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SUPPORTING INFORMATION

Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations†

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1 Computational methods

The molecular structures of the first excited electronic singlet state (S1) of the studied molecules were optimized at the time dependent density functional theory (TD-DFT) level [1] using the B3LYP [2] exchange-correlation functional and def2-TZVP [3] basis sets. The molecular structure optimizations were carried out using Gaussian-09 software [4]. Calculation of singlet and triplet excitation energies were carried out using the extended multi-configuration quasi-degenerate perturbation theory at the second order (XMC-QDPT2) level [5]. In the XMC-QDPT2 calculations, 30 states were included in the effective Hamiltonian. The number of active electrons (e), number of active orbitals (o), and the number of states (s) of the state-average (SA) complete active self-consistent space field (CASSCF) calculations are: PM567 (8 e, 6 o, 5 s), tetraoxa[8]circulene (4B) (10 e, 10 o, 10 s), free-base porphyrin (H2P) (11 e, 14 o, 10 s). The XMC-QDPT2 calculations were carried out using Firefly [6].

Table S1. The calculated excitation energies (in eV) of the studied molecules are compared to available experimental data. Calculated oscillator strengths are given in parenthesis.

Compound	State	XMC-QDPT2	Exp.
PM567	S_1	2.13(0.2)	2.22[a]
	T_1	1.75 -	
	T_2	2.08	-
4B	S_1	2.64	2.99[b]
	T_1	1.89	-
	T_2 (T_3)	2.58	-
H2P	S_1	1.92	2.01[c]
	T_1	1.62	1.58[c]
	T_2	1.8	-

[a] Ref. 7, [b] Ref. 8, [c] Ref. 9.

Table S2. The nonzero matrix elements (in cm-1) of one-electron and two-electron (in parenthesis) spin-orbit coupling interaction between S1 and energetically lower-lying triplets states (Tn).

State	PM567	H2P
$\langle\Psi(S_1)\|H_{SO}\|\Psi(T_1)\rangle$	0.6(0.03)	1.6(0.06)
$\langle\Psi(S_1)\|H_{SO}\|\Psi(T_2)\rangle$	0.3(0.07)	

Table S3. The optimized Cartesian coordinates of the atoms of the S0 and S1 states of H2P.

	S0			S1		
C	2.8963	-1.1305	0.0000	1.1331	2.8973	0.0000
N	2.1175	0.0000	0.0000	-0.0000	2.1154	0.0000
C	2.8963	1.1305	0.0000	-1.1331	2.8973	0.0000
C	0.6782	-4.2592	0.0000	4.2780	0.6814	0.0000
C	-0.6782	-4.2592	0.0000	4.2780	-0.6814	0.0000
C	-1.0849	-2.8564	0.0000	2.8826	-1.0891	0.0000
N	-0.0000	-2.0303	0.0000	2.0516	0.0000	0.0000
C	1.0849	-2.8564	0.0000	2.8827	1.0891	0.0000
C	-0.6782	4.2592	0.0000	-4.2780	-0.6814	0.0000
C	0.6782	4.2592	0.0000	-4.2780	0.6814	0.0000
C	1.0849	2.8564	0.0000	-2.8826	1.0891	0.0000
N	-0.0000	2.0303	0.0000	-2.0516	0.0000	0.0000
C	-1.0849	2.8564	0.0000	-2.8826	-1.0891	0.0000
C	-4.2610	-0.6862	0.0000	0.6875	-4.2620	0.0000
C	-4.2610	0.6862	0.0000	-0.6875	-4.2620	0.0000
C	-2.8963	1.1305	0.0000	-1.1331	-2.8973	0.0000
N	-2.1175	0.0000	0.0000	0.0000	-2.1154	0.0000
C	-2.8963	-1.1305	0.0000	1.1331	-2.8973	0.0000
C	4.2610	0.6862	0.0000	-0.6875	4.2620	0.0000

