Supporting Information

Different mechanisms for lanthanide(III) sensitization and Yb-field-induced single-molecule magnet behaviour in a series of pentagonal bipyramidal and octahedral lanthanide complexes with axial phosphine oxide ligands

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1. Crystallographic data

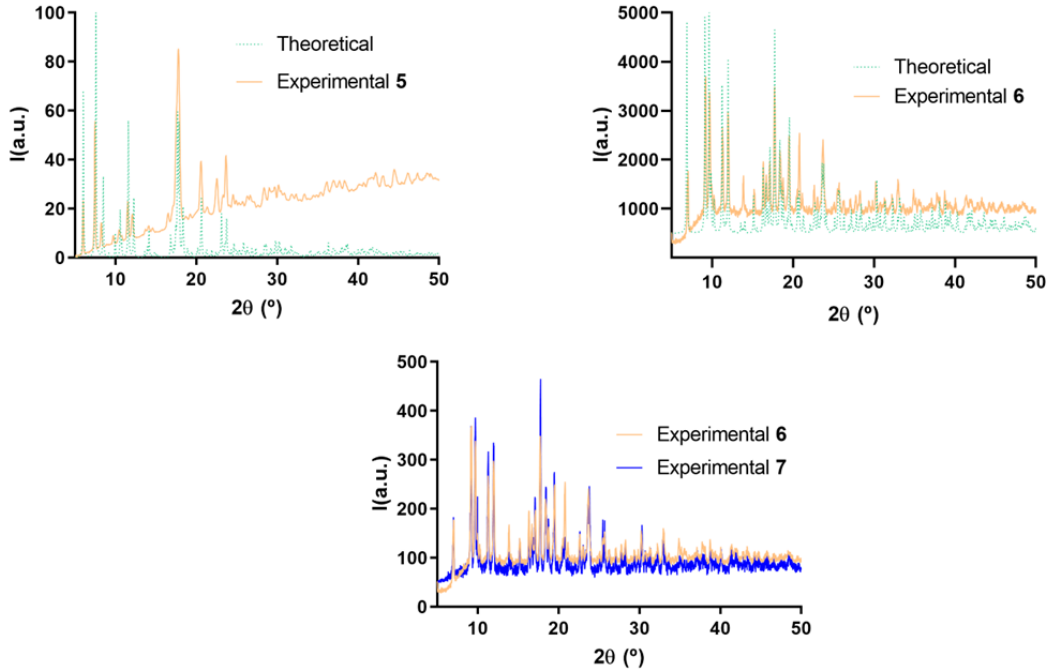

Figure S1. X-ray powder diffractograms for **5-6** (orange), **7** (blue) and the calculated from the X-ray crystal structures (green).

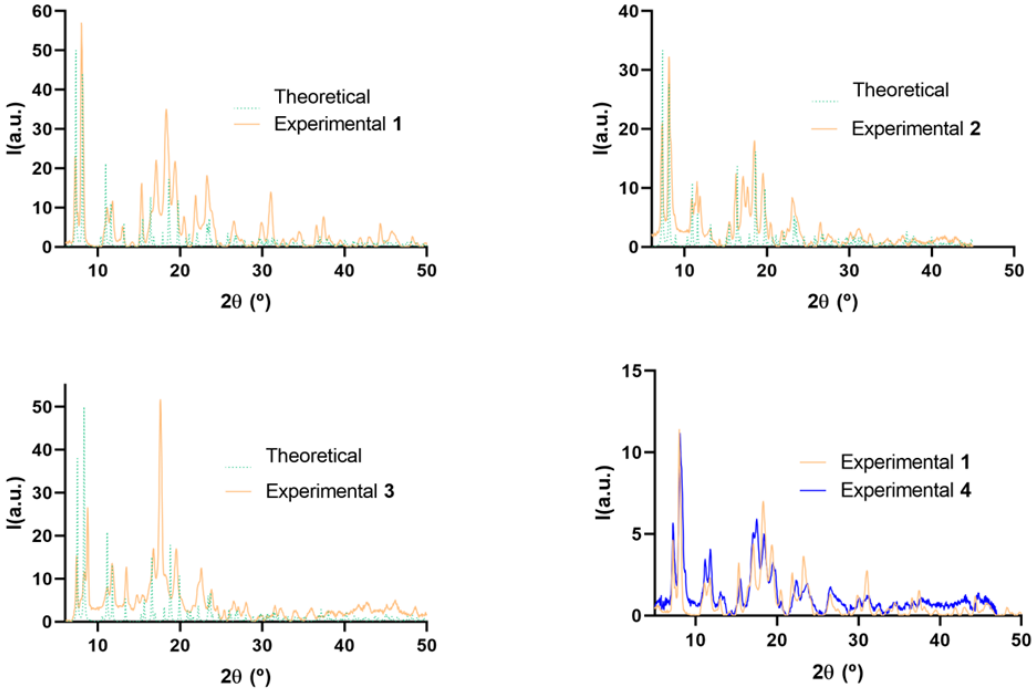

Figure S2. X-ray powder diffractograms for **1-3** (orange), **4** (blue) and the calculated from the X-ray crystal structures (green).

Table S1. Crystallographic data and structural refinement details for complexes **1-3** and **5-6**.

Compound	**1**	**2**	**3**	**5**	**6**
Formula	$C_{31}H_{49}Cl_{1.5}Yb_{0.5}O_4P$	$C_{66}H_{109}Cl_3TbO_{10.5}P_2$	$C_{61.2}H_{96.4}Cl_3GdO_{7.8}P_2$	$C_{59.4}H_{86.8}Cl_3EuO_{4.4}P_2$	$C_{58}H_{82}Cl_3GdO_3P_2$
M_r	656.36	1397.80	1282.49	1191.50	1152.77
Crystal System	Tetragonal	Tetragonal	Tetragonal	Triclinic	Monoclinic
Space Group	I_4	$P4_3$	$P4_3$	P-1	C2/c
a (Å)	24.1565(11)	24.1557(6)	24.2107(8)	12.2190(5)	17.3000(12)
b (Å)	24.1565(11)	24.1557(6)	24.2107(8)	15.2856(5)	11.6907(7)
c (Å)	12.1744(8)	12.2000(4)	12.1822(6)	15.8953(5)	25.6789(18)
α (°)	90	90	90	99.2160(10)	90
β (°)	90	90	90	101.3970(10)	93.668(2)
γ (°)	90	90	90	101.4720(10)	90
V (Å^3)	7104.2(8)	7118.7(4)	7140.7(6)	2790.01(17)	5182.9(6)
Z	8	4	4	2	4
Dc (g cm^{-1})	1.227	1.304	1.190	1.401	1.477
μ(MoK$_α$) (mm^{-1})	1.520	1.204	1.130	1.371	1.541
T (K)	100	100	100	100	100
Observed reflections[a]	10751 (9282)	21231 (20992)	21479 (20458)	13941 (11306)	6431 (5958)
R_{int}[a]	0.0630	0.0266	0.0359	0.1295	0.0479
Parameters	348	766	749	774	314
GOF	1.113	1.185	1.081	1.054	1.113
R_1[b,a]	0.0531 (0.0386)	0.0300 (0.0297)	0.0474 (0.0445)	0.0750 (0.0415)	0.0234 (0.0181)
wR_2[c,a]	0.1109 (0.1046)	0.0775 (0.0773)	0.1142 (0.1212)	0.1090 (0.0993)	0.0440 (0.0431)

[a] Values in parentheses for reflections with I > 2s(I)

[b] $R1 = \sum||Fo| - |Fc||/\sum|Fo|$

[c] $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{½}$

Table S2. Selected bond distances (Å) and angles (°) for complex **1**.

Selected bond distances (Å)			
Yb1-O1	2.163 (4)	Yb1-Cl1	2.673 (2)
Yb1-O2	2.313 (5)	O1-P1	1.524 (4)
Yb1-O3	2.328 (5)		
Selected bond angles (º)			
O1-Yb1-O2	92.44 (19)	O2-Yb1-O3	71.3 (3)
O1-Yb1-O2	87.68 (19)	O2-Yb1-Cl1	75.1 (2)
O1-Yb1-O3	88.43 (17)	O3-Yb1-O3	67.3 (4)
O1-Yb1-O3	91.18 (17)	O1-Yb1-O1	179.5 (2)
O1-Yb1-Cl1	90.24 (11)	Yb1-O1-P1	173.5 (3)

Table S3. Selected bond distances (Å) and angles (°) for complex **2**.

Selected bond distances (Å)			
Tb1-O1	2.234 (3)	Tb1-O6	2.367 (3)
Tb1-O2	2.243 (3)	Tb1-Cl1	2.720 (11)
Tb1-O3	2.3781 (3)	O1-P1	1.520 (3)
Tb1-O4	2.393 (3)	O2-P2	1.509 (3)
Tb1-O5	2.396 (3)		
Selected bond angles (º)			
O1-Tb1-O3	85.96 (12)	O2-Tb1-Cl1	88.21 (10)
O1-Tb1-O4	92.48 (13)	O3-Tb1-O4	70.53 (13)
O1-Tb1-O5	88.51 (13)	O3-Tb1-Cl1	73.94 (9)
O1-Tb1-O6	89.64 (12)	O4-Tb1-O5	67.78 (13)
O1-Tb1-Cl1	92.79 (10)	O5-Tb1-O6	71.17 (13)
O2-Tb1-O3	96.90 (12)	O6-Tb1-Cl1	77.24 (10)
O2-Tb1-O4	88.30 (13)	O1-Tb1-O2	177.14 (12)
O2-Tb1-O5	89.24 (13)	Tb1-O1-P1	171.5 (2)
O2-Tb1-O6	87.96 (12)	Tb1-O2-P2	172.0 (2)

Table S4. Selected bond distances (Å) and angles (°) for complex **3**.

Selected bond distances (Å)			
Gd1-O1	2.256 (3)	Gd1-O6	2.368 (5)
Gd1-O2	2.250 (3)	Gd1-Cl1	2.714 (2)
Gd1-O3	2.388 (5)	O1-P1	1.513 (3)
Gd1-O4	2.408 (5)	O2-P2	1.520 (4)
Gd1-O5	2.390 (5)		
Selected bond angles (º)			
O1-Gd1-O3	85.93 (16)	O2-Gd1-Cl1	90.29 (11)
O1-Gd1-O4	91.38 (16)	O3-Gd1-O4	71.1 (3)
O1-Gd1-O5	87.42 (16)	O3-Gd1-Cl1	73.85 (18)
O1-Gd1-O6	91.42 (19)	O4-Gd1-O5	67.5 (3)
O1-Gd1-Cl1	92.25 (11)	O5-Gd1-O6	71.5 (3)
O2-Gd1-O3	96.14 (17)	O6-Gd1-Cl1	76.6 (2)
O2-Gd1-O4	87.37 (16)	O1-Gd1-O2	177.09 (16)
O2-Gd1-O5	89.67 (17)	Gd1-O1-P1	171.0 (3)
O2-Gd1-O6	87.79 (17)	Gd1-O2-P2	171.1 (3)

Table S5. Obtained S values with the SHAPE software for complexes **1-3**.

