Supplementary Information for

Unusual Singlet Oxygen-dependent Hydroxyl Radical Production by a Unique Ruthenium-Polypyridyl-Hydroxamate Complex under Visible Light Irradiation

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This PDF file includes:

Figures S1 to S10

Table S1

Supporting Figures

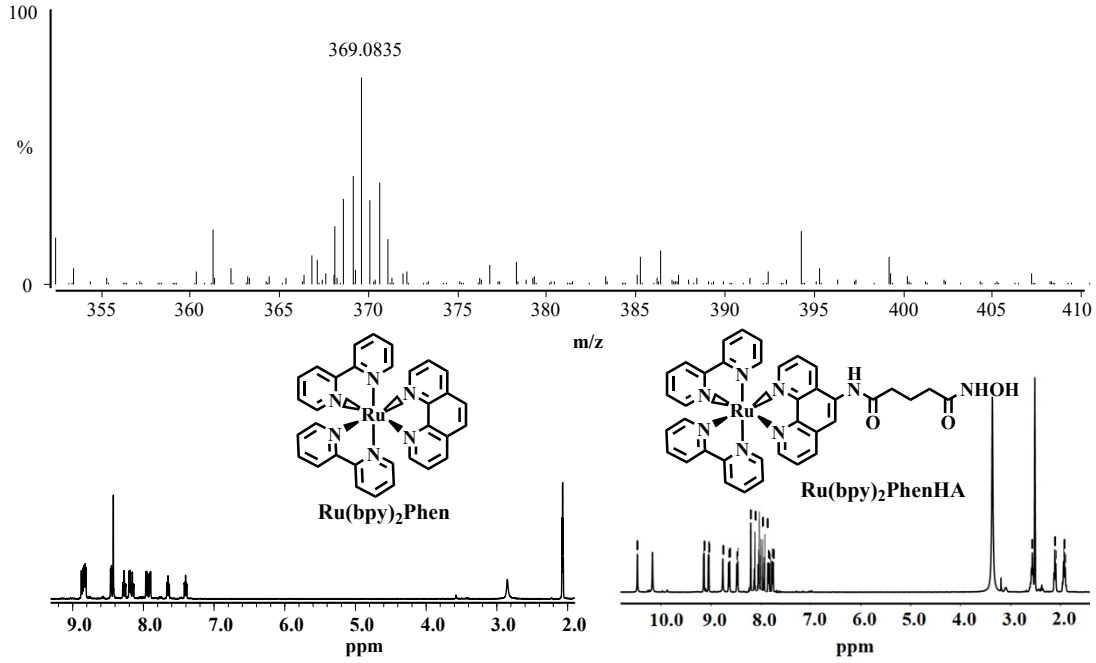

Figure S1. Mass and ^{1}H-NMR spectra of purified Ru(bpy)$_2$PhenHA.

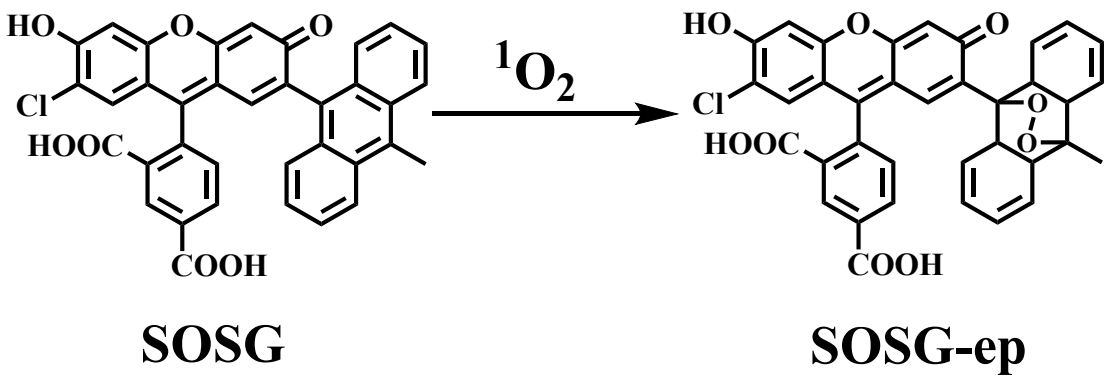

Figure S2. The principle of $^1O_2$ detection by SOSG.

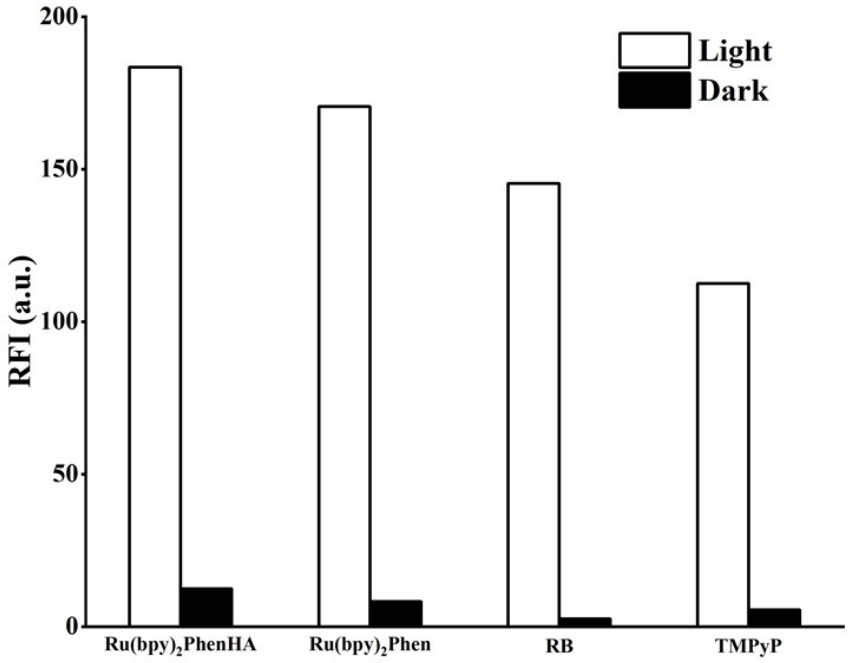

Figure S3. The $^1O_2$-generating ability of Ru(bpy)$_2$PhenHA/VIS is stronger than that of three other photosensitizers as measured by fluorescence analysis with SOSG as the $^1O_2$ probe. All reaction mixtures contained 100 μM photosensitizer and 5 μM SOSG in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4) under 20 min light irradiation before fluorescence detection at room temperature.

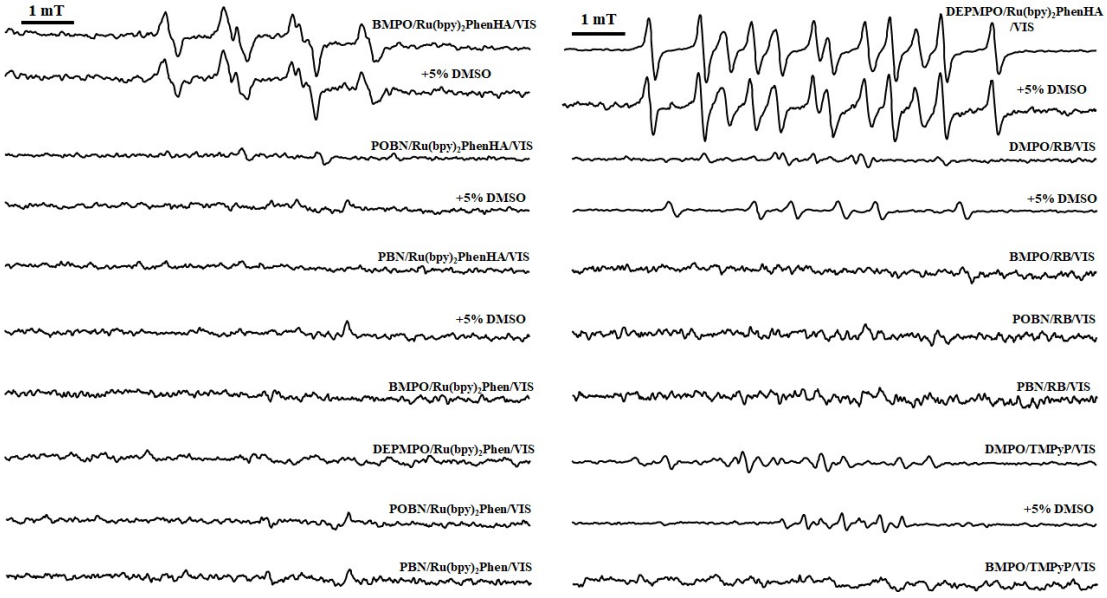

Figure S4. ESR signal of the visible light irradiation of $Ru(bpy)_2PhenHA$ and other photosensitizers in the presence of several other spin trapping agents. All reactions were conducted in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4) under continuous irradiation during the process of ESR detection at room temperature. For all reactions, 100 μM photosensitizers, 5% DMSO and 100 mM spin trapping agents were used.