C	4.2610	−0.6862	0.0000	0.6875	4.2620	0.0000
C	2.4222	−2.4417	0.0000	2.4489	2.4283	0.0000
C	−2.4222	2.4417	0.0000	−2.4489	−2.4283	0.0000
C	−2.4222	−2.4417	0.0000	2.4489	−2.4283	0.0000
C	2.4222	2.4417	0.0000	−2.4489	2.4283	0.0000
H	1.1019	0.0000	0.0000	−0.0000	1.1012	0.0000
H	1.3524	−5.1076	0.0000	5.1277	1.3535	0.0000
H	−1.3524	−5.1076	0.0000	5.1277	−1.3535	0.0000
H	−1.3524	5.1076	0.0000	−5.1277	−1.3535	0.0000
H	1.3524	5.1076	0.0000	−5.1277	1.3535	0.0000
H	−5.1177	−1.3476	0.0000	1.3483	−5.1191	0.0000
H	−5.1177	1.3476	0.0000	−1.3483	−5.1191	0.0000
H	−1.1019	−0.0000	0.0000	0.0000	−1.1012	0.0000
H	5.1177	1.3476	0.0000	−1.3483	5.1191	0.0000
H	5.1177	−1.3476	0.0000	1.3483	5.1191	0.0000
H	3.1800	−3.2203	0.0000	3.2220	3.1919	0.0000
H	−3.1800	3.2203	0.0000	−3.2220	−3.1919	0.0000
H	−3.1800	−3.2203	0.0000	3.2220	−3.1919	0.0000
H	3.1800	3.2203	0.0000	−3.2220	3.1919	0.0000

Table S4. The harmonic frequencies (in cm^{-1}) of of the optimized gemometries of S0 and S1 states of H2P.

S0	S1
57.01	53.87
66.73	65.94
95.16	95.73
105.72	106.27
127.99	118.67
133.51	125.82
157.29	153.52
186.8	181.14
207.63	193.63
208.98	202.93
293.52	286.84
298.96	290.95
310.33	308.16
316.89	312.6
336.88	316.21
359.27	355.97
360.15	356.99
396.37	393.28
422.24	393.46
429.17	418.04
443.86	420.25
480.98	451.23
637.66	599.5
653.57	633.55
678.76	666.58
684.47	668.58
692.54	675.42
710.19	681.93
710.87	685.39
713.25	693.87
713.55	695.12
734.13	723.18
738.52	724.12

740.53	726.49
746.66	742.12
752.63	747.12
786.6	766.59
790.31	773.64
792.42	774.09
793.58	787.15
795.54	790.06
798.21	793.92
808.28	806.92
818.7	816.23
850.23	829
860.62	841.54
861.77	842.86
873.57	857.51
901.54	878.73
906.62	882.84
912.14	896.03
914.5	896.95
972.74	963.09
976.3	971.69
995.44	989.31
1002.14	994.74
1013.51	1008.17
1013.79	1009.91
1023.94	1023.24
1030.04	1026.43
1082.05	1083.56
1086.63	1084.57
1089.7	1092.67
1096.53	1095.01
1174.02	1151.57
1177.28	1156.73
1195.64	1183.5
1216.47	1197.76
1226.22	1210.49
1236.43	1260.26
1266.21	1265.23
1270.35	1290.54
1286.35	1310.61
1325.14	1325.73
1359.55	1344.09
1393.55	1364.1
1395.28	1395.1
1400.6	1396.89
1424.04	1400.57
1447.68	1404.67
1448.91	1428.68
1452	1437.16
1455.73	1449.41
1478.78	1452.14
1541.72	1523.51
1542.43	1527.35
1554.63	1539.85
1558.78	1547.44
1574.4	1562.73

1595.79	1581.22
1607.97	1610.89
1644.35	1611.01
1648.08	1618.32
1656.54	1641.6
3196.37	3195.42
3196.38	3195.43
3196.38	3195.46
3196.58	3195.64
3230.97	3233.01
3230.98	3233.02
3249.93	3250.3
3249.95	3250.35
3251.88	3252.72
3251.99	3252.91
3266.99	3267.05
3267.05	3267.14
3550.43	3573.61
3592.72	3613.11

Table S5. The optimized Cartesian coordinates of the atoms of the S0 and S1 states of 4B.