Complex		JETPY-7	JPBPY-7	CTPR-7	COC-7	PBPY-7	HPY-7	HP-7
1	Yb	24.036	2.612	6.026	7.717	0.648	25.096	33.744
2	Tb	23.139	2.834	5.204	7.015	0.716	24.351	33.548
3	Gd	23.673	2.845	5.456	7.165	0.635	25.000	33.612

JETPY-7 = Johnson elongated triangular pyramid J7; JPBPY-7 = Johnson pentagonal bipyramid J13; CTPR-7 = Capped trigonal prism; COC-7 = Capped octahedron; PBPY-7 = Pentagonal bipyramid; HPY-7 = Hexagonal pyramid; HP-7 = Heptagon

Table S6. Selected bond distances (Å) and angles (°) for complex **5**.

Selected bond distances (Å)			
Eu1-O1	2.289 (2)	Eu1-Cl2	2.648 (10)
Eu1-O2	2.312 (2)	Eu1-Cl3	2.652 (15)
Eu1-O3	2.437 (5)	O1-P1	1.516 (3)
Eu1-Cl1	2.656 (8)	O2-P2	1.513 (3)
Selected bond angles (º)			
O1-Eu1-O3	93.64 (14)	Cl1-Eu1-Cl2	107.57 (3)
O1-Eu1-Cl1	87.79 (7)	Cl2-Eu1-Cl3	91.95 (5)
O1-Eu1-Cl2	90.28 (7)	Cl3-Eu1-O3	76.43 (16)
O1-Eu1-Cl3	89.96 (8)	O1-Eu1-O2	175.37 (8)
O2-Eu1-O3	87.30 (14)	Cl2-Eu1-O3	167.71 (16)
O2-Eu1-Cl1	87.79 (6)	Cl3-Eu1-Cl1	160.36 (5)
O2-Eu1-Cl2	89.73 (7)	Eu1-O1-P1	177.68 (15)
O2-Eu1-Cl3	94.67 (7)	Eu1-O2-P2	172.94 (15)
O3-Eu1-Cl1	84.24 (16)		

Table S7. Selected bond distances (Å) and angles (º) for complex **6**.

Selected bond distances (Å)			
Gd1-O1	2.287 (2)	Gd1-Cl2	2.632 (4)
Gd1-O2	2.501 (15)	O1-P1	1.513 (10)
Gd1-Cl1	2.620 (5)		
Selected bond angles (°)			
O1-Gd1-O2	89.16 (3)	O1-Gd1-O1	178.31 (5)
O1-Gd1-Cl1	90.84 (3)	O2-Gd1-Cl1	180.00 (5)
O1-Gd1-Cl2	92.18 (3)	Cl2-Gd1-Cl2	164.30 (16)
O2-Gd1-Cl2	82.15 (8)	Gd1-O1-P1	168.53 (7)
Cl2-Gd1-Cl1	97.85 (8)		

Table S8. S-parameter values calculated with the Shape software for compounds **5-6**.

Complex		JPPY-6	TPR-6	OC-6	PPY-6	HP-6
5	Eu	26.621	11.310	1.605	23.708	33.265
6	Gd	29.862	15.058	0.896	27.105	32.920

JPPY-6 = Johnson pentagonal pyramid J2; TPR-6 = Trigonal prism; OC-6 = Octahedron; PPY-6 = Pentagonal pyramid; HP-6 = Hexagon

2. Magnetic properties

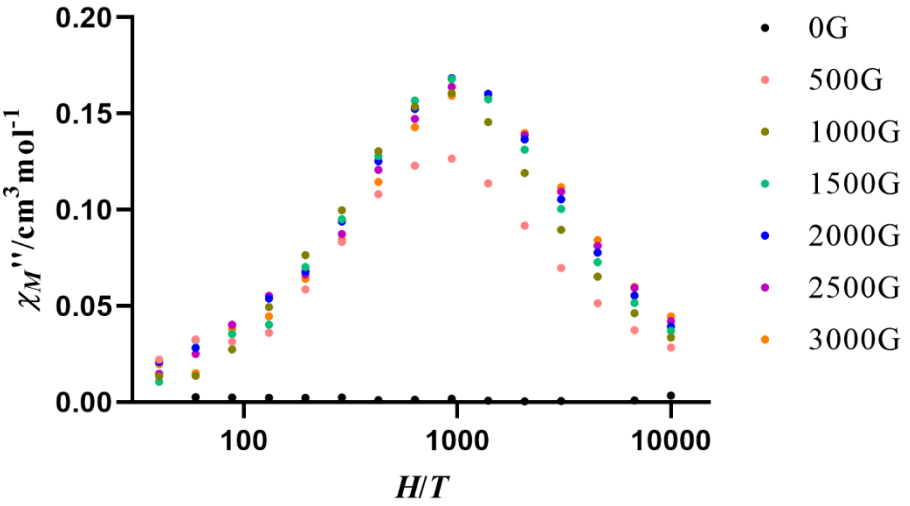

Figure S3. Field dependence of the out-of-phase signals (χ_M'') at different frequencies and 3 K for **1**.

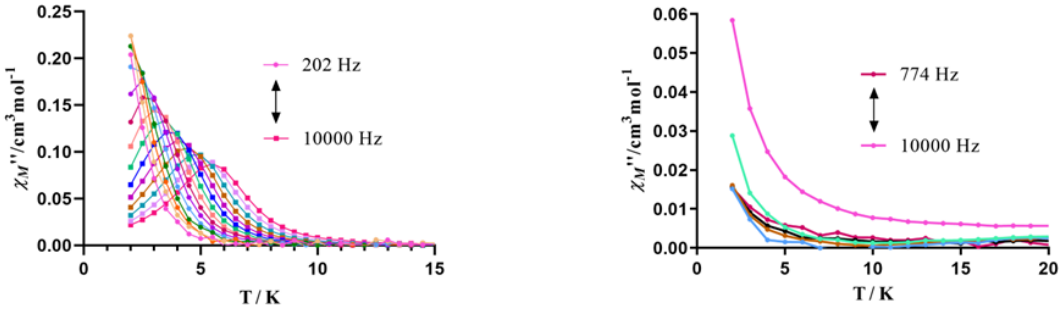

Figure S4. Temperature dependence of the out-of-phase ac susceptibility signals (χ_M'') at 1000 Oe for **1** (left) and **2** (right)

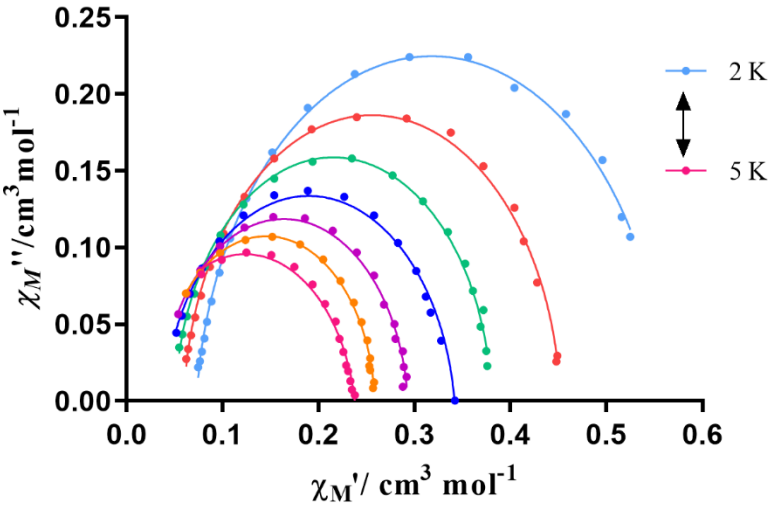

Figure S5. Cole-Cole plot for **1**

Table S9. CASSCF computed relative energies (in cm^{-1}) of the seven Kramers Doublets and g tensors for **1**.

Energy (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	Wavefunction composition
0.0	5.136540	3.942849	1.170722	99.0 |± 1/2 >
282.33	0.000952	1.195925	3.420337	97.5 |± 3/2 >
432.30	0.393152	1.217489	7.104737	63.4 |± 7/2 > + 35.3 |± 5/2 >
564.67	0.206921	0.858752	6.881443	63.3 |± 5/2 > + 35.4 |± 7/2 >
10129.51	2.805975	2.306777	0.808719	
10465.40	0.192571	0.485770	3.322085	
10584.76	0.306269	0.516886	4.036218	

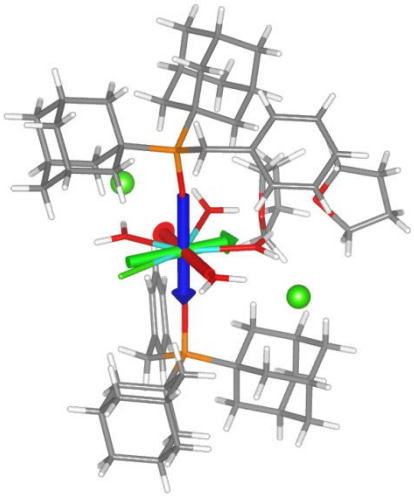

Figure S6. Orientation of the *g*-tensor components obtained from CASSCF calculations for **1**. The reference axis *x*, *y* and *z* of the *g*-tensor are displayed in red, green and blue, respectively. Code colours: yterbium (cyan), oxygen (red), chloride (green), phosphorus (orange), carbon (grey) and hydrogen (white).

Table S10. Computed B_k^q parameters from CASSCF calculations for **1**.

k	q	B(k,q)
2	-2	-0.31
2	-1	-9.52
2	0	11.80
2	1	-1.53
2	2	-2.59
k	**q**	**B(k,q)**
4	-4	0.18
4	-3	0.20
4	-2	-0.27E-01
4	-1	-0.23
4	0	-0.22
4	1	-0.85E-01
4	2	-0.16E-02
4	3	-0.52
4	4	0.23E-01
k	**q**	**B(k,q)**
6	-6	-0.24E-01
6	-5	0.35E-01
6	-4	0.24E-02
6	-3	0.96E-02
6	-2	-0.32E-02
6	-1	-0.19E-02
6	0	0.27E-02
6	1	-0.13E-02
6	2	0.63E-03
6	3	-0.14E-01
6	4	-0.21E-02
6	5	0.66E-02
6	6	0.81E-02

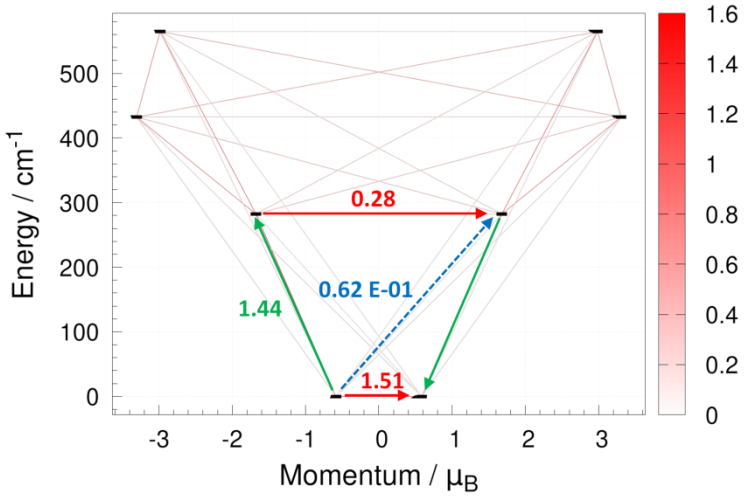

Figure S7. *Ab initio* calculated relaxation pathways in compound **1**. The black lines indicate the KDs as a function of the magnetic moments. Red lines denote QTM in the ground state and TA/QTM through the first and second excited states. Blue dashed lines represent possible Orbach processes.