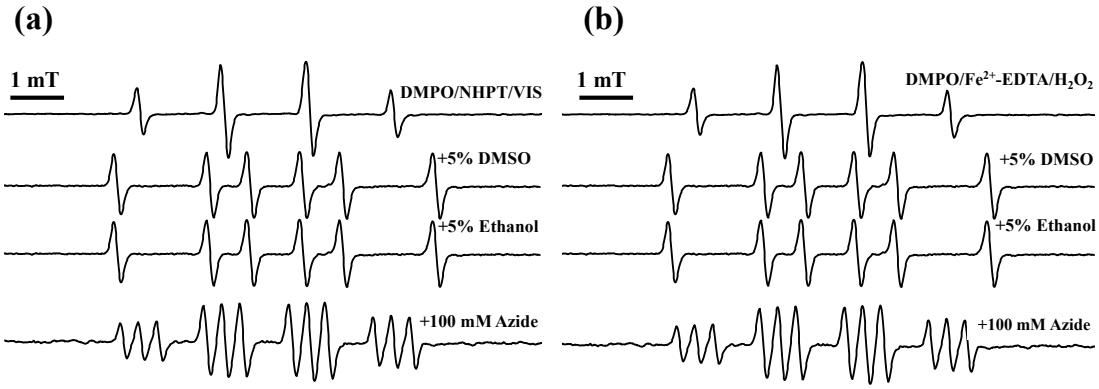

Figure S5. ˙OH production in NHPT/UV (a) and Fe^{2+}-EDTA/H_2O_2 (b) systems can be markedly quenched by the addition of three typical ˙OH scavengers. All reactions were carried out at room temperature in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4). For (a), 1 mM NHPT, and 100 mM DMPO were used. For (b), 1 mM Fe^{2+}-EDTA, 100 mM H_2O_2 and DMPO were used.

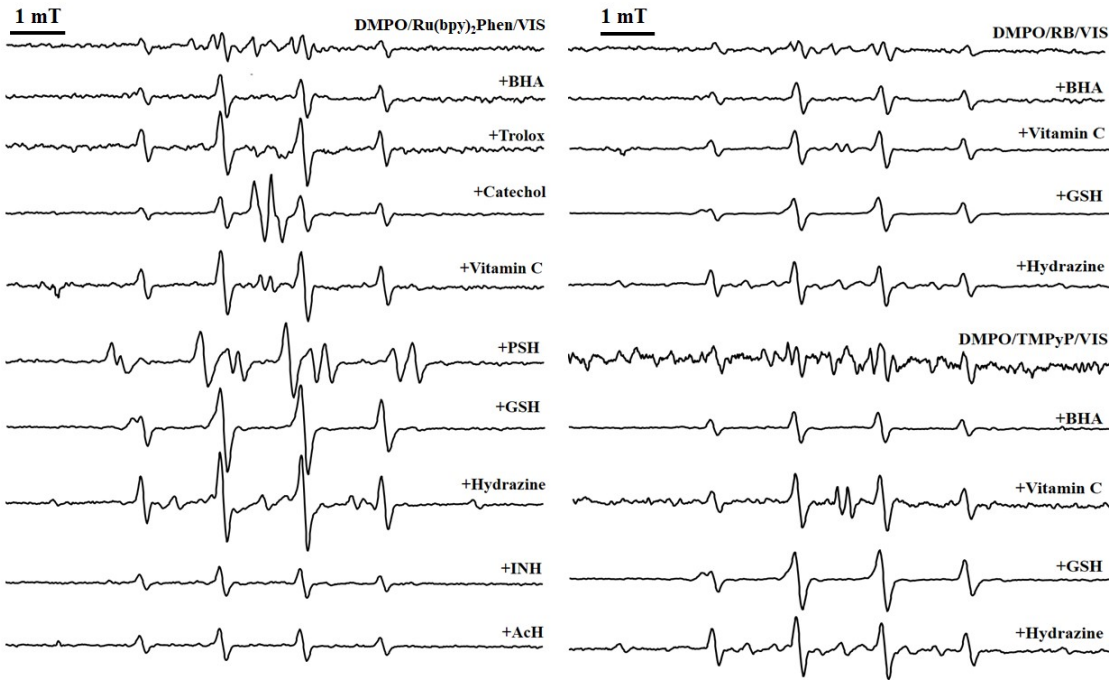

Figure S6. ESR signal of DMPO/photosensitizer/VIS in the presence of several structurally different reducing agents. Three kinds of typical photosensitizers including $Ru(bpy)_2Phen$, rose bengal (RB) and TMPyP were used. All reactions were conducted in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4) under continuous irradiation during the process of ESR detection at room temperature. For all reaction mixtures, 100 μM photosensitizers, 100 μM reducing agents and 100 mM DMPO were used.

