Supporting Information

Photo-excitation energy transfer between a titanium(IV)-porphyrin complex and oxygen molecule

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The minimum structure illustrates the closest approach of oxygen molecule as the Σ^3O_2 state to the C-C portion of the porphyrin ring in the $[TiO(tpypH_4)]^{4+}$ complex.

Atomic Type Coordinates (X, Y, Z) (Angstroms)

С	0.311574	-3.417519	-0.097722
С	-1.027905	-2.922748	-0.021978
С	-2.195664	-3.727032	0.073433
С	-3.261313	-2.888123	0.117752
С	-2.758349	-1.560916	0.044399
С	-3.556043	-0.374715	0.080933
С	-3.079794	0.904600	0.074239
С	-3.881127	2.122167	0.159974
С	-3.049727	3.162535	0.127467
С	-1.690536	2.636257	0.005626
С	-0.515057	3.452324	-0.030430
С	0.761080	2.945545	-0.057601
С	1.992924	3.769342	-0.069714
С	3.029888	2.951767	-0.120035
С	2.515856	1.562420	-0.150855
С	3.309786	0.442608	-0.178808
С	2.796646	-0.893504	-0.153527
С	3.629479	-2.095831	-0.165232
С	2.813459	-3.148922	-0.160250
С	1.440953	-2.652337	-0.141636
Ν	-1.374099	-1.580158	-0.029511
Ν	-1.708563	1.278071	-0.013860
Ν	1.117384	1.592544	-0.098765
Ν	1.480233	-1.229262	-0.135579
С	0.472805	-4.934034	-0.130451
С	0.359459	-5.697370	1.043840
С	0.500423	-7.067684	0.989214
Ν	0.745500	-7.673865	-0.210682
С	0.859709	-6.963278	-1.371863
С	0.728181	-5.590667	-1.345808
С	-5.066575	-0.579085	0.130505
С	-5.782649	-0.409815	1.327013
С	-7.147012	-0.610069	1.346214
Ν	-7.793164	-0.966892	0.196806
С	-7.128719	-1.138277	-0.985158
С	-5.763826	-0.950451	-1.032028
С	-0.712550	4.955078	-0.042780
С	-0.300449	5.758589	1.036897

С	-0.493269	7.122369	1.001882
Ν	-1.080806	7.694403	-0.090860
С	-1.493471	6.950066	-1.160490
С	-1.320362	5.583900	-1.146719
С	4.814916	0.614463	-0.243701
С	5.639576	0.232475	0.831754
С	7.004833	0.395873	0.752670
Ν	7.558214	0.924319	-0.379740
С	6.793667	1.304508	-1.446437
С	5.424648	1.159383	-1.389378
Ti	-0.142591	0.014622	-0.605974
0	-0.197050	0.020878	-2.205105
Н	-2.219565	-4.804051	0.108028
Н	-4.299365	-3.166022	0.201705
Н	-4.957510	2.149168	0.246976
Н	-3.304430	4.207539	0.190487
Н	2.008883	4.847831	-0.041523
Н	4.075708	3.217587	-0.127952
Н	4.706592	-2.102211	-0.182478
Н	3.093389	-4.192357	-0.159842
Н	0.163287	-5.227469	2.000276
Н	0.427468	-7.720100	1.862037
Н	0.846469	-8.703813	-0.240961
Н	1.053319	-7.536640	-2.281125
Н	0.818160	-5.035870	-2.272603
Н	-5.280766	-0.129145	2.245217
Н	-7.763139	-0.500604	2.241290
Н	-8.817714	-1.113289	0.221985
Н	-7.731928	-1.422203	-1.850168
Н	-5.245245	-1.090189	-1.973446
Н	0.160656	5.320218	1.913253
Н	-0.204076	7.796155	1.811047
Н	-1.217893	8.720056	-0.109066
Н	-1.946695	7.495543	-1.990844
Н	-1.647960	5.007163	-2.003308
Н	5.216296	-0.183842	1.737610
Н	7.694990	0.128025	1.555386
Н	8.585556	1.038918	-0.431095
Н	7.324800	1.709941	-2.310213

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Н	4.831566	1.458993	-2.245016
0	2.653256	-0.773255	3.291394
0	3.081349	0.353816	3.356693





The minimum structure illustrates the closest approach of oxygen molecule as the Σ^3O_2 state to the C-N portion of the porphyrin ring in the $[TiO(tpypH_4)]^{4+}$ complex.