3. Isolated ligand calculations

Molecular mechanics calculations were carried out using the MMFF force field.[1] After selecting conformers within an energy window of 20 kJ/mol, three were optimized in the ground state (S_0), both in dichloromethane solution and in the gas phase, using the dispersion-corrected CAM-B3LYP-D3 functional[2,3] with the 6-31+G** basis set (**Figure S8**).

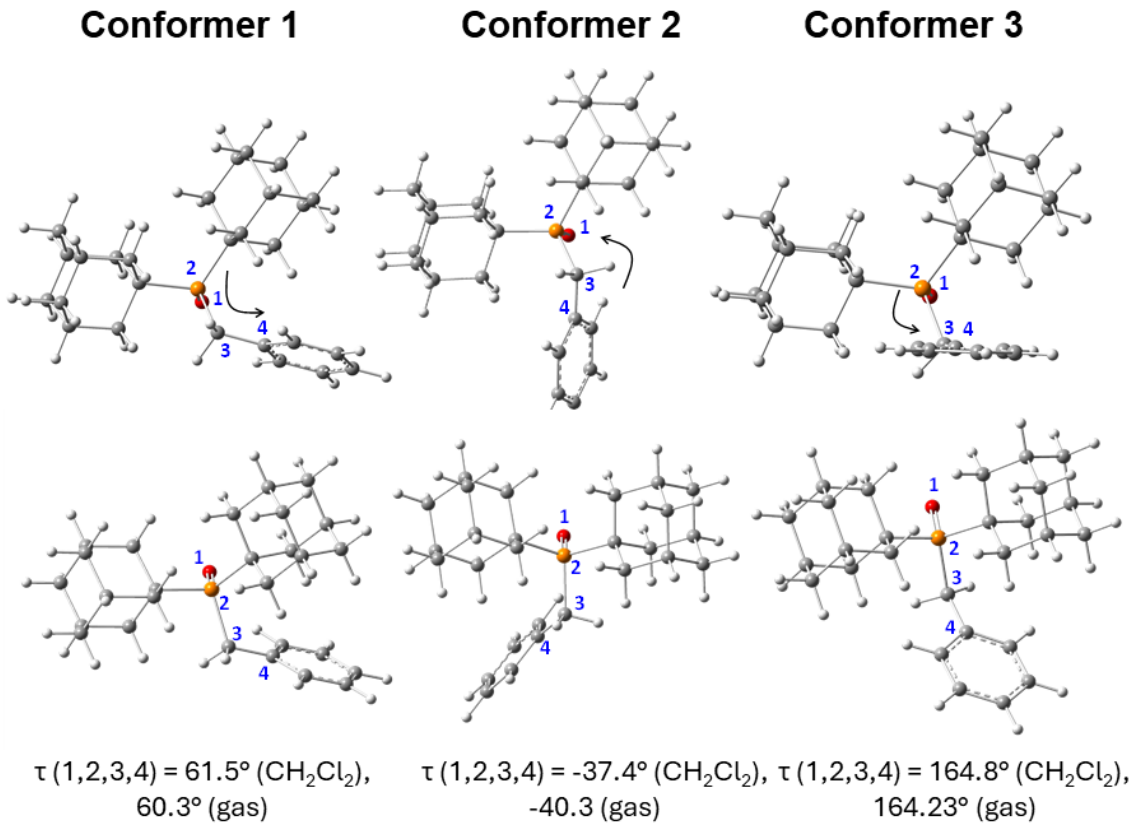

Figure S8. Two different views of the three optimized conformations of the di(1-adamantyl)benzylphosphine oxide ligand ($OPAd_2Bz$) in its ground state (S_0) at the CAM-B3LYP-D3/6-31+G** level of theory in dichloromethane solution and in the gas phase.

Since **conformer 1** was found to be the most stable in both phases (**Table S11**), subsequent calculations focused solely on this conformer. Full geometry optimizations of the S_0 and S_1 states in solution, and the S_0, S_1, and T_1 states (see below) in the gas phase, were performed using the Gaussian 16 program (revision A.03).[4] Three different exchange–correlation functionals were employed: wB97xD,[5] M06-2X-D3,[6,7] and CAM-B3LYP-D3.[2,3] The 6-31+G** basis set was used in all the calculations.

Vibrational frequency analyses were performed for the S_0, S_1, and T_1 states to confirm the absence of imaginary frequencies and validate that each optimized structure corresponds to a true minimum. Solvent effects (dichloromethane) were accounted for using the polarizable continuum model (PCM).[8,9]

Vertical electronic transitions were computed using Time-Dependent DFT (TD-DFT) at the same levels of theory. Specifically, the $S_1 \rightarrow S_0$ transitions in solution were calculated using the energy difference $ES_1(GS_1) - ES_0(GS_1)$, where $ES_1(GS_1)$ represents the energy of the S_1 state at its optimized geometry (state-specific solvation approach),[10] and $ES_0(GS_1)$ corresponds to the S_0 energy evaluated at the optimized S_1 geometry, including static solvation effects from the excited state.[11]

Table S11. Energy (in Hartree) of the ligand conformers, energy difference (AE, kcal/mol) and kJ/mol with respect to the most stable conformer and dipole moment (μ, in Debye), calculated at the CAM-B3LYP-D3(BJ)/6-31+G** level of theory in the gas phase and dichloromethane solution.

Phase	Conformer	Energy	ΔE (kcal/mol)	ΔE (kJ/mol)	μ (D)
Gas	1	-1.466.69957	0.00	0.00	3.69
	2	-1.466.698756	0.51	2.14	3.80
	3	-1.466.69434	3.28	13.73	3.99
CH_2Cl_2	1	-1.466.71027	0.00	0.00	5.58
	2	-1.466.709422	0.53	2.23	5.69
	3	-1.466.705861	2.77	11.58	5.69

The optimized geometries of the S_1 state at the three levels of theory were found to be very similar to their respective S_0 geometries (**Figure S9**). However, full geometry optimization of the T_1 state resulted in a distinct structure, with the benzene ring rotated (torsion angle τ(1,2,3,4) ≈ 61°).

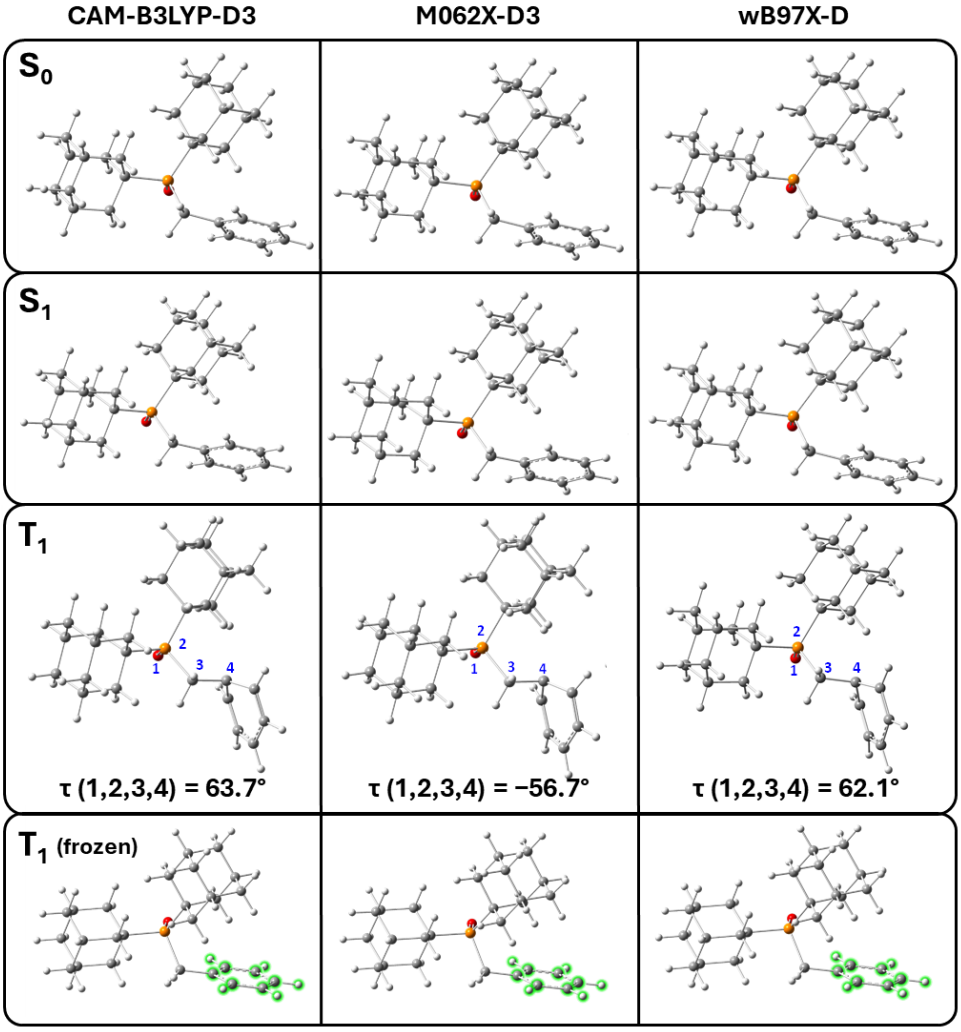

Figure S9. Geometries of the singlet ground (S_0) and lowest-energy (S_1) singlet and triplet (T_1) excited states calculated at the CAM-B3LYP-D3(BJ)/6-31+G**, M062X-D3(BJ)/6-31+G** and wB97X-D/6-31+G** levels of theory in the presence of the solvent (dichloromethane) for the

conformer 1 of the isolated ligand. Atoms marked in green colour were frozen during T_1 optimization.

To approximate the ligand's structure within the crystal environment, a two-layer ONIOM approach was used (**Figure S10**).[12,13] A cluster model was constructed from the crystallographic structure of compound **4**, comprising 12 ligands. The two central ligands were treated at the PBE0/6-31G** level [14] and fully optimized for the S_0, S_1, and T_1 states (**Figure S10**). These were surrounded by 10 additional ligands, modelled semi-empirically with PM6 level [15] and kept frozen to reduce computational cost. Lanthanide ions, chloride, water, and tetrahydrofuran molecules were omitted for simplification.