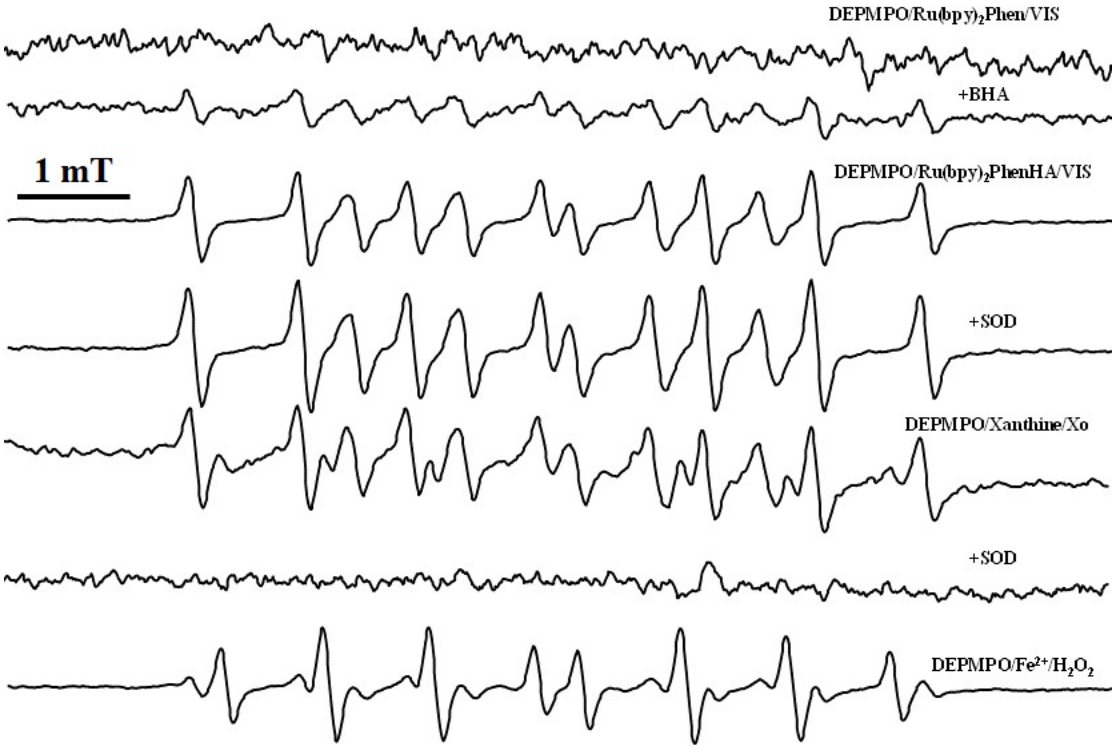

Figure S7. Typical ESR signal of the radical form of DEPMPO-OOH adduct can be detected from DEPMPO/Ru(bpy)$_2$PhenHA/VIS and DEPMPO/Ru(bpy)$_2$Phen/BHA/VIS by ESR spin trapping method. All reactions were conducted in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4) under continuous irradiation during the process of ESR detection at room temperature. 100 μM Ru(bpy)$_2$PhenHA or Ru(bpy)$_2$Phen, 100 μM BHA, 100 mM DEPMPO, 1 mM xanthine and 0.01 U XO, 1000 U SOD, 1 mM Fe^{2+}-EDTA, and 100 mM H_2O_2 were used.

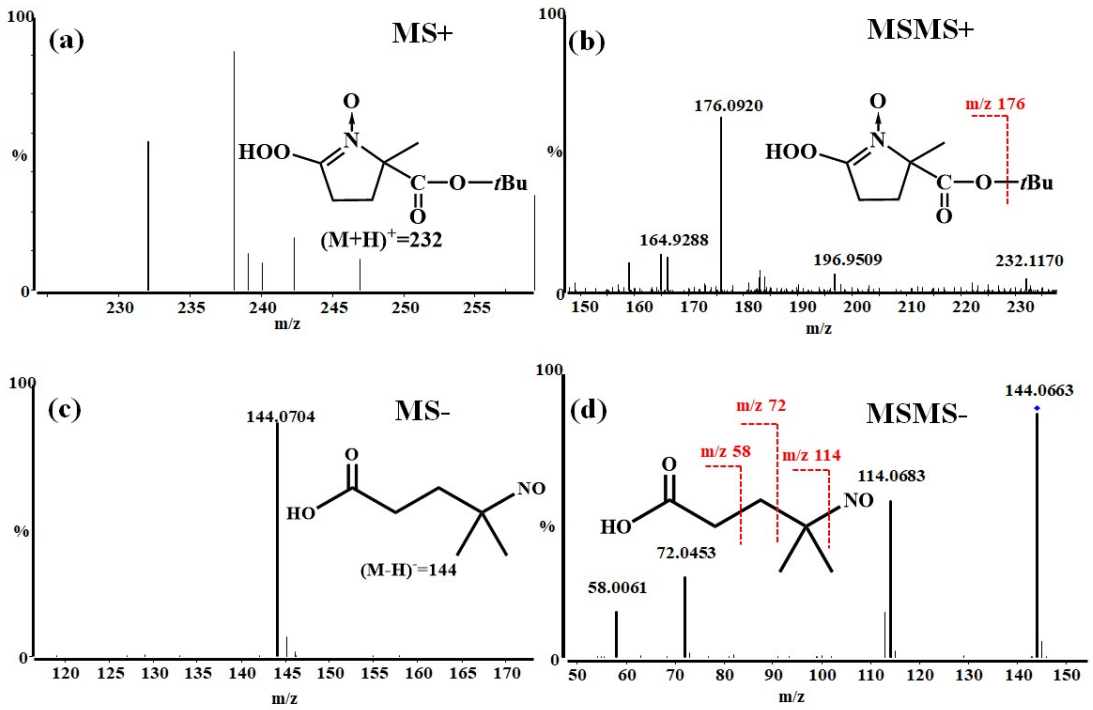

Figure S8. Unequivocal identification of BMPO-OOH adduct and final product from BMPO/Ru(bpy)$_2$PhenHA/VIS by ESI-Q-TOF-MS. (a) The ESI-Q-TOF-MS spectra of BMPO-OOH adduct. (b) MS/MS spectrum of the ion peak at m/z 232. (c) The ESI-Q-TOF-MS spectra of open-ring product. (d) MS/MS spectrum of the ion peak at m/z 144. Reactions were carried out at room temperature in the Chelex-pretreated ammonium acetate buffer (100 mM, pH 7.4).

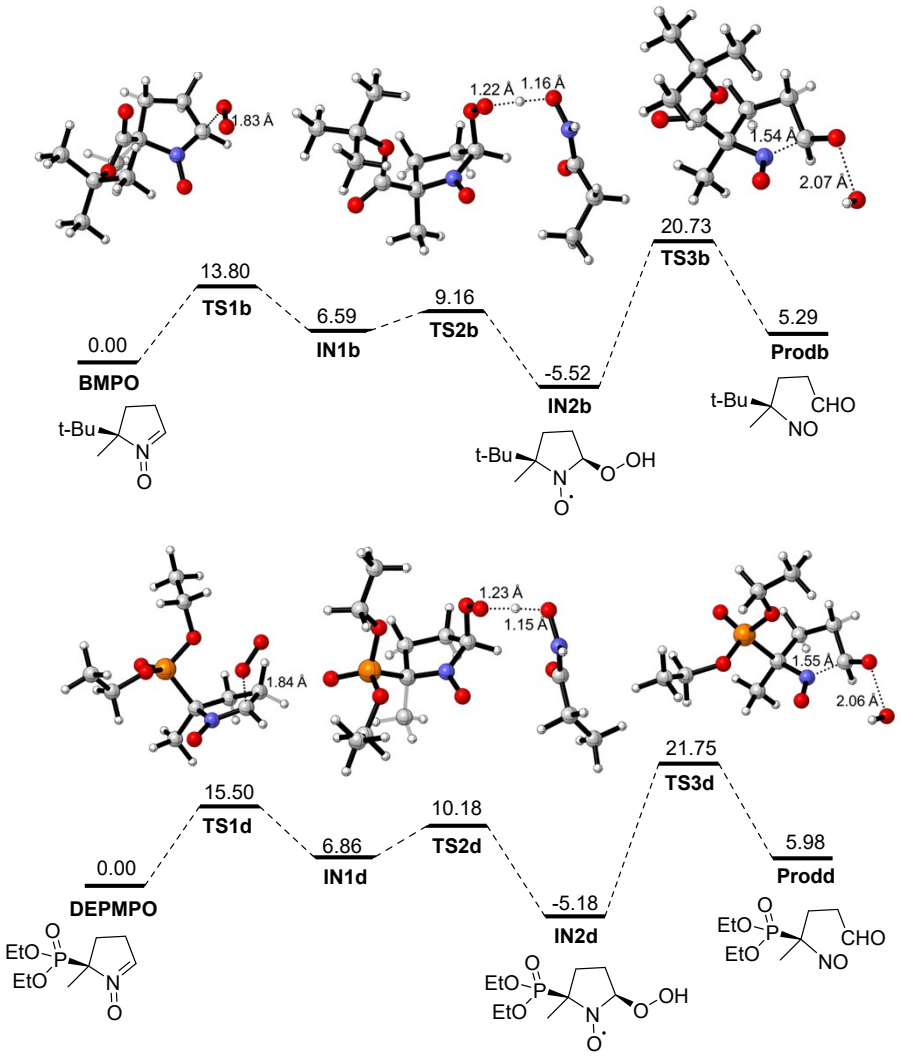

Figure S9. Computational study on the reaction pathway of BMPO (top) and DEPMPO (bottom) with $^1O_2$ and HA.

