.18975500
H	0.60192500	2.31501100	-3.67506200
C	3.08431800	3.41582100	-3.68219200
H	2.35231200	3.88421000	-4.34771700
H	3.78319600	4.19808300	-3.36777900
H	3.63532200	2.66448800	-4.25857500
C	-1.52087900	3.19105200	1.85533000
H	-2.04769400	2.89704900	2.77080200
H	-0.95410300	2.33778000	1.47241700
H	-0.81055600	3.98647200	2.10716500
C	-1.75488400	4.09682300	-0.49867500
H	-2.45103000	4.47198000	-1.25676800
H	-1.03476200	4.89130800	-0.27475600
H	-1.21196400	3.24216800	-0.91197900
C	-3.24349300	4.93679500	1.34192200
H	-2.50584100	5.69987000	1.60980200
H	-3.91594100	5.37805000	0.59822100
H	-3.82170500	4.69856200	2.24164200

Table S91: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 2.013 Å

Cu	1.57547300	0.08771900	-0.10606400
Cu	-1.52398700	0.12207000	-0.11042900
O	0.02067100	-0.81376300	0.00101600
O	0.14386600	1.19323600	-0.09530600
N	4.31875200	0.66925800	0.41414500
N	3.17648100	1.28441400	-0.03609100
N	3.90138000	-1.60790600	-0.14244200
N	2.75342700	-1.35972900	-0.83544300
N	-2.77528300	-1.59181500	0.01345300
N	-3.89921500	-1.42501100	-0.75064000
N	-3.14917400	1.12426500	0.68767100
N	-4.32201300	0.78270400	0.06577900
C	4.32591300	-0.70065000	0.91542300
C	3.54798400	2.54891500	-0.36082900
C	4.92143800	2.72165300	-0.08910900
C	5.37538500	1.51809300	0.39669000
C	2.61606600	3.59396400	-0.94397500
C	2.75109500	-2.22189900	-1.87969000
C	3.90713000	-3.03239500	-1.81300700
C	4.61973400	-2.60580900	-0.71571700
C	1.69971900	-2.24690900	-2.97837400
C	-4.31952100	-0.07717300	-1.11063500
C	-5.38796800	1.38864300	0.65146300
C	-4.89799500	2.15013700	1.68616500
C	-3.49455600	1.96980900	1.68299600
C	-2.49402700	2.66215700	2.58841500
C	-4.68015300	-2.53931200	-0.74302000
C	-4.03266600	-3.47313600	0.02774400
C	-2.85782300	-2.84714900	0.51306700
C	-1.90653100	-3.43610700	1.54521600
H	5.36978000	-0.93977300	1.11875800
H	5.50576700	3.61441400	-0.24404700
H	4.19459300	-3.81252200	-2.49983900
H	-5.35455100	-0.15411700	-1.44267400
H	-5.47495500	2.75951200	2.36383100
H	-4.37091000	-4.47516300	0.23928400
C	3.51798300	-0.84032600	2.19032200
C	4.11122700	-1.24052000	3.38561300
N	2.22093600	-0.52215200	2.07137300
C	3.30961600	-1.30719700	4.52894600
H	5.16724400	-1.48971600	3.42898400
C	1.46179800	-0.58336700	3.17472000
C	1.96225300	-0.96741500	4.42095900
H	3.73327500	-1.61216300	5.48044200
H	0.42254900	-0.31066800	3.04809600
H	1.30569200	-0.99426200	5.28400500
C	-3.48860400	0.54773200	-2.21365600
C	-4.04120800	0.92422500	-3.43354200
N	-2.20095400	0.78395200	-1.90243100
C	-3.22831500	1.58559600	-4.35945700
H	-5.08357500	0.71669600	-3.65366700
C	-1.42652500	1.44456400	-2.77708400
C	-1.90506800	1.86161700	-4.01865200
H	-3.63043300	1.89254900	-5.31960300
H	-0.41942500	1.64659900	-2.43828900
H	-1.24818100	2.39526100	-4.69656400
H	6.35294800	1.19765500	0.72765300
H	5.56755600	-2.92218300	-0.30423500
H	-5.61864200	-2.57099900	-1.27834500
H	-6.39307400	1.22700100	0.28862900
C	-0.56186100	-3.85864300	0.91686000
H	0.05326200	-4.34545900	1.68266200
H	-0.71631700	-4.57494500	0.10287900