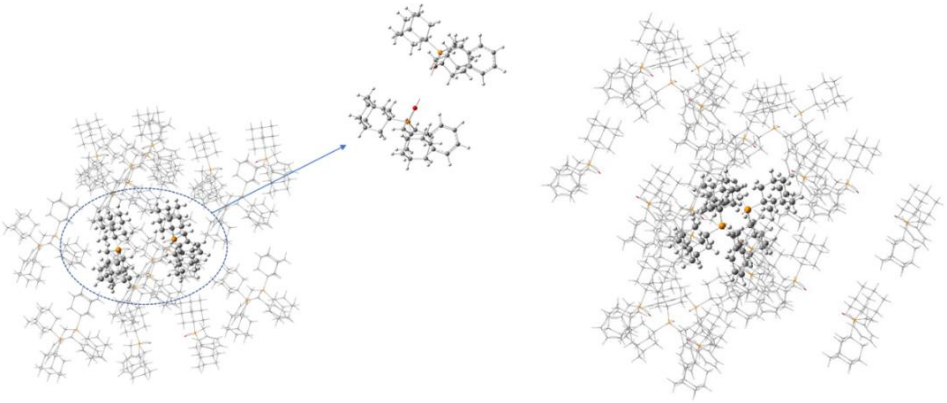

Figure S10. Two different views of the ONIOM cluster for the studied ligand in compound **4**. The active molecule (ball and sticks) is treated as high level (PBE0/6-31G**) and the surrounding molecules (sticks) as low level (PM6).

In this ONIOM model, the S_0, S_1, and T_1 geometries were nearly identical, suggesting no significant rotation of the benzene group in the T_1 state. Therefore, in the final T_1 optimization for the isolated ligand, selected atomic positions were constrained to their crystallographic coordinates (**Figure S9**) to prevent artificial torsional changes of the aromatic ring, while the remaining atoms were allowed to relax during optimization.

Figure S11a displays the experimental absorption spectra of the pure ligand in CH_2Cl_2 solution and solid phase along with the vertical electronic transitions calculated at the TD-CAM-B3LYP-D3/6-31G** level of theory. **Figure S13** presents the frontier molecular orbitals computed using the same theoretical method for both dichloromethane solution and gas phase environments. **Table S12** provides a list of some calculated CAM-B3LYP-D3 vertical electronic transitions with notable oscillator strengths and their assignments, whereas those predicted using M062X-D3 and wB97X-D are gathered in **Table S13**.

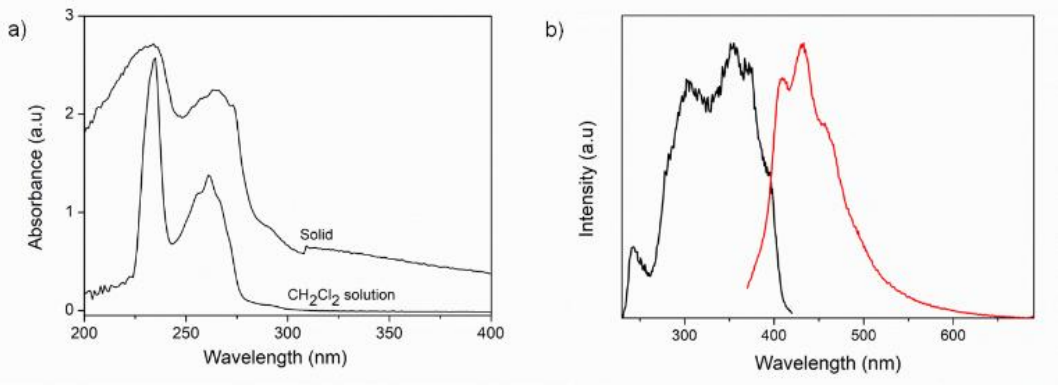

Figure S11. Experimental absorption spectra of the $OPAd_2Bz$ ligand in CH_2Cl_2 solution and solid phase (panel a) and excitation (in black) and emission (in red) spectra in CH_2Cl_2 solution (λ_{exc} = 350 nm, panel b).

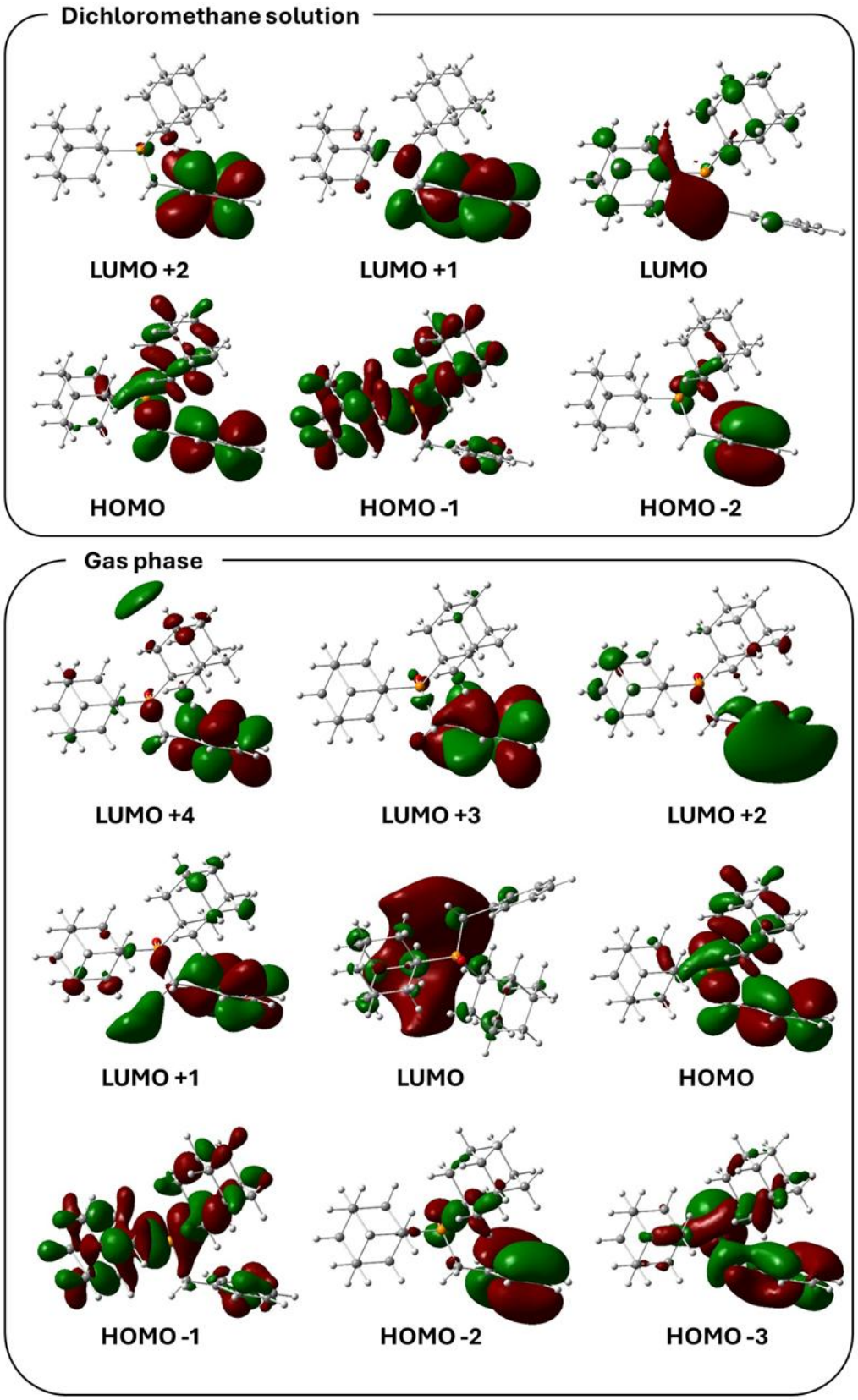

Figure S12. Localization of the HOMO, LUMO, HOMO-1, HOMO-2, LUMO+1 and LUMO+2 orbitals for the ground state S_0 of the $OPAd_2Bz$ ligand at the CAM-B3LYP-D3/6-31+G** level of theory in dichloromethane solution and, additionally, HOMO-3, LUMO+3 and LUMO+4 in the gas phase. Isocontour plots of 0.02 e/a_0^3.

Table S12. Experimental absorption wavelengths (λ_{ab}^{exp}), theoretical vertical electronic transitions ($\lambda_{vert-ab}^{calc}$), oscillator strength (*f*), and the main molecular orbital contributions (≥ 10%) calculated at the CAM-B3LYP-D3(BJ)/6-31+G** levels of theory in dichloromethane solution and in the solid phase for the **conformer 1** of the **ligand**.

Phase	λ_{ab}^{exp} nm (eV)	$\lambda_{vert-ab}^{calc}$ nm (eV)	Transition	*f*	Contribution (%)
Solution	261 (4.75)	231 (5.35)	$S_0 \rightarrow S_1$	0.0018	HOMO → LUMO+2 (49%) HOMO-2 → LUMO+1 (28%)
		212 (5.85)	$S_0 \rightarrow S_2$	0.16	HOMO → LUMO+1 (69%) HOMO-2 → LUMO+2 (14%)
	235 (5.28)	190 (6.53)	$S_0 \rightarrow S_4$	0.31	HOMO-2 → LUMO+2 (44%) HOMO → LUMO+2 (37%)
		188 (6.58)	$S_0 \rightarrow S_5$	0.77	HOMO-2 → LUMO+2 (62%) HOMO → LUMO+1 (16%)
Solid	265 (4.68)	232 (5.35)	$S_0 \rightarrow S_1$	0.0008	HOMO → LUMO+3 (36%) HOMO-2 → LUMO+1 (15%) HOMO → LUMO+3 (12%) HOMO → LUMO+1 (38%)
		211 (5.87)	$S_0 \rightarrow S_2$	0.11	HOMO→ LUMO+4 (15%) HOMO-2 → LUMO+3 (14%) HOMO→ LUMO+3 (11%)
	234 (5.30)	187 (6.62)	$S_0 \rightarrow S_6$	0.20	HOMO-2 → LUMO+1 (15%) HOMO-2 → LUMO+2 (14%) HOMO → LUMO+2 (14%) HOMO-2 → LUMO+3 (29%)
		187 (6.63)	$S_0 \rightarrow S_7$	0.31	HOMO → LUMO+1 (18%) HOMO-2 → LUMO+4 (10%)
		176 (7.06)	$S_0 \rightarrow S_{13}$	0.15	HOMO-3 → LUMO+1 (17%) HOMO-3 → LUMO+4 (9%)
		173 (7.18)	$S_0 \rightarrow S_{18}$	0.11	HOMO-3 → LUMO+1 (8%) HOMO-2 → LUMO (7%)

Table S13. Experimental absorption wavelength (λ_{ab}^{exp}), theoretical vertical electronic transitions ($\lambda_{vert-ab}^{calc}$), oscillator strength (f), and the main molecular orbital contributions (≥ 10%) calculated at the M062X-D3(BJ)/6-31+G** and wB97X-D/6-31+G** levels of theory in dichloromethane solution and in the solid phase for the **conformer 1** of the **ligand**.