	S0			S1		
O	3.8809	-0.0477	0.0000	-3.7724	-0.9657	0.0000
C	3.0341	-1.1443	0.0000	-2.6939	-1.8347	0.0000
C	1.6945	-0.7367	0.0000	-1.4787	-1.0979	0.0000
C	0.6947	-1.7119	0.0000	-0.2522	-1.8243	0.0000
C	1.0692	-3.0611	0.0000	-0.3145	-3.2441	0.0000
O	-0.0477	-3.8808	0.0000	0.9657	-3.7724	0.0000
C	-1.1444	-3.0342	0.0000	1.8347	-2.6939	0.0000
C	-0.7367	-1.6945	0.0000	1.0979	-1.4787	0.0000
C	-1.7118	-0.6947	0.0000	1.8243	-0.2522	0.0000
C	-3.0611	-1.0692	0.0000	3.2441	-0.3145	0.0000
O	-3.8809	0.0477	0.0000	3.7724	0.9657	0.0000
C	-3.0341	1.1443	0.0000	2.6939	1.8347	0.0000
C	-1.6945	0.7367	0.0000	1.4787	1.0979	0.0000
C	-0.6947	1.7119	0.0000	0.2522	1.8243	0.0000
C	-1.0692	3.0611	0.0000	0.3145	3.2441	0.0000
C	1.1443	3.0341	0.0000	-1.8347	2.6939	0.0000
C	0.7367	1.6945	0.0000	-1.0979	1.4787	0.0000
C	1.7119	0.6947	0.0000	-1.8243	0.2522	0.0000
C	3.0611	1.0692	0.0000	-3.2441	0.3145	0.0000
C	3.4725	2.4081	0.0000	-3.9442	1.5031	0.0000
C	2.4930	3.4122	0.0000	-3.2135	2.7367	0.0000
H	2.7762	4.4588	0.0000	-3.7434	3.6825	0.0000
C	-2.4082	3.4725	0.0000	1.5031	3.9442	0.0000
C	-3.4122	2.4930	0.0000	2.7367	3.2135	0.0000
H	-2.6653	4.5258	0.0000	1.5134	5.0283	0.0000
C	-3.4726	-2.4081	0.0000	3.9442	-1.5031	0.0000
C	-2.4931	-3.4122	0.0000	3.2135	-2.7367	0.0000
H	-4.5259	-2.6653	0.0000	5.0283	-1.5134	0.0000
C	2.4082	-3.4725	0.0000	-1.5031	-3.9442	0.0000
C	3.4122	-2.4930	0.0000	-2.7367	-3.2135	0.0000
H	4.4589	-2.7762	0.0000	-3.6825	-3.7434	0.0000
O	0.0477	3.8809	0.0000	-0.9657	3.7724	0.0000
H	4.5259	2.6652	0.0000	-5.0283	1.5134	0.0000

H	−4.4589	2.7762	0.0000	3.6825	3.7434	0.0000
H	−2.7762	−4.4588	0.0000	3.7434	−3.6825	0.0000
H	2.6653	−4.5258	0.0000	−1.5134	−5.0283	0.0000

Table S6. The harmonic frequencies (in cm^{-1}) of of the optimized gemometries of S0 and S1 states of 4B.

S0	S1
98.2958	83.2203
100.8025	87.055
107.2543	90.6944
194.0436	182.8902
194.0436	182.9259
245.5719	236.7952
258.9386	236.9072
258.9386	256.6431
289.8383	272.9526
308.2002	309.2872
326.1492	317.667
370.5905	366.6876
376.1919	372.3867
376.1919	372.3903
427.0945	408.2343
427.0945	422.0198
439.7414	422.0255
452.8985	438.4552
484.6923	459.2513
495.0841	463.8873
510.6864	474.8236
514.8162	474.8724
518.6275	489.6657
518.6275	511.7334
543.0431	520.5698
543.0431	520.5705
609.5417	590.9023
633.043	627.2015
633.0431	632.7749
639.1208	636.8009
661.3405	636.8027
662.5194	643.2265
662.8705	643.2953
662.8705	660.365
673.0353	661.7737
680.5815	691.1308
718.2137	692.5825
718.2137	692.6036
727.9097	693.8553
751.6557	746.7959
751.6557	746.7967
798.7263	791.4639
809.1465	802.3092
814.5131	805.5579
814.5131	805.5958
820.1082	808.9097
858.7382	856.1883
884.2917	870.7601
887.7718	870.7612
887.7719	873.7807