H	-0.01848900	-2.99290700	0.53080500
C	-1.67000900	-2.38741500	2.65044900
H	-1.23369200	-1.47779900	2.22920000
H	-2.60749000	-2.12496200	3.15304000
H	-0.97894700	-2.78985500	3.39937600
C	-2.55836000	-4.68232500	2.18146400
H	-2.68317100	-5.49227900	1.45451500
H	-1.90808800	-5.05636800	2.97866400
H	-3.53421800	-4.45254000	2.62312900
C	0.46141200	-3.05412900	-2.52961200
H	-0.24670000	-3.12276300	-3.36369000
H	0.73790600	-4.07225000	-2.23616100
H	-0.03536000	-2.56853200	-1.68585100
C	1.27633200	-0.81082900	-3.33623100
H	0.80213200	-0.32168500	-2.47906600
H	2.13173300	-0.20682300	-3.65780300
H	0.54654600	-0.83759400	-4.15281500
C	2.29954400	-2.91422900	-4.23490500
H	2.53474800	-3.96947200	-4.06075000
H	1.56656600	-2.87401700	-5.04706600
H	3.20803100	-2.40320200	-4.57138000
C	1.55568200	3.98643700	0.10861400
H	2.03322100	4.40212600	1.00283100
H	0.89425100	4.75398200	-0.30952200
H	0.95078500	3.12187800	0.39911200
C	1.94997500	3.01837000	-2.20925600
H	2.69424200	2.80554900	-2.98462200
H	1.42284000	2.09264000	-1.96397600
H	1.22980900	3.74002500	-2.61130800
C	3.41788700	4.85183500	-1.33368500
H	2.73835600	5.58438600	-1.78044700
H	3.88161100	5.32364800	-0.46060200
H	4.19799100	4.62695100	-2.06951100
C	-1.32658500	1.72326500	2.93525200
H	-1.69086500	0.82490100	3.44809100
H	-0.77120200	1.43483800	2.03615800
H	-0.62984000	2.24030100	3.60420700
C	-1.96166400	3.91190000	1.84474300
H	-2.77706500	4.60154800	1.60212100
H	-1.24586700	4.44270000	2.48225300
H	-1.45545300	3.63078900	0.91608500
C	-3.18893300	3.10595900	3.89205100
H	-2.45174300	3.57525900	4.55132700
H	-3.97500400	3.84515900	3.70563000
H	-3.62873200	2.25551600	4.42467800

Table S92: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 1.881 Å

Cu	1.57400000	0.14458500	0.09052700
Cu	-1.61565800	0.09263900	0.10810200
O	-0.01666900	-0.71399600	-0.05600300
O	-0.16977800	1.15999700	0.00578000
N	4.35263800	0.79215400	-0.02445200
N	3.18903300	1.13167700	-0.66248100
N	3.91692500	-1.42778000	0.75070100
N	2.79977500	-1.58740100	-0.02575100
N	-2.77912300	-1.35971000	0.84786000
N	-3.93570300	-1.60618100	0.16775000
N	-3.21988700	1.28217100	0.03038800
N	-4.36223100	0.66377500	-0.41162900
C	4.33117300	-0.08532500	1.13960000
C	3.54320900	1.97714100	-1.65427900
C	4.94590000	2.15995600	-1.63914700
C	5.42457600	1.39864900	-0.59809800
C	2.54593300	2.66106400	-2.56949600
C	2.88679800	-2.83780000	-0.53476400
C	4.05688900	-3.46921800	-0.04537500
C	4.69738800	-2.54257700	0.74024800
C	1.93772000	-3.41392900	-1.57590800
C	-4.36435900	-0.71108100	-0.89958400
C	-5.41909300	1.51288200	-0.39759700
C	-4.96306300	2.72063400	0.07705200
C	-3.58861600	2.54888100	0.34488300
C	-2.64479800	3.59553700	0.90495600
C	-4.65325100	-2.59656600	0.75469200
C	-3.93217600	-3.02037500	1.84786100
C	-2.77135400	-2.21620300	1.89644300
C	-1.70176500	-2.23997800	2.97684300
H	5.36120000	-0.16858000	1.48543700
H	5.53023500	2.77106300	-2.30896300
H	4.39653400	-4.46958900	-0.26254300
H	-5.40721500	-0.95689900	-1.10008800
H	-5.54663000	3.61490800	0.22664900
H	-4.21633900	-3.79543900	2.54182200
C	3.48589800	0.52616100	2.24152900
C	4.02203100	0.87146300	3.47803000
N	2.20592000	0.78236700	1.91355000
C	3.20042800	1.52247100	4.40376700
H	5.05820600	0.64846700	3.71199300
C	1.42446300	1.43204100	2.78969500
C	1.88561800	1.81928100	4.04750700
H	3.58979700	1.80587800	5.37631900
H	0.42359500	1.65118500	2.44191000
H	1.22339500	2.34609700	4.72558700
C	-3.55437400	-0.86169100	-2.17297400
C	-4.14379400	-1.27055800	-3.36722000
N	-2.25732800	-0.54558700	-2.05239300
C	-3.33669300	-1.34808000	-4.50619300
H	-5.20001900	-1.51833100	-3.41368300
C	-1.49234800	-0.61779100	-3.15061900
C	-1.98858500	-1.01110500	-4.39571700
H	-3.75688400	-1.65987600	-5.45702900
H	-0.45261100	-0.34694500	-3.01925800
H	-1.32914000	-1.04738400	-5.25624200
H	6.42546900	1.23894000	-0.22307300
H	5.63006200	-2.58042500	1.28527100
H	-5.60630400	-2.91125500	0.35414700
H	-6.39784200	1.19011700	-0.72273300
C	-0.45032800	-3.00015800	2.48518900
H	0.27906000	-3.06331800	3.30124700
H	-0.70342500	-4.02025700	2.17803500