M062X-D3(BJ)/6-31+G**					
Phase	λ_{ab}^{exp} nm (eV)	$\lambda_{vert-ab}^{calc}$ nm (eV)	Transition	f	Contribution (%)
Solution	261 (4.75)	231 (5.37)	$S_0 \rightarrow S_1$	0.0028	HOMO → LUMO+2 (39%) HOMO-2 → LUMO+1 (23%) HOMO → LUMO+3 (10%) HOMO-2 → LUMO+4 (10%)
		210 (5.89)	$S_0 \rightarrow S_2$	0.25	HOMO → LUMO+1 (69%) HOMO → LUMO+4 (15%)
	235 (5.28)	192 (6.47)	$S_0 \rightarrow S_5$	0.26	HOMO-2 → LUMO+1 (38%) HOMO → LUMO+2 (25%)
		188 (6.58)	$S_0 \rightarrow S_6$	0.60	HOMO-2 → LUMO+2 (55%) HOMO-2 → LUMO+3 (11%)
Solid	265 (4.68)	231 (5.37)	$S_0 \rightarrow S_1$	0.0012	HOMO → LUMO+5 (30%) HOMO → LUMO+3 (17%) HOMO-2 → LUMO+5 (10%)
		210 (5.90)	$S_0 \rightarrow S_2$	0.15	HOMO → LUMO+1 (34%) HOMO → LUMO+3 (22%) HOMO → LUMO+5 (14%) HOMO → LUMO+4 (10%)
	234 (5.30)	185 (6.67)	$S_0 \rightarrow S_{10}$	0.32	HOMO-2 → LUMO+5 (14%) HOMO-2 → LUMO+3 (11%) HOMO- → LUMO+4 (11%)
		175 (7.08)	$S_0 \rightarrow S_{20}$	0.11	HOMO-3 → LUMO+3 (27%) HOMO-3 → LUMO+5 (11%)
		174 (7.11)	$S_0 \rightarrow S_{22}$	0.13	HOMO -3 → LUMO+1 (18%) HOMO-3 → LUMO+5 (10%)
wB97X-D/6-31+G**					
Phase	λ_{ab}^{exp} nm (eV)	$\lambda_{vert-ab}^{calc}$ nm (eV)	Transition	f	Contribution (%)
Solution	261 (4.75)	232 (5.35)	$S_0 \rightarrow S_1$	0.0018	HOMO→ LUMO+2 (48%) HOMO-2 → LUMO (32%)
		211 (5.88)	$S_0 \rightarrow S_2$	0.17	HOMO→ LUMO (74%) HOMO-2 → LUMO+2 (14%)
	235 (5.28)	189 (6.57)	$S_0 \rightarrow S_3$	0.35	HOMO-2 → LUMO (47%) HOMO → LUMO+2 (38%)
		188 (6.61)	$S_0 \rightarrow S_4$	0.80	HOMO-2 → LUMO+2 (64%) HOMO→ LUMO (17%)
Solid	265 (4.68)	232 (5.35)	$S_0 \rightarrow S_1$	0.0009	HOMO → LUMO+2 (47%) HOMO-2→ LUMO+1 (31%)
		210 (5.90)	$S_0 \rightarrow S_2$	0.12	HOMO→ LUMO+1 (68%) HOMO-2 → LUMO+2 (17%)
	234 (5.30)	187 (6.65)	$S_0 \rightarrow S_4$	0.21	HOMO → LUMO+2 (39%) HOMO-2 → LUMO+1 (36%)
		186 (6.66)	$S_0 \rightarrow S_5$	0.49	HOMO-2 → LUMO+2 (50%) HOMO → LUMO+1 (19%)
		174 (7.15)	$S_0 \rightarrow S_{12}$	0.21	HOMO-3 → LUMO+1 (30%) HOMO-3 → LUMO+2 (25%)

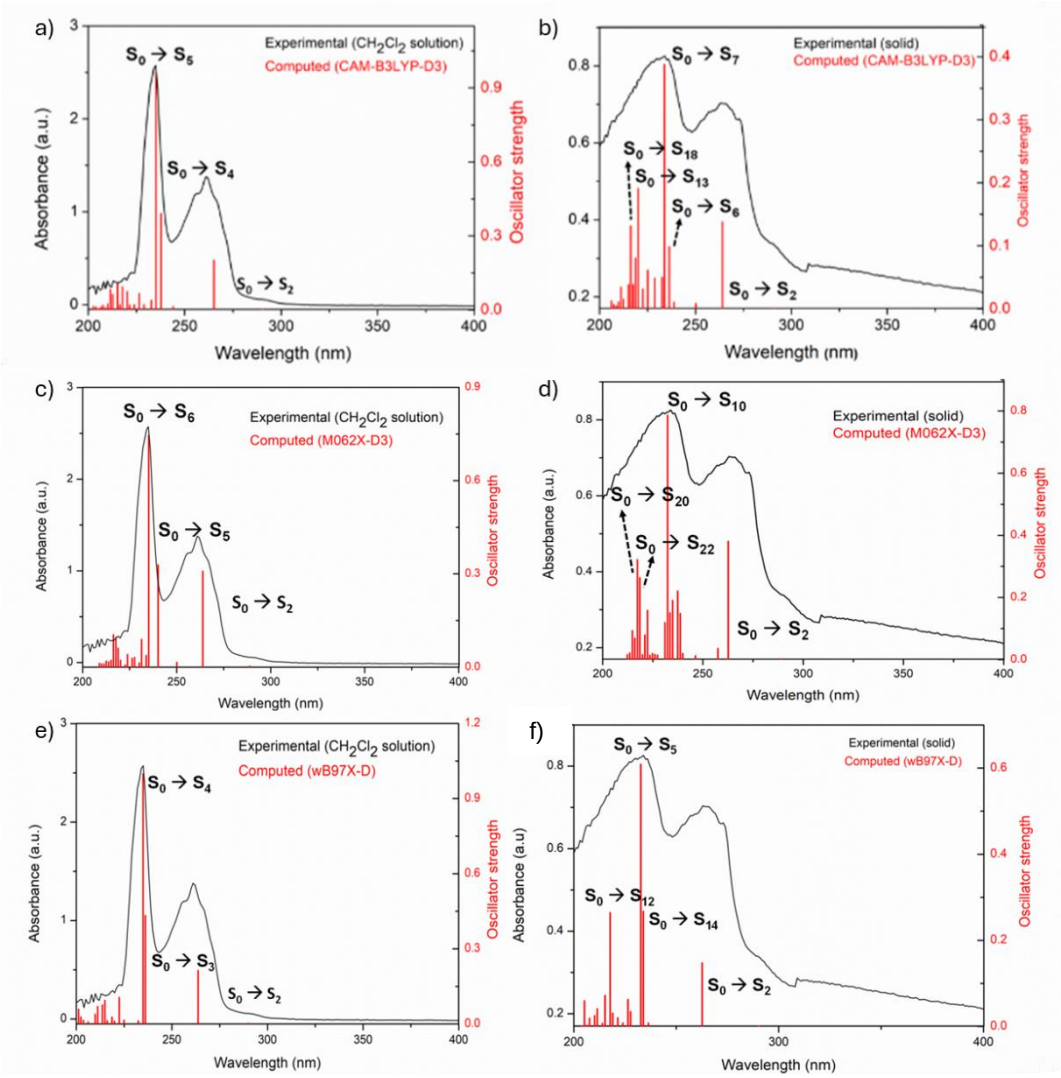

Figure S13. Experimental absorption spectra of the $OPAd_2Bz$ ligand in CH_2Cl_2 solution and in the solid state (black colour), along with the oscillator strengths of vertical electronic transitions (red lines) calculated at different levels of theory. Panels (a) and (b) present the results obtained using the TD-CAM-B3LYP-D3/6-31+G** level in CH_2Cl_2 solution and in the gas phase, respectively. Panels (c) and (d) show the corresponding results using the TD-M06-2X-D3(BJ)/6-31+G** level, while panels (e) and (f) display the spectra calculated at the TD-ωB97XD/6-31+G** level in solution and gas phase, respectively. The theoretical energies in panels (a) - (e) were scaled by a factor of 1.25, while those of panel (f) was scaled by a factor of 1.20.

In solution, the weaker experimental absorption band at 261 nm (**Figure S13**) could be assigned to the $S_0 \rightarrow S_2$ electronic transition (calculated at 212 nm), in agreement with the lower oscillator strength predicted for it (f = 0.16), with 69% contribution of HOMO → LUMO+1. The strong and sharp absorption band observed at 235 nm was attributed to the $S_0 \rightarrow S_4$ and $S_0 \rightarrow S_5$ electronic transitions, which were predicted at 190 nm (f = 0.31) and 188 nm (f = 0.77), corresponding mainly to HOMO−2 → LUMO+2 with 44% and 62% and contributions, respectively. **Figure S14a** displays the frontier molecular orbitals involved in the most intense $S_0 \rightarrow S_5$ transition, whereas **Figure S12** shows those involved in the dominant transitions described in **Table S12**. The HOMO-2, LUMO+1 and LUMO+2 are mainly localized on the aromatic ring, whereas the HOMO resides in the benzene and one of the adamantyl moieties. This indicates, as expected, that the aromatic ring is the main responsible for the absorption properties of the ligand, with minor participation of one of the adamantyl moieties.

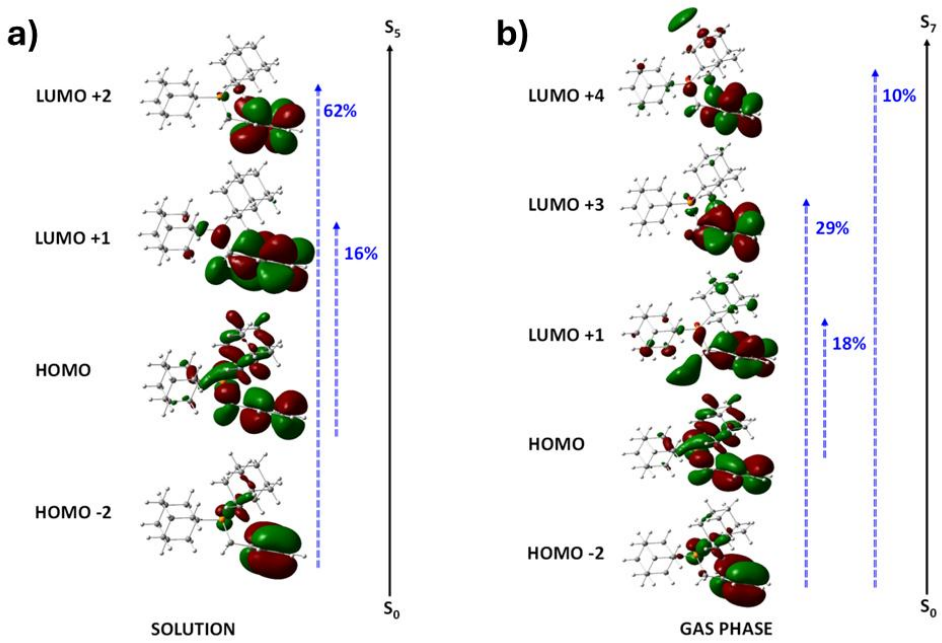

Figure S14. (a) Schematic representation of the $S_0 \rightarrow S_5$ electronic transition in dichloromethane solution and the (b) $S_0 \rightarrow S_7$ electronic transition in the gas phase for the ligand (isocontour plots of 0.02 e/a_0^3).