931.9333	883.0801
932.9568	883.2135
932.9568	883.4141
933.3162	883.4222
1015.7668	988.8606
1041.7853	1031.6669
1041.7853	1031.6707
1052.9732	1045.1902
1100.9029	1104.3389
1126.9675	1104.9424
1126.9675	1106.7947
1134.4127	1106.801
1170.0681	1146.1592
1206.5245	1178.0972
1206.5245	1178.1017
1243.7176	1211.8806
1246.6153	1238.8801
1252.414	1240.9721
1258.048	1240.9728
1258.048	1244.1526
1284.7024	1252.9089
1304.5078	1301.9225
1304.5078	1301.9256
1391.1079	1396.4316
1411.9409	1415.862
1411.9409	1428.9925
1434.7672	1428.9961
1459.1185	1455.1108
1461.1972	1456.869
1467.3558	1469.2783
1474.3188	1469.2808
1474.3188	1483.9519
1495.3572	1502.211
1523.925	1502.2146
1523.925	1529.7121
1548.0428	1542.6752
1655.2478	1582.9435
1655.2478	1635.0811
1657.3456	1649.7715
1666.8725	1649.7755
1668.9166	1653.0662
1707.3566	1653.0752
1707.3566	1670.1766
1721.1573	1718.6884
3251.7638	3225.0299
3252.094	3225.0305
3252.094	3225.5231
3252.2842	3225.5643
3264.3734	3236.6518
3264.4827	3236.7577
3264.4827	3236.7588
3264.6347	3237.1605

Table S7. The optimized Cartesian coordinates of the atoms of the S0 and S1 states of PM567

	S0			S1		
C	1.2147	0.8288	-0.1589	1.2328	0.8590	-0.2214
N	1.2456	-0.5673	-0.1495	1.2640	-0.5579	-0.2879
B	0.0117	-1.5108	-0.0877	-0.0002	-1.4761	-0.2423
N	-1.2279	-0.5893	0.0818	-1.1945	-0.5640	0.0614
C	-1.2234	0.8070	0.0649	-1.2089	0.8493	0.0088
C	-0.0143	1.5135	-0.0918	-0.0538	1.5735	-0.2140
C	-2.4925	-1.0224	0.2436	-2.4559	-1.0073	0.2863
C	-3.3633	0.0887	0.3611	-3.3262	0.0990	0.4108
C	-2.5780	1.2417	0.2464	-2.5713	1.2601	0.2405
C	2.5733	1.2865	-0.2238	2.5193	1.2962	-0.1604
C	3.3843	0.1477	-0.2655	3.3894	0.0784	-0.2470
C	2.5249	-0.9785	-0.2209	2.5443	-1.0173	-0.3186
C	-3.1142	2.6412	0.3490	-3.0976	2.6558	0.3647
C	3.0936	2.6961	-0.2096	3.0966	2.6645	-0.0365
C	2.8842	-2.4292	-0.2456	2.8865	-2.4678	-0.4048
C	-2.8219	-2.4800	0.2790	-2.7894	-2.4569	0.3466
C	-5.6522	0.1400	-0.7668	-5.6508	0.0534	-0.6207
C	-4.8549	0.0142	0.5498	-4.8030	0.0152	0.6621
C	5.5447	-0.0025	1.0806	5.4475	0.0069	1.2240
C	4.8882	0.0908	-0.3091	4.8722	0.0793	-0.2122
C	-0.0371	3.0186	-0.1923	-0.0631	3.0439	-0.5108
F	-0.0923	-2.2490	-1.2671	-0.1370	-2.1280	-1.4771
F	0.1247	-2.3639	1.0105	0.1712	-2.4297	0.7721
H	-2.5483	3.2559	1.0554	-2.4551	3.2854	0.9835
H	-4.1519	2.6236	0.6907	-4.0865	2.6492	0.8243
H	-3.1075	3.1645	-0.6155	-3.2048	3.1563	-0.6038
H	2.6670	3.2884	0.6054	2.3664	3.4035	0.2755
H	4.1779	2.6996	-0.0782	3.9122	2.6724	0.6919
H	2.8838	3.2314	-1.1443	3.5284	2.9998	-0.9870
H	2.3296	-2.9420	-1.0367	2.3288	-2.9541	-1.2068
H	3.9544	-2.5670	-0.4087	3.9519	-2.5925	-0.5985
H	2.6015	-2.9095	0.6961	2.6385	-2.9926	0.5200
H	-3.8962	-2.6415	0.3949	-3.8579	-2.6013	0.4966
H	-2.4855	-2.9652	-0.6445	-2.4976	-2.9636	-0.5777
H	-2.2897	-2.9709	1.1008	-2.2492	-2.9537	1.1564
H	-6.7297	0.0771	-0.5807	-6.7163	-0.0106	-0.3863
H	-5.3820	-0.6576	-1.4715	-5.3979	-0.7779	-1.2816
H	-5.4480	1.1001	-1.2592	-5.4811	0.9782	-1.1756
H	-5.1803	0.8021	1.2455	-5.1102	0.8366	1.3156
H	-5.1147	-0.9346	1.0390	-5.0297	-0.9002	1.2134
H	6.6359	-0.0487	0.9982	6.5387	0.0220	1.1897
H	5.2069	-0.8958	1.6153	5.1297	-0.9099	1.7212
H	5.2869	0.8650	1.6966	5.1127	0.8503	1.8295
H	5.2027	-0.7697	-0.9114	5.2554	-0.7709	-0.7809
H	5.2773	0.9705	-0.8338	5.2549	0.9833	-0.6947
H	-0.9604	3.3703	-0.6471	-1.0304	3.3663	-0.8836
H	0.7864	3.3872	-0.7992	0.6730	3.2847	-1.2807
H	0.0445	3.4873	0.7966	0.1704	3.6670	0.3621