H	0.01352500	-2.48490300	1.63996200
C	-1.31282600	-0.79993300	3.35922800
H	-0.87085200	-0.27844100	2.50358600
H	-2.17899100	-0.22800100	3.70913700
H	-0.56641900	-0.82207000	4.16077300
C	-2.25846300	-2.95350500	4.22683300
H	-2.47379800	-4.00881300	4.02857300
H	-1.50937900	-2.91793900	5.02436000
H	-3.17067200	-2.47298700	4.59672400
C	0.57222400	-3.78893500	-0.96330800
H	-0.04801900	-4.26246100	-1.73332800
H	0.69337900	-4.50277200	-0.14163200
H	0.05039200	-2.90344200	-0.59209400
C	1.74665100	-2.37157400	-2.69678300
H	1.32253600	-1.44692100	-2.29530400
H	2.69929500	-2.13511000	-3.18333400
H	1.06216600	-2.76705400	-3.45540900
C	2.56429500	-4.68503500	-2.18672100
H	2.66325100	-5.48595300	-1.44584100
H	1.91307900	-5.05594200	-2.98460100
H	3.54936000	-4.48556600	-2.62270600
C	1.97676200	3.89247900	-1.82253400
H	2.77484400	4.59352000	-1.55609300
H	1.26426800	4.41766300	-2.46825200
H	1.45686100	3.59190700	-0.90743100
C	1.40227400	1.70288800	-2.94502800
H	1.78965400	0.81776100	-3.46323500
H	0.83872300	1.39249100	-2.05792300
H	0.70436100	2.21483200	-3.61658300
C	3.25484000	3.13119400	-3.85597400
H	2.52130800	3.59602200	-4.52238300
H	4.02525800	3.88087900	-3.64709300
H	3.71737000	2.29430300	-4.39076400
C	-1.93881800	3.02093900	2.14848600
H	-2.65825600	2.79963300	2.94456900
H	-1.41161500	2.10015300	1.88374900
H	-1.21148700	3.74575000	2.53150500
C	-1.61450200	3.98820000	-0.17783200
H	-2.11749300	4.40084600	-1.05933500
H	-0.94281900	4.75781900	0.21966000
H	-1.01663600	3.12414900	-0.48394700
C	-3.43891000	4.85074800	1.31730400
H	-2.75094800	5.58421800	1.74946300
H	-3.92452800	5.32351600	0.45674500
H	-4.20103300	4.62152100	2.07044400