In the absorption spectrum of the solid, the second lowest energy transition observed at 265 nm in the solid spectrum could be assigned to the $S_0 \rightarrow S_2$ transition predicted at 211 nm with f=0.11 and 38% contribution of HOMO → LUMO+1. The absorption band at 234 nm could be assigned mainly to the $S_0 \rightarrow S_6$ and $S_0 \rightarrow S_7$ electronic transitions, which were calculated both at 187 nm. The $S_0 \rightarrow S_7$ transition is predicted to be the most intense one with f=0.31 and contributions of HOMO−2 → LUMO+3 (29%), HOMO → LUMO+1 (18%) and HOMO−2 → LUMO+4 (10 %) (**Figure S14b**).

4. Spectroscopic measurements

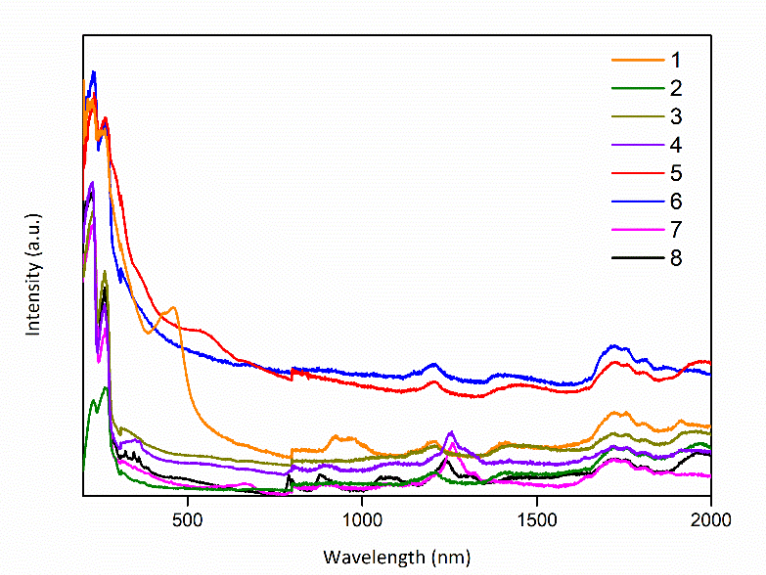

Figure S15. Experimental absorption spectra of compounds **1**-**8** in the solid phase.

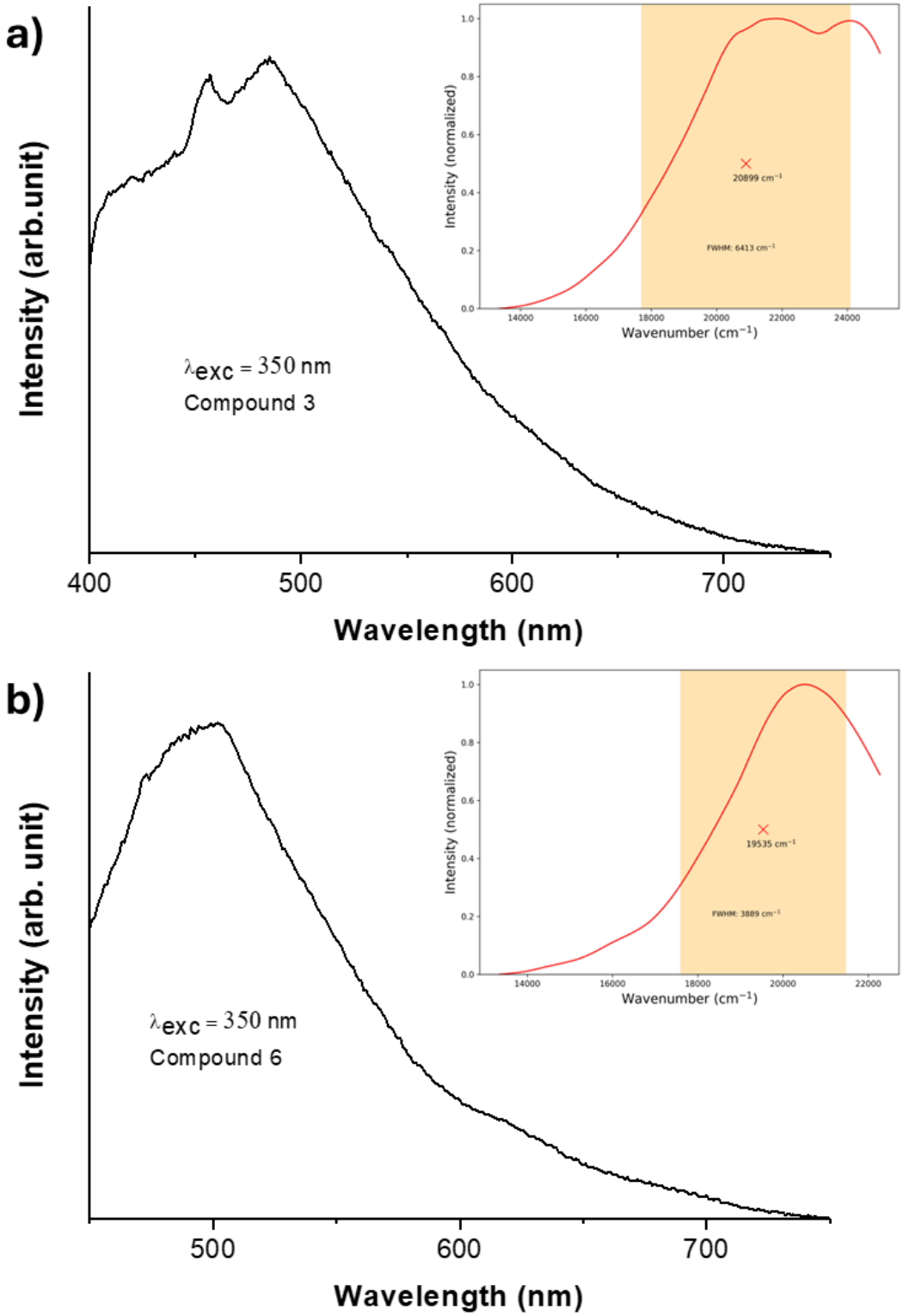

Figure S16. Emission spectra of **3** (a) and **6** (b) at λ_{exc} = 350 nm in solid state at room temperature. The insets display the corresponding phosphorescence spectra processed via Jacobian transformation. Red crosses indicate the barycenter positions of the T_1 states, while the shaded orange regions represent the full width at half maximum (FWHM) of the emission bands.

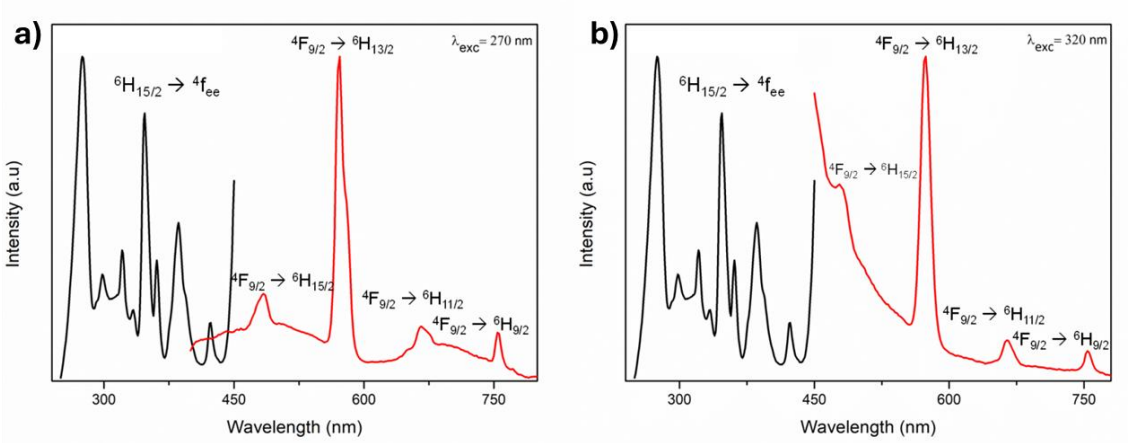

Figure S17. Excitation (monitoring λ_{em} = 575 nm) and emission spectra of **4** at λ_{exc} = 270 nm (a) and λ_{exc} = 320 nm (b) in solid state at room temperature.

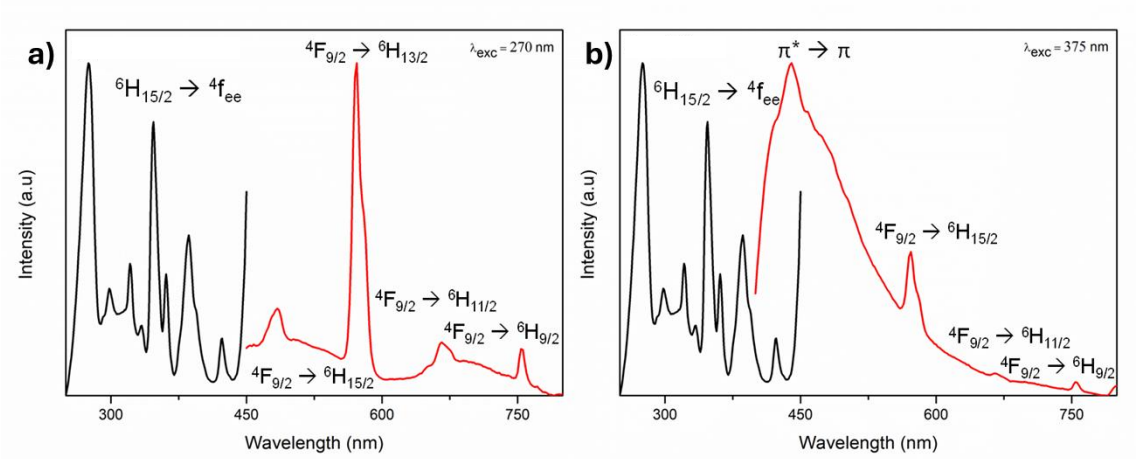

Figure S18. Excitation (monitoring λ_{em} = 570 nm) and emission spectra of **7** at λ_{exc} = 270 nm (a) and λ_{exc} = 375 nm (b) in solid state at room temperature.