Table S8. The harmonic frequencies (in cm^{-1}) of of the optimized gemometries of S0 and S1 states of PM567.

29.7188	26.06
41.863	43.00
54.377	51.72
58.3602	56.69

64.7955	61.20
76.3366	65.66
81.1303	81.01
89.1687	93.93
97.4608	98.35
121.5742	101.52
138.8692	140.53
157.8011	157.91
164.5316	163.92
179.4652	180.92
183.9278	185.43
198.9602	205.49
210.6795	215.19
219.3301	222.92
222.3884	228.18
242.7367	247.79
256.5914	257.79
294.1799	294.77
299.3654	300.07
304.0437	307.86
308.6826	308.98
325.6463	326.69
330.4056	331.71
335.1245	336.10
367.7973	372.56
376.0242	379.17
393.0753	394.48
412.1283	412.77
448.0384	449.75
465.0567	469.09
487.3325	488.77
550.5741	548.83
551.6531	555.59
555.5138	557.76
568.0892	570.47
572.1426	576.60
648.7535	648.47
657.4159	659.92
691.8113	692.87
703.0364	708.78
709.3293	718.91
722.0536	735.68
741.56	740.84
762.8587	765.37
776.9601	776.17
788.7286	787.89
840.8399	846.22
873.2829	876.25
909.0182	910.77
967.3872	972.11
970.378	974.73
993.293	1001.32
1007.4868	1012.15
1037.97	1040.78
1042.4261	1045.11
1044.934	1046.38

1047.1037	1049.34
1049.6127	1051.98
1054.916	1058.74
1055.6684	1059.55
1062.7546	1076.74
1083.6312	1086.95
1085.7949	1088.58
1093.9027	1118.83
1118.6741	1129.80
1129.512	1151.86
1149.7629	1152.81
1151.3501	1155.24
1187.3702	1194.33
1192.1905	1199.61
1224.9439	1238.50
1243.9973	1255.57
1298.0258	1299.07
1300.6775	1301.72
1345.6616	1355.06
1356.801	1360.56
1361.8333	1372.99
1389.9626	1400.88
1410.1434	1414.37
1413.1738	1418.58
1416.9042	1421.55
1417.5587	1422.63
1420.2174	1424.19
1423.5126	1428.93
1425.2587	1432.28
1433.2664	1446.27
1436.4995	1453.05
1471.0387	1477.69
1473.2783	1481.22
1475.6018	1483.24
1480.5085	1485.13
1482.6614	1486.15
1493.3011	1499.62
1494.5847	1501.45
1498.2342	1506.57
1499.5948	1507.15
1500.3504	1508.94
1500.8705	1510.60
1501.4756	1511.29
1505.7327	1514.24
1508.4542	1518.53
1510.4856	1520.35
1518.6138	1528.08
1519.7703	1530.26
1525.0494	1535.10
1529.5471	1540.56
1559.1689	1572.87
1572.7165	1587.16
1579.3927	1594.56
3026.2213	3034.45
3027.3088	3035.49
3029.5536	3042.61

3029.7909	3042.81
3036.4875	3044.31
3037.7348	3045.89
3038.0579	3047.93
3047.0007	3061.62
3049.306	3062.03
3062.613	3075.59
3063.0042	3076.82
3082.036	3095.56
3082.3816	3096.01
3093.1854	3115.04
3093.626	3115.16
3099.9904	3120.48
3100.6998	3120.72
3101.4832	3122.89
3102.036	3123.48
3115.4626	3130.45
3117.033	3131.73
3132.7452	3153.29
3136.6613	3155.30
3149.5377	3162.05
3182.9007	3198.61

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