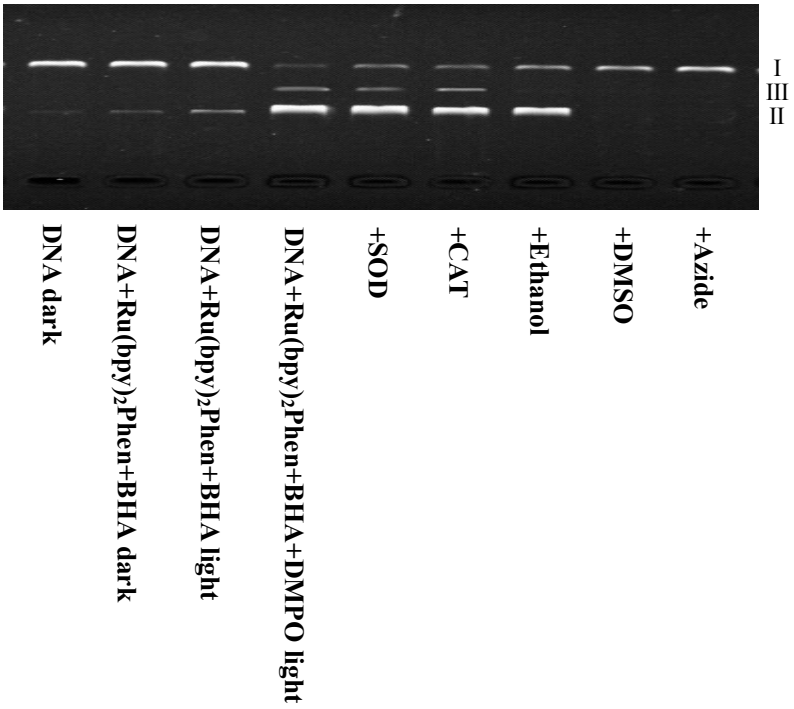

Figure S10. Gel-electrophoretic detection of DNA strand breaks induced by Ru(bpy)$_2$Phen/DMPO/VIS. Different DNA forms: Form I, closed circular supercoiled DNA; Form II, open circle DNA; Form III, linear DNA. All reactions were conducted in the Chelex-pretreated phosphate buffer (100 mM, pH 7.4) under dark or the indicated VIS irradiation (1.5 mW/cm^2 at 450 nm) at room temperature. Reaction mixtures contained 100 μM Ru(bpy)$_2$Phen and 100 μM DMPO. 100 μM BHA, 1000U SOD or catalase, 5% ethanol or DMSO, or 100 mM azide were used.

Supporting Tables

Table S1. XYZ coordinates related to the optimized species.

DMPO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.427886	0.888822	-0.023311
2	6	0	1.945512	-0.514144	-0.008697
3	1	0	1.996537	1.808766	0.020224
4	6	0	0.684564	-1.34475	-0.359242
5	1	0	2.350199	-0.777224	0.979948
6	1	0	2.757317	-0.669697	-0.728077
7	6	0	-0.518253	0.44096	-0.012187
8	1	0	0.679202	-1.568874	-1.430853
9	1	0	0.644463	-2.29592	0.17878
10	7	0	0.122306	0.948072	-0.027247
11	8	0	-0.623017	1.979421	0.010307
12	6	0	-1.058353	0.668944	1.406228
13	1	0	-1.580347	1.630113	1.453779
14	1	0	-0.24938	0.680003	2.144405
15	1	0	-1.760165	0.125749	1.672917
16	6	0	-1.639937	0.474162	-1.047489
17	1	0	-2.091215	1.471799	-1.065875
18	1	0	-2.409576	0.260653	-0.800778
19	1	0	-1.257554	0.248582	-2.047998

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.886503	0.622797	0.824372
2	6	0	-0.318044	1.871753	0.213516
3	1	0	-1.481719	0.606492	1.730469
4	6	0	0.683444	1.313473	-0.827287
5	1	0	0.180495	2.470783	0.98613
6	1	0	-1.096999	2.494057	-0.235678
7	6	0	1.149291	-0.054925	-0.269747
8	1	0	0.171832	1.168459	-1.783243
9	1	0	1.526832	1.987611	-0.996931
10	7	0	0.034084	-0.374548	0.697335
11	8	0	-0.04969	-1.506304	1.284434
12	6	0	2.452227	0.042192	0.53891

13	1	0	3.294723	0.227907	-0.134783
14	1	0	2.410621	0.856319	1.27037
15	1	0	2.633543	-0.893642	1.074894
16	8	0	-2.259894	0.25692	-0.315026
17	8	0	-2.386705	-0.983146	-0.582212
18	6	0	1.23683	-1.154517	-1.330709
19	1	0	2.01694	-0.902072	-2.056345
20	1	0	1.485458	-2.113136	-0.868071
21	1	0	0.28653	-1.265346	-1.860093

IN1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.053725	-0.06145	-0.595441
2	6	0	0.716069	1.420633	-0.555644
3	1	0	1.548386	-0.4464	-1.487144
4	6	0	-0.478275	1.492475	0.421125
5	1	0	0.428109	1.741843	-1.562524
6	1	0	1.576528	2.017487	-0.245937
7	6	0	-1.273426	0.184806	0.191504
8	1	0	-0.112316	1.529032	1.452276
9	1	0	-1.098254	2.377277	0.255269
10	7	0	-0.199164	0.715298	-0.347137
11	8	0	-0.396424	1.94648	-0.620674
12	6	0	-2.365982	0.334193	-0.881185
13	1	0	-3.188744	0.943649	-0.494148
14	1	0	-1.978264	0.814079	-1.785894
15	1	0	-2.758694	0.648672	-1.155975
16	8	0	1.961598	-0.419088	0.546341
17	8	0	3.202423	-0.050555	0.289546
18	6	0	-1.848526	0.418764	1.476952
19	1	0	-2.611006	0.247864	1.892867
20	1	0	-2.309197	1.38844	1.269068
21	1	0	-1.06469	0.563002	2.226534

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.785698	-0.681178	0.652206
2	6	0	-1.914543	-0.814085	1.665062
3	1	0	0.203185	-0.402765	1.029053
4	6	0	-3.183708	-0.495733	0.844235
5	1	0	-1.756215	-0.080983	2.462282
6	1	0	-1.932078	-1.807871	2.118783
7	6	0	-2.751025	0.581835	-0.177996

8	1	0	-3.51999	-1.395938	0.320071
9	1	0	-4.008706	-0.147185	1.471615
10	7	0	-1.276309	0.323064	-0.274881
11	8	0	-0.502809	1.04095	-0.994189
12	6	0	-2.962684	2.011979	0.348321
13	1	0	-4.032002	2.244668	0.378498
14	1	0	-2.555337	2.132472	1.357651
15	1	0	-2.465711	2.730607	-0.308987
16	8	0	-0.667003	-1.994731	0.01846
17	8	0	0.214294	-1.966061	-1.033578
18	8	0	2.459051	-2.115411	-0.272545
19	1	0	1.34977	-2.074115	-0.600568
20	7	0	3.039846	-0.944107	-0.518205
21	1	0	3.512836	-0.862459	-1.41294
22	6	0	2.926356	0.13753	0.336607
23	8	0	2.264787	0.075434	1.365104
24	6	0	3.693101	1.372746	-0.105305
25	1	0	4.578763	1.442412	0.539454
26	1	0	4.058538	1.255596	-1.132624
27	6	0	2.844557	2.645044	0.026481
28	1	0	2.512303	2.77312	1.059571
29	1	0	3.431549	3.521813	-0.262788
30	1	0	1.956183	2.591278	-0.60942
31	6	0	-3.39311	0.408642	-1.559138
32	1	0	-4.47452	0.56864	-1.492293
33	1	0	-2.977119	1.133108	-2.265097
34	1	0	-3.212247	-0.597213	-1.949514