Atomic Type Coordinates (X, Y, Z) (Angstroms)

С	1.439552	-3.082967	-0.111931
С	0.011289	-3.056613	-0.047783
С	-0.828082	-4.200951	0.026935
С	-2.110553	-3.759256	0.065843
С	-2.071053	-2.339703	0.009805
С	-3.214515	-1.481899	0.047069
С	-3.185064	-0.117150	0.056957
С	-4.342681	0.768493	0.143643
С	-3.899080	2.024548	0.129871
С	-2.441465	1.975467	0.019593
С	-1.599169	3.132758	0.004416
С	-0.227189	3.073675	-0.012014
С	0.665600	4.256497	-0.002518
С	1.914019	3.825598	-0.047585
С	1.885355	2.344969	-0.096372
С	3.003376	1.548526	-0.124531
С	2.957592	0.117795	-0.116758
С	4.139333	-0.743992	-0.128918
С	3.714667	-2.006683	-0.142595
С	2.255096	-1.988782	-0.135946
Ν	-0.756785	-1.902267	-0.047908
Ν	-2.012021	0.687068	-0.011734
Ν	0.554262	1.913401	-0.060551
Ν	1.824513	-0.631958	-0.117239
С	2.090430	-4.461851	-0.155738
С	2.224419	-5.234057	1.010552
С	2.808297	-6.481261	0.945863
Ν	3.248962	-6.958887	-0.256202
С	3.133011	-6.236372	-1.409824
С	2.557529	-4.983557	-1.373572
С	-4.574365	-2.171712	0.077041
С	-5.316255	-2.261399	1.266411
С	-6.539156	-2.898946	1.267776
Ν	-7.022558	-3.434441	0.107801
С	-6.328854	-3.363885	-1.067654
С	-5.101137	-2.737571	-1.096787
С	-2.279396	4.487274	0.002604
С	-2.163242	5.368584	1.093915

С	-2.793199	6.593655	1.068305
N	-3.526942	6.953975	-0.026364
С	-3.663157	6.128245	-1.107129
С	-3.050854	4.894701	-1.103014
С	4.368935	2.206040	-0.170164
С	5.264319	2.103306	0.911648
С	6.500675	2.707055	0.850100
N	6.859105	3.401474	-0.271126
С	6.021013	3.522151	-1.343486
С	4.775282	2.934687	-1.303850
Ti	-0.112952	0.015338	-0.596104
0	-0.153097	0.022496	-2.195655
Н	-0.497031	-5.226385	0.052020
Н	-3.000303	-4.363715	0.135144
Н	-5.368849	0.439362	0.218151
Н	-4.483549	2.927056	0.198824
Н	0.326040	5.279958	0.035093
Н	2.814441	4.420292	-0.040870
Н	5.158832	-0.395982	-0.133491
Н	4.321916	-2.900182	-0.147815
Н	1.876755	-4.866160	1.968592
Н	2.946500	-7.131835	1.812144
Н	3.683018	-7.898068	-0.294104
Н	3.511859	-6.703386	-2.321612
Н	2.467932	-4.418938	-2.294455
Н	-4.942152	-1.842450	2.192849
Н	-7.164485	-3.008675	2.156415
Н	-7.942277	-3.909567	0.119620
Н	-6.798026	-3.819833	-1.942130
Н	-4.557599	-2.687922	-2.033174
Н	-1.591022	5.095556	1.971872
Н	-2.748238	7.315312	1.886569
Н	-3.993294	7.877817	-0.037404
Н	-4.263513	6.504466	-1.938078
Н	-3.163581	4.252651	-1.968320
Н	4.993805	1.560235	1.808841
Н	7.233799	2.671199	1.658591
Н	7.792130	3.847800	-0.309357
Н	6.396612	4.089869	-2.197424

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Н	4.123844	3.033063	-2.163837
0	2.768079	0.141269	3.087557
0	1.780482	-0.552519	3.121080