Table S93: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 1.749 Å

Cu	-1.69161300	0.06786400	0.05908000
Cu	1.68843500	0.05474700	0.01836400
O	-0.00233700	-0.64124700	0.66296900
O	-0.00186700	1.07199500	0.30296100
N	-4.36186700	0.92569200	-0.48077100
N	-3.23761600	1.35706900	0.16664200
N	-4.09634000	-1.43499100	-0.28781000
N	-2.98245600	-1.42429800	0.50531900
N	2.89357500	-1.51956700	-0.43943700
N	4.06162000	-1.51915800	0.27286100
N	3.24788400	1.26562000	-0.38331100
N	4.42742900	0.83034400	0.15890500
C	-4.35780300	-0.33547900	-1.20755100
C	-3.58751900	2.50984600	0.78259900
C	-4.94353100	2.79770000	0.50887300
C	-5.40455300	1.77250000	-0.28551000
C	-2.62693700	3.34126000	1.61126100
C	-3.13803100	-2.45497600	1.37094700
C	-4.35440800	-3.12015100	1.09495900
C	-4.94190400	-2.44035600	0.05315300
C	-2.16392700	-2.79167700	2.48797400
C	4.47493500	-0.33868300	1.02642500
C	5.46416600	1.62516400	-0.20888600
C	4.94864300	2.61322300	-1.01574200
C	3.56222100	2.36185700	-1.11076800
C	2.53669300	3.20916200	-1.83817400
C	4.80904400	-2.61850100	0.00486100
C	4.10377800	-3.37178900	-0.90617000
C	2.92194900	-2.65113100	-1.18311500
C	1.89001100	-2.98544800	-2.24634200
H	-5.37457800	-0.48101800	-1.57207700
H	-5.51122300	3.64621500	0.85672900
H	-4.75624900	-3.97933900	1.60814300
H	5.52549200	-0.49216800	1.27271200
H	5.49957100	3.41320700	-1.48472400
H	4.40873900	-4.31358600	-1.33431900
C	-3.40691000	-0.30486500	-2.39151400
C	-3.88627000	-0.41915800	-3.69456500
N	-2.10520200	-0.13530600	-2.09547400
C	-2.97330600	-0.34681400	-4.75015900
H	-4.94617800	-0.55700700	-3.88484300
C	-1.23787100	-0.06306600	-3.11734800
C	-1.62402100	-0.16110100	-4.45443700
H	-3.31298800	-0.42944000	-5.77755200
H	-0.20057200	0.08157800	-2.84461600
H	-0.87985700	-0.09042000	-5.24028400
C	3.68262200	-0.13079900	2.30452200
C	4.28647900	-0.16875500	3.55852100
N	2.37645700	0.10954900	2.11970200
C	3.48457300	0.06236800	4.68062200
H	5.34847900	-0.36902500	3.66329200
C	1.61233500	0.33234000	3.19839000
C	2.12676600	0.32079800	4.49661400
H	3.91682800	0.04416000	5.67596700
H	0.56606000	0.52575100	2.99643100
H	1.47374000	0.51303600	5.34106900
H	-6.37291400	1.58023900	-0.72503100
H	-5.87815900	-2.58640100	-0.46646100
H	5.76927100	-2.77157500	0.47654400
H	6.46990500	1.42548000	0.13229000
C	0.47093700	-3.04603300	-1.65130200
H	-0.25516500	-3.23413200	-2.45034700
H	0.39218000	-3.85933900	-0.92291600

H	0.19888600	-2.11487500	-1.14598100
C	1.97845600	-1.89903300	-3.34378300
H	1.80260600	-0.89916300	-2.93005800
H	2.96904400	-1.89494600	-3.81054800
H	1.23456300	-2.09416600	-4.12449300
C	2.21436300	-4.35232000	-2.88072800
H	2.19423800	-5.15610000	-2.13662600
H	1.46315000	-4.58421600	-3.64252000
H	3.19364900	-4.35151900	-3.37115400
C	-0.86151400	-3.38127300	1.90529700
H	-0.18919500	-3.66261500	2.72372700
H	-1.06836100	-4.27777100	1.31049300
H	-0.34442400	-2.65148200	1.27391000
C	-1.85796300	-1.51992800	3.30586400
H	-1.38903700	-0.75715700	2.67856600
H	-2.77139600	-1.10456100	3.74500000
H	-1.16736400	-1.76516600	4.12040900
C	-2.79917300	-3.84052500	3.42434100
H	-2.98647200	-4.78800500	2.90718800
H	-2.11022800	-4.04731600	4.24931700
H	-3.74060200	-3.48279800	3.85556600
C	-1.57376100	3.96877300	0.67131100
H	-2.04931000	4.61051400	-0.07846200
H	-0.87712500	4.58176600	1.25365700
H	-1.00065200	3.19257000	0.15432700
C	-1.93630200	2.45334900	2.66658300
H	-2.66989000	1.99437100	3.33820800
H	-1.34952300	1.66591400	2.18414200
H	-1.25344600	3.06327900	3.26837700
C	-3.39664600	4.46775000	2.32781000
H	-2.69812600	5.04968400	2.93716900
H	-3.86448800	5.15662800	1.61589300
H	-4.17160100	4.06966000	2.99213100
C	1.46587000	2.31604000	-2.48573900
H	1.90767100	1.66947000	-3.25323000
H	0.97817400	1.69415500	-1.72770700
H	0.69583500	2.93621600	-2.95682500
C	1.88413000	4.15885100	-0.80474600
H	2.63346400	4.81797000	-0.35405500
H	1.13332200	4.78484800	-1.29967900
H	1.39587800	3.59445100	-0.00444000
C	3.22475100	4.04722700	-2.93408400
H	2.46785600	4.62034200	-3.47921400
H	3.93452200	4.76561500	-2.51097900
H	3.75517400	3.41370900	-3.65340000