IN2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.013467	0.575997	-0.457797
2	6	0	0.208161	1.829275	-0.110833
3	1	0	1.443258	0.559363	-1.466028
4	6	0	-1.267536	1.42636	-0.323227
5	1	0	0.509046	2.685152	-0.718347
6	1	0	0.40422	2.078162	0.937163
7	6	0	-1.349155	0.070217	0.05053
8	1	0	-1.951067	2.031913	0.278083
9	1	0	-1.546117	1.557781	-1.374932
10	7	0	0.022263	-0.516214	-0.332547
11	8	0	0.40515	-1.73575	-0.236376
12	6	0	-2.387008	0.851975	-0.75961
13	1	0	-3.394904	0.505505	-0.50908
14	1	0	-2.229658	0.715804	-1.834059
15	1	0	-2.320159	1.919993	-0.534735
16	8	0	2.055928	0.42064	0.48285

17	8	0	2.961162	-0.60812	-0.006188
18	6	0	-1.552739	0.294235	1.561412
19	1	0	-2.565842	0.005137	1.849647
20	1	0	-1.419002	1.352246	1.803218
21	1	0	-0.837798	0.283102	2.155118
22	1	0	2.383122	-1.398949	0.056646

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.034338	0.64785	-0.130135
2	6	0	0.06158	1.842681	0.09114
3	1	0	1.161905	0.533231	-1.230933
4	6	0	-1.252105	1.356421	-0.545583
5	1	0	0.472973	2.734883	-0.38312
6	1	0	-0.035366	2.033647	1.164269
7	6	0	-1.393961	0.126927	-0.122119
8	1	0	-2.117856	1.940796	-0.222081
9	1	0	-1.189781	1.435181	-1.636649
10	7	0	0.042898	-0.497131	0.142738
11	8	0	0.360692	-1.549302	0.684824
12	6	0	-1.966397	1.048942	-1.205572
13	1	0	-3.00143	0.762976	-1.417747
14	1	0	-1.390902	0.974469	-2.132997
15	1	0	-1.956536	2.089856	-0.870141
16	8	0	2.151381	0.621448	0.526515
17	8	0	3.205532	-0.755498	-0.561976
18	6	0	-2.165833	0.27908	1.200286
19	1	0	-3.217713	0.031823	1.02773
20	1	0	-2.099583	1.30633	1.566879
21	1	0	-1.775425	0.389857	1.972795
22	1	0	3.202869	-1.307415	0.239824

Prod

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.201222	-0.31374	-0.350513
2	6	0	1.504716	1.033234	-0.354124
3	1	0	1.965258	-0.979946	-1.207876
4	6	0	0.039836	1.03052	-0.824738
5	1	0	2.076378	1.655295	-1.060389
6	1	0	1.628626	1.490353	0.631688
7	6	0	-0.999068	0.305731	0.073617
8	1	0	-0.293656	2.070702	-0.917138
9	1	0	-0.021337	0.601693	-1.834081

10	7	0	-0.558648	1.140617	0.068628
11	8	0	-1.414235	1.94772	-0.211051
12	6	0	-2.414683	0.500528	-0.466227
13	1	0	-2.690748	1.557752	-0.403075
14	1	0	-2.49037	0.186217	-1.512005
15	1	0	-3.139968	0.080976	0.108245
16	8	0	3.016498	-0.648201	0.483475
17	6	0	-0.888138	0.731315	1.551396
18	1	0	-0.974803	1.820244	1.629314
19	1	0	-1.694446	0.279321	2.136865
20	1	0	0.064191	0.425506	1.992203

BMPO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.124095	0.595691	-0.618545
2	6	0	3.510994	-0.78367	-0.199784
3	1	0	3.733995	1.33447	-1.122239
4	6	0	2.160377	-1.407813	0.242414
5	1	0	4.243097	-0.756442	0.62039
6	1	0	3.975621	-1.350517	-1.014461
7	6	0	1.213119	-0.213033	0.485917
8	1	0	1.760962	-2.026706	-0.562865
9	1	0	2.258751	-2.023219	1.140206
10	7	0	1.909324	0.918358	-0.26532
11	8	0	1.295193	2.021848	-0.424218
12	6	0	1.095443	0.204974	1.952319
13	1	0	0.536828	-0.547116	2.515464
14	1	0	2.094754	0.297868	2.390217
15	1	0	0.579052	1.161897	2.037961
16	6	0	-0.14262	0.410538	-0.237122
17	8	0	-0.207789	0.897876	-1.348435
18	8	0	-1.171868	0.001807	0.502696
19	6	0	-2.567439	0.000533	-0.012292
20	6	0	-2.657669	0.891224	-1.253693
21	6	0	-3.013228	1.440501	-0.283604
22	6	0	-3.34794	0.604828	1.156046
23	1	0	-2.240078	1.880097	-1.043265
24	1	0	-2.122039	0.457733	-2.099114
25	1	0	-3.710478	1.011593	-1.530466
26	1	0	-2.884847	2.057582	0.611879
27	1	0	-4.07633	1.443472	-0.546572
28	1	0	-2.450292	1.883829	-1.106061
29	1	0	-4.411371	0.659326	0.903346
30	1	0	-3.237137	0.007568	2.056178
31	1	0	-2.990833	1.614944	1.376365

TS1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.766543	-0.126227	-0.525596
2	6	0	3.178363	0.850171	0.535202
3	1	0	3.418262	-0.46666	-1.322215
4	6	0	1.828371	1.272884	1.164471
5	1	0	3.70553	1.695296	0.074806
6	1	0	3.856327	0.394726	1.2626
7	6	0	0.769027	1.076513	0.057255
8	1	0	1.587034	0.621124	2.005558
9	1	0	1.841488	2.30602	1.519622
10	7	0	1.481813	0.141924	-0.894536
11	8	0	0.907996	-0.371354	-1.913826
12	6	0	0.422267	2.361821	-0.704635
13	1	0	-0.152853	3.03569	-0.062697
14	1	0	1.341297	2.873755	-1.008188
15	1	0	-0.169151	2.134265	-1.592307
16	6	0	-0.489866	0.342203	0.597748
17	8	0	-0.489171	-0.281072	1.640605
18	8	0	-1.523389	0.49113	-0.228638
19	6	0	-2.81448	-0.221954	-0.023506
20	6	0	-2.571685	-1.733464	-0.029386
21	6	0	-3.470836	0.267862	1.270381
22	6	0	-3.622384	0.208639	-1.249033
23	1	0	-2.022901	-2.028141	-0.928586
24	1	0	-2.008885	-2.054829	0.848006
25	1	0	-3.538039	-2.248861	-0.031351
26	1	0	-3.573756	1.358009	1.260309
27	1	0	-4.473695	-0.164961	1.350157
28	1	0	-2.894146	-0.027949	2.147926
29	1	0	-4.613315	-0.254957	-1.220554
30	1	0	-3.749514	1.295407	-1.26878
31	1	0	-3.118903	-0.099671	-2.169638
32	8	0	2.757662	-1.709519	0.386277
33	8	0	1.874479	-2.523239	-0.029458

IN1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.713552	0.048347	0.506276
2	6	0	2.978742	-0.97549	-0.584553
3	1	0	3.361397	0.028701	1.38276
4	6	0	1.600656	-1.166809	-1.255249
5	1	0	3.330784	-1.901063	-0.116028
6	1	0	3.753252	-0.632116	-1.273462