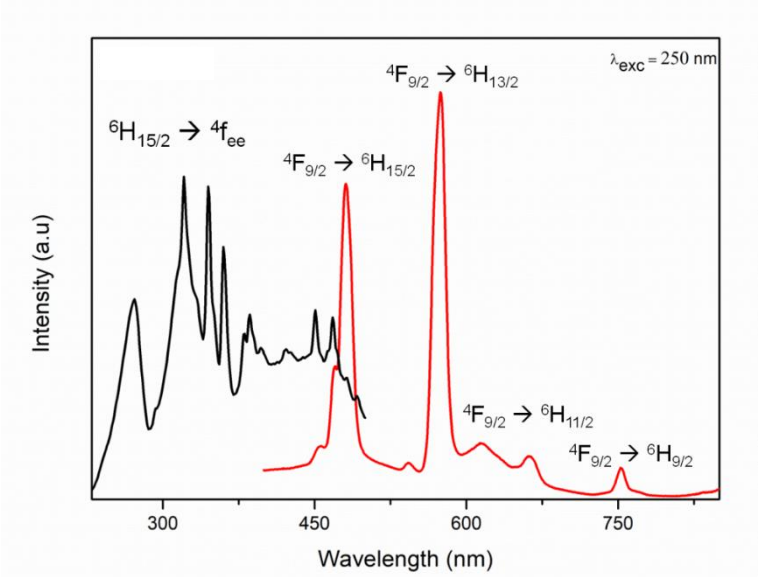

Figure S19. Excitation and emission spectra of **8** at λ_{exc} = 250 nm in solid state at room temperature.

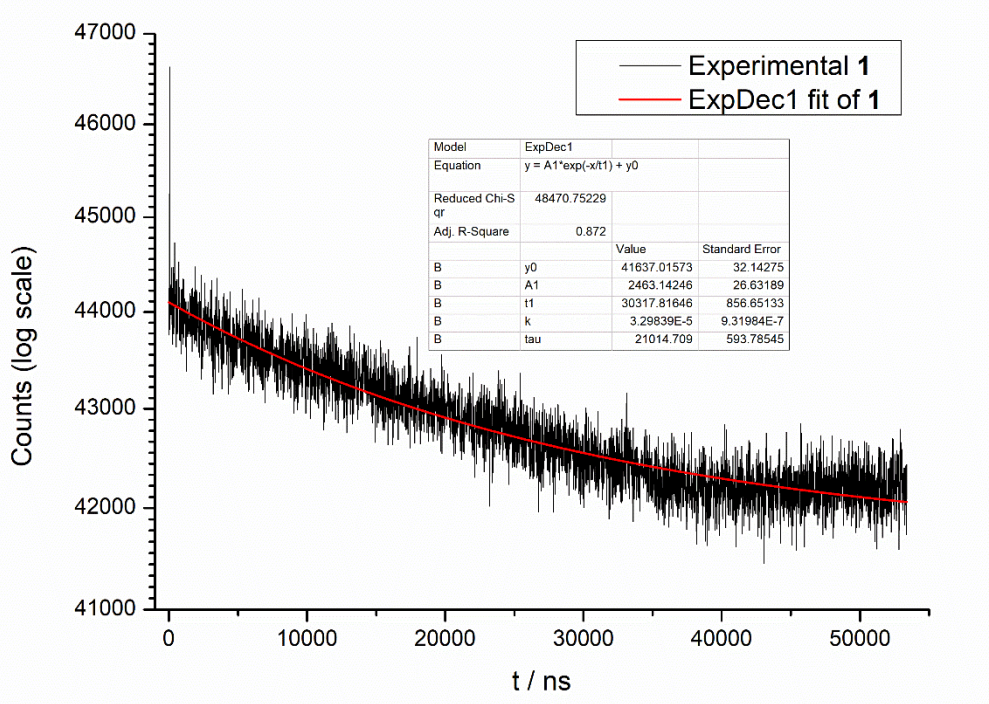

Figure S20. Experimental exponential fitting of the excited state lifetime of **1** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (l_{exc} = 375 nm; l_{emi} = 978 nm).

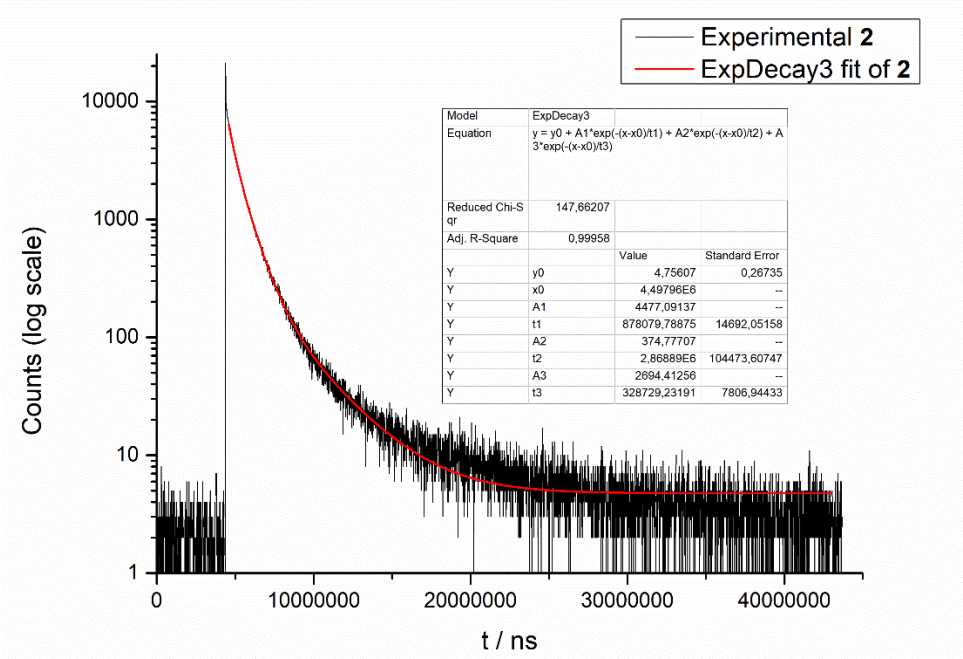

Figure S21. Experimental exponential fitting of the excited state lifetime of **2** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (l_{exc} = 350 nm; l_{emi} = 500 nm).

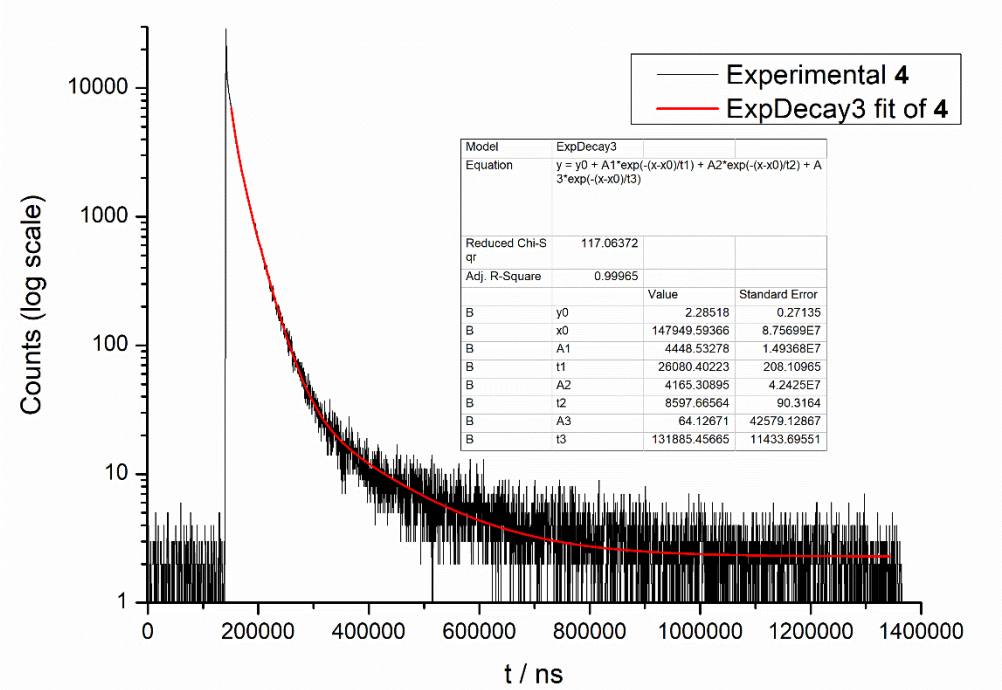

Figure S22. Experimental exponential fitting of the excited state lifetime of **4** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (l_{exc} = 320 nm; l_{emi} = 575 nm).

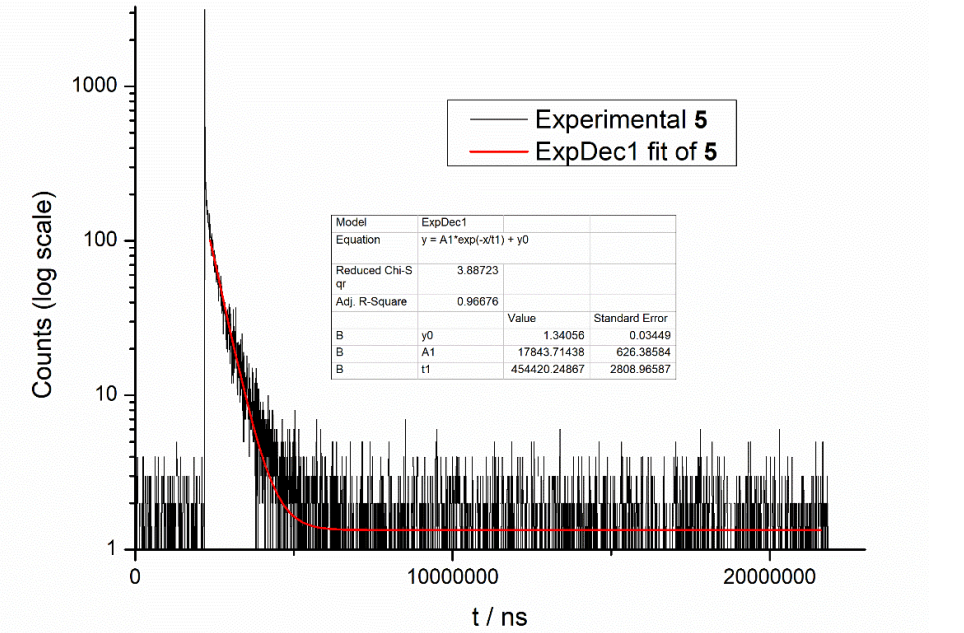

Figure S23. Experimental exponential fitting of the excited state lifetime of **5** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (l_{exc} = 350 nm; l_{emi} = 620 nm).