Table S94: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 1.618 Å

Cu	-1.66475600	-0.13212000	0.18003700
Cu	1.73568600	0.24111700	-0.20175300
O	-0.06080000	0.95282400	0.39807700
O	-0.04814800	0.00202900	-0.91271300
N	-4.06137800	-1.67442900	0.18222400
N	-2.82849100	-1.65011900	-0.41254900
N	-4.60439700	0.65632600	0.09343300
N	-3.45581000	1.20557400	-0.39888700
N	3.27728900	1.41403400	0.34239800
N	4.49511000	0.94271400	-0.06577600
N	2.97714900	-1.44954600	0.56895800
N	4.19343400	-1.43059900	-0.06285100
C	-4.54394100	-0.52315300	0.93683300
C	-2.81320700	-2.70214500	-1.26624700
C	-4.04464100	-3.38969300	-1.19184200
C	-4.81544300	-2.70256200	-0.28368300
C	-1.65505900	-3.02950800	-2.19244500
C	-3.85718300	2.27066800	-1.12015700
C	-5.26948200	2.38645600	-1.07950400
C	-5.71298100	1.34328200	-0.30099200
C	-2.87910000	3.20036900	-1.81570500
C	4.59738900	-0.27876400	-0.85384300
C	4.99521800	-2.45229900	0.34888700
C	4.27486100	-3.17886800	1.26316600
C	3.02839400	-2.51609600	1.39055000
C	1.93459700	-2.90414000	2.36383000
C	5.50534900	1.74017000	0.36466100
C	4.92985700	2.76917800	1.07517900
C	3.53671400	2.53956700	1.04738500
C	2.45400700	3.39580100	1.67602700
H	-5.56970600	-0.75965400	1.21939800
H	-4.32935900	-4.27614400	-1.73581800
H	-5.88079400	3.13479200	-1.55927900
H	5.65676600	-0.41442500	-1.07110200
H	4.60346000	-4.06492800	1.78509000
H	5.44489200	3.58808800	1.55193900
C	-3.73879500	-0.25767200	2.19434100
C	-4.35284200	-0.18799600	3.44171700
N	-2.42241900	-0.02459100	2.02075800
C	-3.57939800	0.14955700	4.55495800
H	-5.41544500	-0.38474000	3.54179400
C	-1.68406600	0.32134600	3.09226800
C	-2.22357900	0.41865900	4.37277400
H	-4.03156400	0.21051800	5.53956900
H	-0.64061800	0.52739300	2.89495300
H	-1.58786100	0.70117500	5.20456800
C	3.84011600	-0.14813700	-2.16188500
C	4.47572000	-0.26051000	-3.39467500
N	2.52491900	0.11311000	-2.04660400
C	3.71716000	-0.08528200	-4.55578500
H	5.53826200	-0.47491400	-3.45000400
C	1.79521300	0.28836400	-3.16349000
C	2.35751800	0.19953100	-4.43594200
H	4.18460900	-0.16283000	-5.53213600
H	0.74581300	0.50681000	-3.00541700
H	1.73562600	0.35589300	-5.31038800
H	-5.82461300	-2.85995000	0.06939200
H	-6.70456000	1.03733300	0.00152900
H	6.53570700	1.51440600	0.12970600
H	5.99567600	-2.57384000	-0.04203000
C	1.51846100	3.92825200	0.56863400
H	0.75262400	4.57270200	1.01394500
H	2.07801600	4.52072100	-0.16317700