7	6	0	0.56941	-1.001321	-0.117594
8	1	0	1.432458	-0.392351	-2.006364
9	1	0	1.506083	-2.142931	-1.737222
10	7	0	1.337099	-0.166182	0.867147
11	8	0	0.846737	0.243746	1.970448
12	6	0	0.171033	-2.324542	0.549155
13	1	0	-0.45733	-2.913375	-0.125308
14	1	0	1.067243	-2.907334	0.785204
15	1	0	-0.383817	-2.13837	1.469527
16	6	0	-0.653248	-0.160057	-0.580847
17	8	0	-0.594141	0.626383	-1.505038
18	8	0	-1.72349	-0.404582	0.175118
19	6	0	-2.992336	0.361501	0.028281
20	6	0	-2.72585	1.846149	0.290064
21	6	0	-3.592794	0.102829	-1.356391
22	6	0	-3.866323	-0.241727	1.129244
23	1	0	-2.229153	1.979847	1.255705
24	1	0	-2.105731	2.287143	-0.491551
25	1	0	-3.681316	2.380397	0.318892
26	1	0	-3.708408	-0.97204	-1.53034
27	1	0	-4.58606	0.561225	-1.407324
28	1	0	-2.973173	0.527598	-2.147333
29	1	0	-4.847431	0.243102	1.130942
30	1	0	-4.011013	-1.314193	0.966904
31	1	0	-3.405113	-0.097523	2.110449
32	8	0	2.813148	1.440125	-0.030327
33	8	0	4.077818	1.798488	-0.148426

TS2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.713764	-0.631177	-1.275814
2	6	0	0.094474	-1.614888	-2.258255
3	1	0	1.791326	-0.70789	-1.100587
4	6	0	-1.358878	-1.780839	-1.759025
5	1	0	0.646567	-2.558077	-2.204659
6	1	0	0.15198	-1.24644	-3.285125
7	6	0	-1.257549	-1.681355	-0.213674
8	1	0	-1.977525	-0.969853	-2.151153
9	1	0	-1.802236	-2.73152	-2.06416
10	7	0	-0.010007	-0.884384	-0.039503
11	8	0	0.455218	-0.596968	1.112955
12	6	0	-1.100343	-3.044078	0.469971
13	1	0	-2.036001	-3.602568	0.40502
14	1	0	-0.301712	-3.616438	-0.011752
15	1	0	-0.849361	-2.909796	1.524388
16	8	0	0.442635	0.697923	-1.811604

17	8	0	0.863907	1.678955	-0.949051
18	8	0	3.194418	2.066841	-1.189001
19	1	0	2.055045	1.864369	-1.124778
20	7	0	3.778269	1.689669	-0.054884
21	1	0	3.903925	2.416866	0.642462
22	6	0	4.1044	0.372026	0.212421
23	8	0	3.855143	-0.523761	-0.584445
24	6	0	4.792151	0.151766	1.549111
25	1	0	5.847648	-0.055478	1.330935
26	1	0	4.767808	1.066408	2.153707
27	6	0	4.173839	-1.023657	2.319432
28	1	0	4.230985	-1.938484	1.724631
29	1	0	4.711677	-1.183952	3.258521
30	1	0	3.12065	-0.834762	2.547035
31	6	0	-2.462814	-0.920639	0.387473
32	8	0	-3.325788	-1.467801	1.045076
33	8	0	-2.425207	0.369522	0.048824
34	6	0	-3.427037	1.356019	0.527758
35	6	0	-4.814922	0.988552	-0.005598
36	6	0	-3.383413	1.422579	2.057076
37	6	0	-2.924439	2.659836	-0.094676
38	1	0	-4.791957	0.886856	-1.095605
39	1	0	-5.179813	0.058	0.431755
40	1	0	-5.518247	1.79062	0.242495
41	1	0	-2.362884	1.618068	2.400083
42	1	0	-4.022872	2.243184	2.39921
43	1	0	-3.737754	0.494706	2.508969
44	1	0	-3.572665	3.488705	0.20672
45	1	0	-1.90249	2.873034	0.230102
46	1	0	-2.927941	2.59489	-1.186745

IN2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.418514	0.688126	-0.0284
2	6	0	2.735154	-0.200797	-1.230657
3	1	0	3.254048	0.950946	0.626888
4	6	0	1.431637	-0.99932	-1.455699
5	1	0	3.566181	-0.863337	-0.969035
6	1	0	3.028348	0.387534	-2.103265
7	6	0	0.876363	-1.252907	-0.028761
8	1	0	0.728589	-0.397361	-2.036474
9	1	0	1.602013	-1.939787	-1.984996
10	7	0	1.472107	-0.122776	0.736081
11	8	0	1.334604	-0.015178	1.999919
12	6	0	1.340361	-2.586631	0.568646
13	1	0	0.842694	-3.415008	0.061113

14	1	0	2.424254	-2.692226	0.458768
15	1	0	1.091266	-2.62901	1.631131
16	6	0	-0.667769	1.169545	-0.000417
17	8	0	-1.377488	2.149446	0.116486
18	8	0	-1.078932	0.089411	-0.159396
19	6	0	-2.510746	0.479268	-0.112616
20	6	0	-3.26821	0.184688	-1.266354
21	6	0	-3.090261	0.117817	1.257958
22	6	0	-2.442176	1.996341	-0.297965
23	1	0	-2.784031	0.041499	-2.222165
24	1	0	-3.320983	1.267203	-1.140979
25	1	0	-4.287824	0.213566	-1.303006
26	1	0	-2.481135	0.55507	2.054858
27	1	0	-4.103825	0.524902	1.338864
28	1	0	-3.137664	0.963032	1.399984
29	1	0	-3.450512	2.42068	-0.260838
30	1	0	-1.836171	2.453027	0.489104
31	1	0	-1.993379	2.248596	-1.263327
32	8	0	1.842342	1.875217	-0.575
33	8	0	1.469745	2.752561	0.524646
34	1	0	2.094014	3.484055	0.383148

TS3b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.256531	-0.432108	-0.623402
2	6	0	-1.416665	-0.045746	-1.873276
3	1	0	-3.127204	0.265398	-0.590689
4	6	0	-0.920061	1.375083	-1.553115
5	1	0	-2.051094	-0.087221	-2.759909
6	1	0	-0.595597	-0.756525	-1.986
7	6	0	-0.568647	1.370874	-0.036572
8	1	0	-0.061026	1.670912	-2.160554
9	1	0	-1.714234	2.107968	-1.730592
10	7	0	-1.384899	0.222664	0.463645
11	8	0	-1.286734	-0.204284	1.608379
12	6	0	-0.930545	2.651861	0.716838
13	1	0	-0.315395	3.474972	0.347796
14	1	0	-1.986556	2.890089	0.563446
15	1	0	-0.74117	2.535481	1.786443
16	8	0	-2.591981	-1.668686	-0.437805
17	8	0	-4.15821	-1.453341	0.896937
18	1	0	-3.572582	-1.876039	1.549965
19	6	0	0.937862	1.044356	0.158817
20	8	0	1.746125	1.895718	0.460992
21	8	0	1.18682	-0.238236	-0.104945
22	6	0	2.549866	-0.838385	0.024

23	6	0	3.496771	-0.173875	-0.977812
24	6	0	3.027457	-0.701775	1.471681
25	6	0	2.29605	-2.302501	-0.336775
26	1	0	3.093396	-0.242128	-1.993367
27	1	0	3.671571	0.87466	-0.731758
28	1	0	4.457544	-0.698804	-0.962789
29	1	0	2.284896	-1.116377	2.160076
30	1	0	3.957081	-1.267029	1.593975
31	1	0	3.218962	0.338984	1.737568
32	1	0	3.230612	-2.866671	-0.262015
33	1	0	1.564016	-2.748506	0.342038
34	1	0	1.919578	-2.393878	-1.359915

