Supporting information:

Table S1. The energies, dipole moments, and configuration contributions for the ground state, 8 singlet excited states, and 8 triplet excited states as calculated by CISD with 4 electrons and 11 molecular orbitals in active space.

State	Energy / cm^{-1}	Dipole Moment / D	Coefficients of the MO configurations
S_0	0	4.235	0.99 of 1
S_1	27683.5	1.493	-0.65 of 5, 0.14 of 7, -0.2 of 14
S_2	30516.5	12.643	0.57 of 2, 0.33 of 3, -0.15 of 11, 0.15 of 12
S_3	32614.9	1.548	-0.14 of 5, -0.65 of 7, -0.21 of 16
S_4	36408.3	11.143	-0.69 of 6
S_5	38305.0	10.970	-0.11 of 2, 0.43 of 3, -0.12 of 9, 0.52 of 11
S_6	40209.7	13.288	0.45 of 4, -0.52 of 13
S_7	41404.2	17.284	-0.22 of 2, 0.34 of 3, -0.38 of 11, -0.15 of 12, 0.18 of 20, -0.29 of 57, -0.12 of 58, -0.18 of 66, -0.14 of 67, 0.1 of 77
S_8	45100.7	1.656	-0.54 of 8, 0.41 of 17
T_1	20540.7	1.137	0.64 of 5, -0.16 of 7, 0.23 of 14
T_2	24600.4	10.586	0.54 of 2, 0.34 of 3, -0.24 of 11, 0.12 of 12
T_3	27175.1	2.049	0.15 of 5, 0.64 of 7, 0.24 of 18
T_4	28692.4	11.593	0.44 of 3, -0.13 of 9, 0.52 of 11, -0.13 of 12
T_5	31977.3	10.323	-0.7 of 6
T_6	35318.7	12.518	-0.39 of 4, 0.59 of 13
T_7	43074.9	27.478	0.35 of 2, -0.36 of 3, 0.35 of 11, -0.19 of 20, -0.16 of 58, -0.15 of 66
T_8	43970.8	3.798	0.53 of 8, -0.43 of 17

Table S2. The energy and configuration assignment for the lowest-energy transitions as calculated by single and double excitation from occupied orbitals to the virtual orbitals.

Transition	Assignment[a]	Energy/eV	Transition	Assignment[a]	Energy/eV
1[b]		0	14	H(-1) →L(3)	6.843
2	H →L	4.566	15	H(-1) →L(4)	6.692
3	H →L(1)	4.764	16	H(-1) →L(5)	7.555
4	H →L(2)	6.296	17	H(-1) →L(6)	6.696
5	H →L(3)	3.460	18	H(-1) →L(7)	7.229
6	H →L(4)	4.273	19	H(-1) →L(8)	7.623
7	H →L(5)	4.142	20[c]	H →L(1), H(-1) →L	8.014
8	H →L(6)	6.472	57[c]	H →L	12.865
9	H →L(7)	7.150	58[c]	H →L, H →L(1)	11.629
10	H →L(8)	8.374	66[c]	H →L, H(-1) →L	9.890
11	H)-1) →L	4.694	67[c]	H →L, H(-1) →L(1)	9.755
12	H(-1) →L(1)	5.994	77[c]	H →L(1)	13.376
13	H(-1) →L(1)	5.369			

a. H is for HOMO, and L is for LUMO. b In the first configuration, all of the electrons are paired in occupied orbitals and there is no transition to the virtual orbitals. c Refers to double excitation.