H	1.01254900	3.10878200	0.05007500
C	1.65696500	2.54800500	2.69067300
H	1.20188600	1.68521800	2.19286600
H	2.30396600	2.18742900	3.49813000
H	0.85808500	3.15419400	3.13197100
C	3.09273200	4.58859900	2.41330200
H	3.65079700	5.23472900	1.72687500
H	2.30415700	5.19457600	2.87016200
H	3.76674000	4.26020100	3.21236900
C	-2.10205300	3.99610700	-0.74145500
H	-1.40629300	4.69008700	-1.22688800
H	-2.78545300	4.58176000	-0.11689300
H	-1.52783200	3.32400500	-0.09669300
C	-1.89294500	2.38568100	-2.67709200
H	-1.31410500	1.69079400	-2.06155800
H	-2.42366800	1.81533200	-3.44814800
H	-1.19490300	3.06798200	-3.17625900
C	-3.64379200	4.18561900	-2.72007000
H	-4.31802900	4.82740900	-2.14217800
H	-2.92989600	4.83801600	-3.23326200
H	-4.23018100	3.66183200	-3.48339200
C	-0.36407800	-3.23897800	-1.37854300
H	-0.47358200	-4.08692800	-0.69442200
H	0.47147500	-3.45121900	-2.05507400
H	-0.11674700	-2.34611900	-0.79831800
C	-1.48129600	-1.87209300	-3.20247000
H	-2.38406000	-1.74562000	-3.80949100
H	-1.27461100	-0.92574500	-2.69352200
H	-0.64667500	-2.09776500	-3.87622800
C	-1.96062400	-4.32275000	-2.97416800
H	-1.11769200	-4.55115200	-3.63414400
H	-2.10105400	-5.17805900	-2.30407600
H	-2.85235900	-4.21744000	-3.60146000
C	0.76951700	-1.91020400	2.31781400
H	1.11156100	-0.90434100	2.58705900
H	0.31034500	-1.86957200	1.32409900
H	-0.00021700	-2.21489900	3.03505900
C	1.43466200	-4.32960800	2.03725100
H	2.24700900	-5.06060600	2.10282500
H	0.66129500	-4.62427100	2.75527100
H	1.01107700	-4.38252800	1.02986200
C	2.53517800	-2.89620700	3.79161000
H	1.76352900	-3.17831700	4.51656300
H	3.35826600	-3.61131500	3.88635400
H	2.91373900	-1.90319600	4.05785800

Table S95: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 1.488 Å

Cu	-1.91212200	0.11389000	-0.13829100
Cu	1.99363900	0.16363100	0.00121100
O	0.16424500	0.19273900	-0.23340400
O	-0.54030700	0.81365000	0.92245100
N	-4.70726600	0.74347100	-0.29957300
N	-3.54489400	1.34996700	0.09032900
N	-4.29200500	-1.58883100	0.08898900
N	-3.06274300	-1.52416800	0.68077700
N	3.10540100	-1.48605200	-0.63945800
N	4.27770400	-1.58126800	0.05713600
N	3.59523200	1.30031800	-0.18411500
N	4.73047500	0.74962100	0.33258700
C	-4.68649000	-0.58807800	-0.88935600
C	-3.91025900	2.55442000	0.58237400
C	-5.31538800	2.69586200	0.49848400
C	-5.78826000	1.53169400	-0.06192500
C	-2.92329300	3.57161800	1.12663700
C	-3.07265300	-2.48409700	1.62738500
C	-4.31693900	-3.15808600	1.62437300
C	-5.07166800	-2.55587500	0.64421700
C	-1.90527800	-2.71059500	2.56887300
C	4.65273300	-0.54041900	1.00696700
C	5.80718500	1.54912500	0.11666000
C	5.35138500	2.66045400	-0.55976400
C	3.96104000	2.47635700	-0.73456700
C	2.95689300	3.42314000	-1.36216900
C	5.03636600	-2.62201700	-0.37815100
C	4.32770300	-3.23814900	-1.38517400
C	3.13292200	-2.49727100	-1.53180100
C	2.02422800	-2.71787500	-2.54456800
H	-5.71561500	-0.81781500	-1.16492400
H	-5.90406900	3.54747600	0.80098300
H	-4.62030700	-3.97932800	2.25466100
H	5.66173900	-0.77893500	1.34239700
H	5.94480600	3.49904300	-0.88919500
H	4.63450500	-4.10635600	-1.94717800
C	-3.82426300	-0.61648900	-2.14014300
C	-4.36332300	-0.89396400	-3.39304300
N	-2.51965900	-0.32255000	-1.96463200
C	-3.52367700	-0.85682500	-4.50935600
H	-5.41761300	-1.12892000	-3.49795600
C	-1.71325900	-0.28115100	-3.04185400
C	-2.17750800	-0.53931200	-4.32943200
H	-3.91790000	-1.06497200	-5.49874200
H	-0.67830700	-0.02877900	-2.84668200
H	-1.49434800	-0.48656100	-5.16990200
C	3.72878000	-0.46657200	2.21534000
C	4.19855400	-0.71872200	3.50045700
N	2.45167500	-0.11009500	1.96655000
C	3.31142100	-0.58807800	4.57388300
H	5.23245200	-1.00538400	3.66533300
C	1.60008500	0.01561200	2.99832300
C	1.99460000	-0.21077900	4.31767500
H	3.65007900	-0.77184100	5.58848000
H	0.59120300	0.30885800	2.72650800
H	1.27827100	-0.08686400	5.12239000
H	-6.78759700	1.20543600	-0.31261300
H	-6.07884900	-2.73616400	0.29600700
H	5.99992000	-2.83794300	0.06116800
H	6.79319000	1.26744100	0.45736400
C	0.69183200	-2.98678200	-1.81426800
H	-0.10682300	-3.14956900	-2.54738500
H	0.76472500	-3.88344700	-1.18992000