Prodb

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.921646	-1.477971	-0.304925
2	6	0	2.442777	-0.881009	1.003849
3	1	0	3.597227	-0.835622	-0.911211
4	6	0	2.173829	0.633377	0.998581
5	1	0	3.254304	-1.068696	1.723825
6	1	0	1.579664	-1.450836	1.358735
7	6	0	0.948509	1.116758	0.184845
8	1	0	2.011669	0.960673	2.029579
9	1	0	3.054507	1.172206	0.625523
10	7	0	1.211123	0.649082	-1.23232
11	8	0	1.176387	1.515132	-2.072881
12	6	0	0.749759	2.631775	0.298134
13	1	0	0.553238	2.898017	1.339958
14	1	0	1.648456	3.156954	-0.037809
15	1	0	-0.08545	2.968718	-0.320164
16	8	0	2.659462	-2.605796	-0.667097
17	6	0	-0.332787	0.409603	0.68189
18	8	0	-0.529033	0.16564	1.855243
19	8	0	-1.170643	0.180478	-0.330277
20	6	0	-2.502969	-0.465296	-0.147019
21	6	0	-2.314531	-1.872575	0.425149
22	6	0	-3.380254	0.42223	0.739467
23	6	0	-3.037093	-0.519701	-1.578967
24	1	0	-1.618516	-2.447964	-0.192885
25	1	0	-1.941734	-1.844319	1.450156
26	1	0	-3.279323	-2.390323	0.421419
27	1	0	-3.440267	1.435465	0.329287
28	1	0	-4.393955	0.009198	0.76767
29	1	0	-2.997833	0.472414	1.760138
30	1	0	-4.029039	-0.981744	-1.585214
31	1	0	-3.119704	0.485924	-2.00162

32	1	0	-2.373809	-1.110414	-2.21707

DEPMPO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.156426	-0.843641	-1.487408
2	6	0	-2.90074	0.140651	-0.644974
3	1	0	-2.336171	-1.109039	-2.521058
4	6	0	-2.373433	-0.163364	0.77978
5	1	0	-3.986036	0.008389	-0.718757
6	1	0	-2.675728	1.171102	-0.947228
7	6	0	-1.02881	-0.899162	0.568589
8	1	0	-2.271894	0.733653	1.39265
9	1	0	-3.058654	-0.844745	1.294969
10	7	0	-1.164188	-1.413885	-0.855336
11	8	0	-0.352822	-2.29777	-1.285701
12	6	0	-0.807011	-2.078121	1.517465
13	1	0	-0.699528	-1.709948	2.539831
14	1	0	-1.66492	-2.756095	1.461519
15	1	0	0.086979	-2.643498	1.248018
16	15	0	0.427888	0.274048	0.696353
17	8	0	0.888431	0.425124	2.105751
18	8	0	1.566251	-0.146168	-0.361545
19	8	0	-0.164734	1.593506	-0.023954
20	6	0	2.529253	-1.205121	-0.092865
21	1	0	2.790253	-1.182241	0.970068
22	1	0	2.040936	-2.151998	-0.339199
23	6	0	3.744543	-0.966573	-0.968647
24	1	0	4.473304	-1.769013	-0.80972
25	1	0	3.462975	-0.961846	-2.025742
26	1	0	4.223369	-0.012579	-0.727175
27	6	0	0.654819	2.791647	-0.12799
28	1	0	1.071164	3.018322	0.858814
29	1	0	1.475922	2.584907	-0.821708
30	6	0	-0.224863	3.920694	-0.630332
31	1	0	-0.647055	3.68026	-1.610841
32	1	0	-1.045349	4.116264	0.066583
33	1	0	0.370425	4.834993	-0.727088

TS1d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.428582	-0.562384	0.665538
2	6	0	2.812193	0.28933	-0.503672
3	1	0	3.143498	-1.03134	1.332031

4	6	0	1.865301	-0.155467	-1.651994
5	1	0	3.866283	0.158574	-0.763435
6	1	0	2.672941	1.343231	-0.228555
7	6	0	0.73029	-0.974463	-0.984933
8	1	0	1.486338	0.692953	-2.223516
9	1	0	2.397221	-0.812869	-2.346981
10	7	0	1.35929	-1.353554	0.319999
11	8	0	0.89913	-2.290722	1.053339
12	6	0	0.350903	-2.243005	-1.75726
13	1	0	-0.090923	-1.968126	-2.717043
14	1	0	1.246703	-2.84892	-1.927113
15	1	0	-0.367758	-2.849105	-1.201646
16	8	0	1.809391	0.559863	1.982969
17	8	0	2.170377	1.770683	1.841903
18	15	0	-0.815378	0.058879	-0.728911
19	8	0	-1.690943	0.054385	-1.934963
20	8	0	-0.160563	1.450584	-0.268198
21	8	0	-1.529603	-0.420454	0.635044
22	6	0	-0.931439	2.548201	0.302031
23	1	0	-0.233719	3.041646	0.982261
24	1	0	-1.752785	2.133279	0.893278
25	6	0	-1.428414	3.491246	-0.780998
26	1	0	-2.111007	2.980562	-1.465746
27	1	0	-1.960039	4.330257	-0.317514
28	1	0	-0.591267	3.894021	-1.359276
29	6	0	-2.514416	-1.491145	0.666073
30	1	0	-3.047486	-1.510455	-0.28936
31	1	0	-1.967906	-2.429688	0.801353
32	6	0	-3.456977	-1.234808	1.826914
33	1	0	-2.904831	-1.182514	2.769758
34	1	0	-4.004607	-0.297695	1.687834
35	1	0	-4.183456	-2.051857	1.896393

IN1d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.548561	-0.313793	-0.234971
2	6	0	-2.507932	0.692332	0.916593
3	1	0	-3.456326	-0.912504	-0.335273
4	6	0	-1.504828	0.105915	1.937021
5	1	0	-3.499869	0.843699	1.347436
6	1	0	-2.150175	1.647504	0.527911
7	6	0	-0.544591	-0.794469	1.122842
8	1	0	-0.979838	0.885327	2.493767
9	1	0	-2.024089	-0.526355	2.665491
10	7	0	-1.391345	-1.158806	-0.041098
11	8	0	-1.191494	-2.193065	-0.759419

12	6	0	-0.100875	-2.054331	1.875556
13	1	0	0.515529	-1.773397	2.732239
14	1	0	-0.982819	-2.59978	2.225977
15	1	0	0.47089	-2.723835	1.229373
16	8	0	-2.402661	0.371105	-1.541273
17	8	0	-3.574638	0.535392	-2.128384
18	15	0	0.989693	0.14038	0.586348
19	8	0	1.974773	0.313408	1.69243
20	8	0	0.326978	1.463141	-0.047192
21	8	0	1.574776	-0.586073	-0.730858
22	6	0	1.1175	2.475533	-0.735914
23	1	0	0.455634	2.856011	-1.517704
24	1	0	1.972827	1.993338	-1.218441
25	6	0	1.550981	3.574331	0.220115
26	1	0	2.199377	3.177017	1.005633
27	1	0	2.101656	4.343722	-0.333046
28	1	0	0.682061	4.046648	0.688704
29	6	0	2.624578	-1.590884	-0.668877
30	1	0	3.205313	-1.442368	0.246295
31	1	0	2.135265	-2.569781	-0.635082
32	6	0	3.489292	-1.457779	-1.908583
33	1	0	2.887149	-1.567351	-2.815202
34	1	0	3.989402	-0.484809	-1.934737
35	1	0	4.256779	-2.239532	-1.906004

TS2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.970951	-1.086231	1.173931
2	6	0	0.355019	-1.516856	2.496306
3	1	0	2.033787	-0.824132	1.181122
4	6	0	-1.127086	-1.092184	2.382186
5	1	0	0.865417	-0.98475	3.30515
6	1	0	0.476452	-2.58911	2.667501
7	6	0	-1.104295	0.202418	1.523159
8	1	0	-1.697856	-1.880434	1.887666
9	1	0	-1.586883	-0.902375	3.354185
10	7	0	0.188212	0.082299	0.79078
11	8	0	0.692667	1.050284	0.126723
12	6	0	-1.100911	1.484788	2.373752
13	1	0	-2.077327	1.624844	2.843513
14	1	0	-0.337424	1.410016	3.155218
15	1	0	-0.866852	2.355681	1.75694
16	8	0	0.788746	-2.198582	0.252699
17	8	0	1.117244	-1.842992	-1.03147
18	8	0	3.468172	-1.825017	-1.37514
19	1	0	2.334432	-1.880677	-1.164396

20	7	0	3.82688	-0.550484	-1.509657
21	1	0	3.805717	-0.181485	-2.455749
22	6	0	4.052692	0.278194	-0.42411
23	8	0	3.990069	-0.140056	0.724669
24	6	0	4.338397	1.723707	-0.791548
25	1	0	4.658583	1.799224	-1.838092
26	1	0	3.375479	2.246145	-0.715173
27	6	0	5.367137	2.371965	0.141007
28	1	0	6.347585	1.895024	0.043092
29	1	0	5.478113	3.433814	-0.097384
30	1	0	5.049928	2.278995	1.182234
31	15	0	-2.561407	0.241749	0.359362
32	8	0	-3.849672	0.447834	1.082769
33	8	0	-2.344322	-1.141371	-0.425695
34	8	0	-2.271369	1.327808	-0.802294
35	6	0	-3.132403	-1.508226	-1.589725
36	1	0	-4.192666	-1.492993	-1.314883
37	1	0	-2.95509	-0.762197	-2.370721
38	6	0	-2.687853	-2.889621	-2.031285
39	1	0	-3.240689	-3.183348	-2.930293
40	1	0	-1.617978	-2.89462	-2.257671
41	1	0	-2.880935	-3.630114	-1.249381
42	6	0	-2.788408	2.68252	-0.743321
43	1	0	-2.000399	3.31652	-0.322445
44	1	0	-3.659632	2.704317	-0.082055
45	6	0	-3.145815	3.123841	-2.151097
46	1	0	-3.494059	4.162577	-2.134623
47	1	0	-2.275281	3.061232	-2.810935
48	1	0	-3.943806	2.499774	-2.564723

IN2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.549018	-0.216034	-0.113699
2	6	0	-2.401858	0.890332	0.928523
3	1	0	-3.434297	-0.852773	0.002521
4	6	0	-1.444481	0.312709	1.994447
5	1	0	-3.368702	1.178228	1.346089
6	1	0	-1.956156	1.760595	0.442472
7	6	0	-0.503293	-0.661881	1.240961
8	1	0	-0.897781	1.094602	2.525698
9	1	0	-2.004263	-0.262911	2.740319
10	7	0	-1.341658	-1.04426	0.087383
11	8	0	-1.056638	-2.003852	-0.711343
12	6	0	-0.116458	-1.902049	2.060362
13	1	0	0.507351	-1.609648	2.907478
14	1	0	-1.023935	-2.3924	2.426893

15	1	0	0.432887	-2.623382	1.450869
16	8	0	-2.564413	0.346285	-1.407896
17	8	0	-2.987276	-0.683262	-2.345508
18	1	0	-2.225121	-1.297935	-2.303148
19	15	0	1.082506	0.19452	0.702515
20	8	0	2.083381	0.275075	1.804896
21	8	0	0.515275	1.584043	0.116991
22	8	0	1.611136	-0.514282	-0.647749
23	6	0	1.417382	2.56523	-0.470453
24	1	0	2.195497	2.803775	0.261758
25	1	0	1.882314	2.115934	-1.353407
26	6	0	2.513124	-1.653841	-0.632431
27	1	0	3.130084	-1.607702	0.270216
28	1	0	1.896143	-2.557856	-0.608503
29	6	0	3.361327	-1.605949	-1.889747
30	1	0	3.982064	-0.705082	-1.908976
31	1	0	4.020505	-2.480371	-1.9217
32	1	0	2.730436	-1.616297	-2.78344
33	6	0	0.601255	3.789511	-0.837907
34	1	0	0.137703	4.231731	0.049217
35	1	0	1.254015	4.541011	-1.294873
36	1	0	-0.184315	3.532274	-1.554352

TS3d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.67386	-0.047557	0.141063
2	6	0	-2.210385	0.487752	1.52126
3	1	0	-3.253032	-0.98271	0.331686
4	6	0	-1.234479	-0.593208	2.017512
5	1	0	-3.07711	0.60908	2.172641
6	1	0	-1.722617	1.454838	1.387185
7	6	0	-0.429285	-1.040535	0.76781
8	1	0	-0.57252	-0.243023	2.812251
9	1	0	-1.788969	-1.455884	2.404857
10	7	0	-1.356826	-0.700855	-0.341483
11	8	0	-1.086466	-0.88019	-1.526286
12	6	0	-0.054506	-2.528876	0.733098
13	1	0	0.660321	-2.751526	1.530007
14	1	0	-0.95073	-3.136966	0.889283
15	1	0	0.383213	-2.798373	-0.230849
16	8	0	-3.269567	0.745526	-0.692039
17	8	0	-4.219927	-0.599394	-1.930769
18	1	0	-3.529048	-0.385102	-2.582866
19	15	0	1.149132	-0.023544	0.639492
20	8	0	1.960595	-0.122034	1.885265
21	8	0	0.540959	1.405909	0.23814

22	8	0	1.921826	-0.475098	-0.700272
23	6	0	1.395512	2.53746	-0.107864
24	1	0	2.089003	2.71477	0.720498
25	1	0	1.964216	2.268071	-1.003036
26	6	0	3.120673	-1.304532	-0.676392
27	1	0	3.547591	-1.281707	0.329718
28	1	0	2.808621	-2.32742	-0.91124
29	6	0	4.092733	-0.778488	-1.715566
30	1	0	4.420364	0.235754	-1.468341
31	1	0	4.976113	-1.425498	-1.750175
32	1	0	3.63414	-0.766634	-2.708568
33	6	0	0.501061	3.7359	-0.356683
34	1	0	-0.056189	4.004222	0.545526
35	1	0	1.115584	4.593931	-0.649382
36	1	0	-0.212286	3.528085	-1.158933

Prodd

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.350981	-0.112304	-0.054666
2	6	0	-2.521066	-0.49461	1.154442
3	1	0	-3.666454	-0.95105	-0.71143
4	6	0	-1.530261	-1.655967	0.964357
5	1	0	-3.249871	-0.820186	1.91317
6	1	0	-2.042472	0.403456	1.550797
7	6	0	-0.327779	-1.457591	0.001402
8	1	0	-1.113028	-1.9121	1.942699
9	1	0	-2.071731	-2.544229	0.610735
10	7	0	-0.935579	-1.167646	-1.352839
11	8	0	-0.421888	-1.751679	-2.278344
12	6	0	0.583429	-2.689396	0.000375
13	1	0	1.040394	-2.823173	0.984902
14	1	0	-0.006986	-3.582713	-0.228351
15	1	0	1.367233	-2.606295	-0.753552
16	8	0	-3.724543	1.01963	-0.283202
17	15	0	0.676424	0.037303	0.512906
18	8	0	0.931105	0.087268	1.981103
19	8	0	-0.174022	1.221814	-0.145987
20	8	0	2.014908	0.006916	-0.39445
21	6	0	0.13417	2.627536	0.088419
22	1	0	0.074309	2.816524	1.164819
23	1	0	1.158298	2.818111	-0.250179
24	6	0	3.322109	-0.332459	0.150448
25	1	0	3.262898	-0.330842	1.242101
26	1	0	3.559089	-1.34441	-0.194249
27	6	0	4.33983	0.671862	-0.358329
28	1	0	4.110356	1.678449	0.004154

29	1	0	5.337974	0.396934	0.000221
30	1	0	4.358351	0.689936	-1.452021
31	6	0	-0.874267	3.453195	-0.686583
32	1	0	-1.893938	3.208012	-0.37769
33	1	0	-0.692473	4.517499	-0.501328
34	1	0	-0.784838	3.266866	-1.760665