H	0.40912100	-2.14548500	-1.17326500
C	1.90255100	-1.45960600	-3.43266400
H	1.64591200	-0.57580100	-2.83626800
H	2.84183700	-1.25233300	-3.95601100
H	1.12170000	-1.61070400	-4.18709400
C	2.36207600	-3.92802300	-3.43604900
H	2.45623400	-4.84693300	-2.84710900
H	1.55923500	-4.08110900	-4.16452600
H	3.29215300	-3.77285400	-3.99369200
C	-0.58493000	-2.73237300	1.77698100
H	0.25745900	-2.87841700	2.46287000
H	-0.57866100	-3.55278400	1.05166200
H	-0.43188100	-1.79208300	1.23920800
C	-1.88538000	-1.56027100	3.60389700
H	-1.75377400	-0.59081000	3.11161400
H	-2.81810100	-1.53006200	4.17685800
H	-1.06047300	-1.71248800	4.31021600
C	-2.07593700	-4.05094300	3.30929400
H	-2.14090600	-4.89206800	2.61028200
H	-1.21237100	-4.22018500	3.96093400
H	-2.96978600	-4.05387200	3.94246600
C	-1.79149600	3.80312700	0.10344800
H	-2.19358600	4.16488800	-0.84970200
H	-1.10046100	4.56000600	0.49067800
H	-1.22526100	2.88410500	-0.06980100
C	-2.34099100	3.06356700	2.46624300
H	-3.13616200	2.89380800	3.20025900
H	-1.78445300	2.13155100	2.33043400
H	-1.65547400	3.81451500	2.87478400
C	-3.64761700	4.90905300	1.38013100
H	-2.92433000	5.64664300	1.74208600
H	-4.10012800	5.30456000	0.46391000
H	-4.42804400	4.81155500	2.14298700
C	1.94474200	2.63046100	-2.21027900
H	2.44038400	2.11284700	-3.03913500
H	1.42189000	1.88799600	-1.59541900
H	1.19159900	3.30858400	-2.62488200
C	2.21522200	4.17015200	-0.22606900
H	2.91802800	4.72612100	0.40312800
H	1.50635200	4.88479500	-0.65816000
H	1.65621200	3.47465100	0.41035000
C	3.68495800	4.44579900	-2.25538600
H	2.94989300	5.10391300	-2.72953500
H	4.36424300	5.07917300	-1.67479600
H	4.25923200	3.95224100	-3.04704700

Table S96: XYZ coordinates for optimised structure: Triplet minimum path, O...O = 1.359 Å

Cu	1.95302800	0.08315900	0.13685400
Cu	-2.02366300	0.13949700	-0.00658900
O	-0.17416100	0.23585100	0.14254400
O	0.53264100	0.69967500	-0.92208300
N	4.72520000	0.79141900	0.28531900
N	3.55449900	1.37194200	-0.11867400
N	4.33875600	-1.55272800	-0.06802300
N	3.10442900	-1.51918100	-0.65337900
N	-3.12064500	-1.48443800	0.64848500
N	-4.30311600	-1.57833600	-0.03080200
N	-3.61680900	1.30244000	0.18965200
N	-4.75474800	0.75224500	-0.32210600
C	4.72188100	-0.53132000	0.89496400
C	3.90313900	2.57167100	-0.63187500
C	5.30567900	2.73799000	-0.54716300
C	5.79514600	1.59177700	0.03580800
C	2.89846000	3.55676600	-1.20168400
C	3.12623800	-2.48972500	-1.58948300
C	4.38340000	-3.13850800	-1.58660100
C	5.13258600	-2.51067700	-0.61825300
C	1.95653900	-2.75272200	-2.51889800
C	-4.68440400	-0.54370300	-0.98596200
C	-5.83126900	1.55280800	-0.10560600
C	-5.37268100	2.66585800	0.56577300
C	-3.98192500	2.47922900	0.73704000
C	-2.97364100	3.42570800	1.35896400
C	-5.06636900	-2.60374300	0.43193200
C	-4.35014200	-3.21160300	1.43880500
C	-3.14620800	-2.48095200	1.55705300
C	-2.02581800	-2.69415400	2.55841100
H	5.75447300	-0.74444200	1.17084100
H	5.88190900	3.59297800	-0.86414900
H	4.69861600	-3.96126900	-2.20900400
H	-5.69773800	-0.78343400	-1.30734700
H	-5.96455100	3.50599600	0.89416900
H	-4.65742100	-4.06822900	2.01805900
C	3.86458700	-0.55476200	2.14994300
C	4.41548100	-0.79839200	3.40471900
N	2.55259700	-0.29173500	1.97559600
C	3.58083500	-0.76077900	4.52470100
H	5.47516200	-1.00838900	3.50837400
C	1.75117300	-0.25044000	3.05716500
C	2.22703400	-0.47655300	4.34641000
H	3.98437500	-0.94360800	5.51532600
H	0.70934700	-0.02525000	2.86503500
H	1.54651100	-0.42575700	5.18913300
C	-3.77640000	-0.48796500	-2.20770800
C	-4.27198000	-0.74602400	-3.48245300
N	-2.49141500	-0.14501600	-1.98125200
C	-3.40286100	-0.63817400	-4.57245400
H	-5.31221600	-1.02087200	-3.62654200
C	-1.65922000	-0.04062000	-3.03145100
C	-2.07703900	-0.27544800	-4.34190800
H	-3.76104400	-0.82804500	-5.57916200
H	-0.64132400	0.24410800	-2.78757300
H	-1.37251900	-0.16928700	-5.15956500
H	6.79880900	1.28598900	0.29497400
H	6.14525600	-2.66786200	-0.27488200
H	-6.03815200	-2.81627400	0.00950700
H	-6.81842700	1.27063100	-0.44257900
C	-0.70107200	-2.96108100	1.81453500
H	0.10765600	-3.11614500	2.53826100
H	-0.77675600	-3.86005900	1.19402500

H	-0.43161400	-2.12046400	1.16681100
C	-1.89640100	-1.43034400	3.43771300
H	-1.64693600	-0.55047000	2.83218300
H	-2.83051500	-1.21994800	3.96891900
H	-1.10788000	-1.57593900	4.18536700
C	-2.34942100	-3.90068800	3.45971500
H	-2.45152500	-4.82200400	2.87588200
H	-1.53627300	-4.05004200	4.17750500
H	-3.27157800	-3.74390500	4.02987800
C	0.64419500	-2.79956800	-1.71498600
H	-0.20237000	-2.96005200	-2.39219900
H	0.66005100	-3.61930200	-0.98913200
H	0.47904100	-1.86257800	-1.17546000
C	1.89883800	-1.61498000	-3.56639800
H	1.74636100	-0.64290700	-3.08552800
H	2.82545200	-1.56795200	-4.14797600
H	1.07184300	-1.79684000	-4.26297200
C	2.15279300	-4.09611300	-3.24753200
H	2.24288400	-4.92859500	-2.54106400
H	1.28810200	-4.29159300	-3.89020300
H	3.04124900	-4.08424100	-3.88810400
C	1.75037200	3.77567400	-0.19447800
H	2.13118600	4.17087100	0.75405200
H	1.03814800	4.50002700	-0.60445400
H	1.21249200	2.84344600	-0.00170400
C	2.34243500	3.01138600	-2.53795700
H	3.14881000	2.85203700	-3.26188800
H	1.81177500	2.06627300	-2.39177700
H	1.64020700	3.73600200	-2.96529000
C	3.59198800	4.90731700	-1.46924700
H	2.85506900	5.62202000	-1.84916200
H	4.02672500	5.32719200	-0.55530600
H	4.38151600	4.81645800	-2.22342400
C	-1.95524300	2.63081600	2.19735200
H	-2.44335200	2.11998500	3.03478400
H	-1.45086900	1.88019300	1.57701200
H	-1.19094000	3.30472300	2.59833600
C	-2.24022800	4.17368400	0.21843600
H	-2.94724900	4.73186000	-0.40403000
H	-1.52548800	4.88621700	0.64460500
H	-1.68986500	3.47705100	-0.42442800
C	-3.69401300	4.44747900	2.25916800
H	-2.95545100	5.10495000	2.72895100
H	-4.37769200	5.08162800	1.68459800
H	-4.26275700	3.95286600	3.05414600