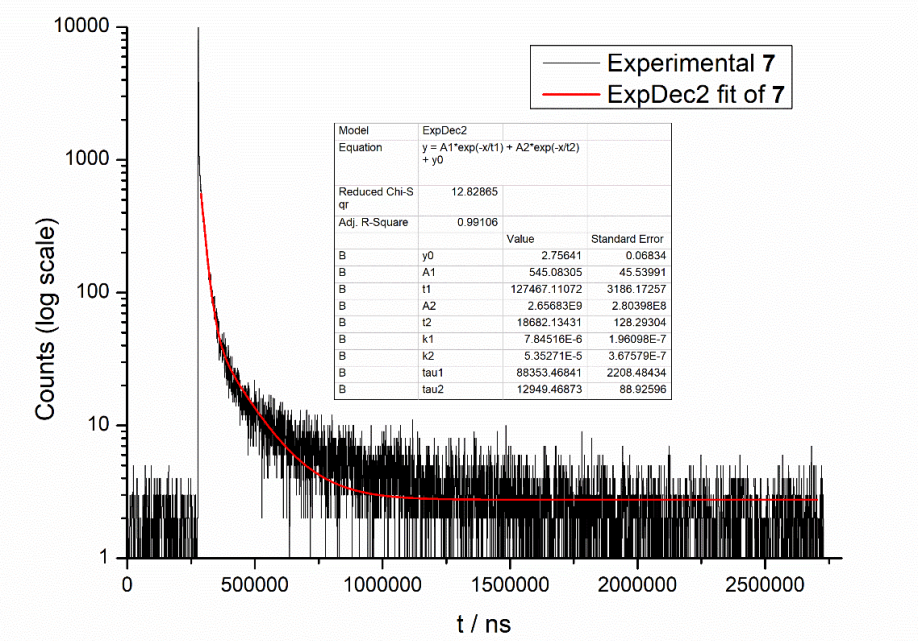

Figure S24. Experimental exponential fitting of the excited state lifetime of **7** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (l_{exc} = 250 nm; l_{emi} = 575 nm).

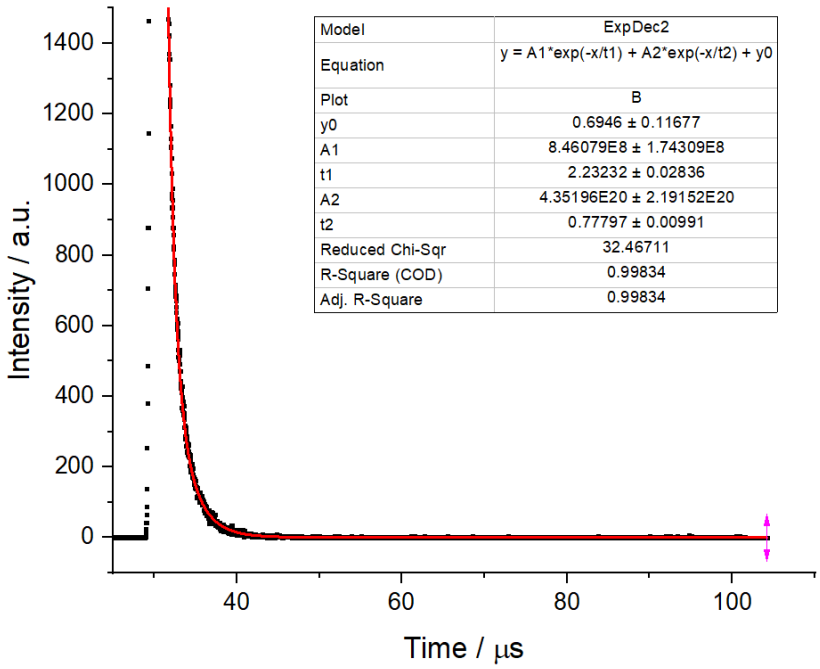

Figure S25. Experimental exponential fitting of the excited state lifetime of **8** using a flash lamp light source (1 µs pulse, HORIBA Scientific) in the solid state (λ_{exc} = 250 nm; λ_{emi} = 576 nm). The black dots correspond to the experimental data and the red trace to fitted data. The fitting parameters are depicted in the associated table.

5. Photophysical properties of the complexes

5.1. Donor-acceptor distances

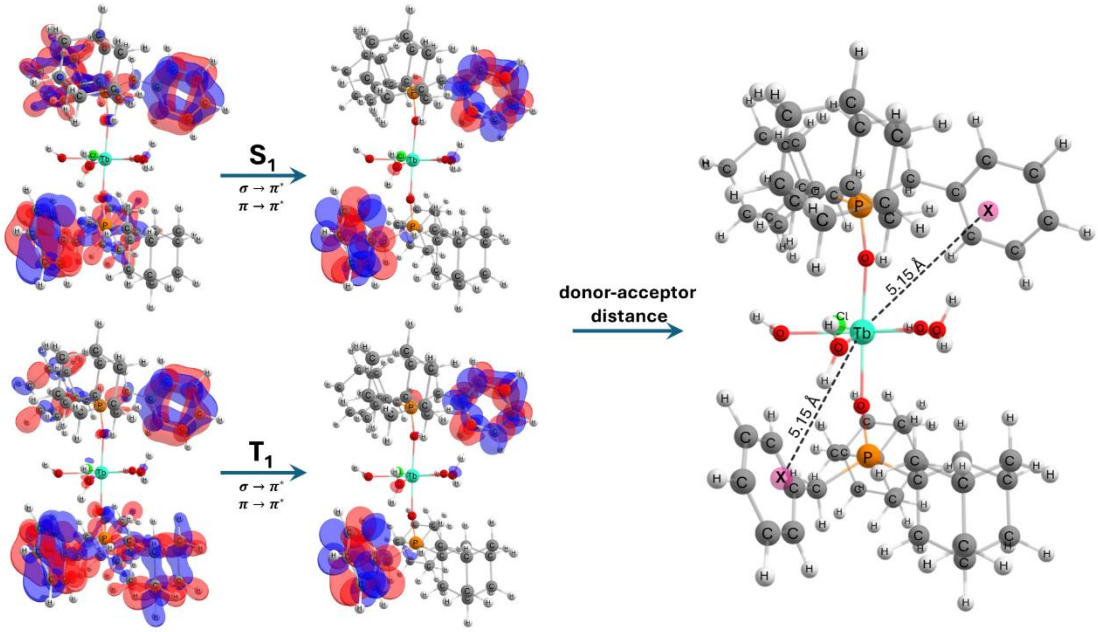

Figure S26. Kohn–Sham molecular orbitals composition of the S_1 and T_1 excited states for the representative compound **2**. The nature of the transitions (σ → π* and π → π*) is indicated for each state. Donor–acceptor distances, extracted from the atomic coefficients (Eq. 1), are shown on the right. M06-L/def2-SVP/MWB54 level of theory was used and the isosurfaces were generated with isovalues of 0.03 a_0^3.

Table S14. Calculated values of donor-acceptor distances (in units of Å) for [Yb(OPAd$_2$Bz)$_2$(H$_2$O)$_4$Cl] (**1**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Compound	$R_L(S_1)$	$R_L(T_1)$
1	5.04	5.15
2	5.04	5.15
4	5.04	5.15
5	5.39	5.46
7	5.39	5.46

5.2. Intramolecular energy transfer rates

Table S15. Forward IET rates (in units of s^{-1}) for $[Yb(OPAd_2Bz)_2(H_2O)_4Cl]$ (**1**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Pathway	Donor	Acceptor	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$S_1 \rightarrow S_0$	$^2F_{7/2} \rightarrow {}^2F_{5/2}$	29760	1.72E-07	5.87E-11	1.36E-08	1.59E-07
			W^S	**1.72E-07**			
2	$T_1 \rightarrow S_0$	$^2F_{7/2} \rightarrow {}^2F_{5/2}$	10659	1.43E+07	5.83E-01	1.30E+02	1.43E+07
			W^T	**1.43E+07**			

Table S16. Backward IET rates (in units of s^{-1}) for $[Yb(OPAd_2Bz)_2(H_2O)_4Cl]$ (**1**). The Δ is the donor-acceptor energy difference. W_b^S and W_b^T are the total energy transfer to the S_1 and T_1 states.

Pathway	Donor	Acceptor	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$^2F_{5/2} \rightarrow {}^2F_{7/2}$	$S_0 \rightarrow S_1$	-29760	2.49E-69	8.50E-73	1.97E-70	2.30E-69
			W_b^S	**2.49E-69**			
2	$^2F_{5/2} \rightarrow {}^2F_{7/2}$	$S_0 \rightarrow T_1$	-10659	1.26E-15	5.14E-23	1.15E-20	1.26E-15
			W_b^T	**1.26E-15**			

Table S17. Forward IET rates (in units of s^{-1}) for $[Tb(OPAd_2Bz)_2(H_2O)_4Cl]$ (**2**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_4$	0.0	19556	2.2E-01	5.1E-04	2.2E-01	0.0E+00
2	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_3$	0.0	13764	1.9E+00	1.8E+00	1.3E-01	0.0E+00
3	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_6$	0.1	13577	2.0E+05	1.8E+02	2.1E+03	2.0E+05
4	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_{10}$	0.0	13029	1.7E+02	1.7E+02	8.2E-01	0.0E+00
5	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_5$	0.0	12233	6.7E+04	9.6E+01	7.1E+03	6.0E+04
6	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_2$	0.0	11893	0.0E+00	0.0E+00	0.0E+00	0.0E+00
7	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_4$	0.0	11713	1.1E+03	1.0E+02	1.0E+03	0.0E+00
8	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_9$	0.0	11592	6.3E+02	6.2E+02	1.5E+01	0.0E+00
9	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_3$	0.0	11023	3.7E+01	3.4E+01	2.5E+00	0.0E+00
10	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_8$	0.0	10810	6.6E+02	6.5E+02	2.9E+00	0.0E+00
11	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_7$	0.0	10543	1.9E+04	4.5E+02	1.9E+04	3.3E+00
12	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_2$	0.0	10469	0.0E+00	0.0E+00	0.0E+00	0.0E+00
13	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_6$	0.0	10330	9.1E+04	0.0E+00	0.0E+00	9.1E+04
14	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_1$	0.0	9390	0.0E+00	0.0E+00	0.0E+00	0.0E+00
15	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_0$	0.0	8776	0.0E+00	0.0E+00	0.0E+00	0.0E+00
16	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_7$	0.1	8621	4.1E+05	0.0E+00	0.0E+00	4.1E+05
17	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_6$	2.9	7109	9.3E+06	0.0E+00	0.0E+00	9.3E+06
18	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_5$	0.0	6233	1.7E-01	0.0E+00	0.0E+00	1.7E-01
19	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_4$	0.0	5661	0.0E+00	0.0E+00	0.0E+00	0.0E+00
20	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_5$	17.3	5066	5.6E+07	0.0E+00	0.0E+00	5.6E+07
21	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_3$	0.0	5064	0.0E+00	0.0E+00	0.0E+00	0.0E+00
22	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_8$	0.0	4869	0.0E+00	0.0E+00	0.0E+00	0.0E+00
23	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_4$	0.0	4626	0.0E+00	0.0E+00	0.0E+00	0.0E+00
24	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_3$	0.0	3450	0.0E+00	0.0E+00	0.0E+00	0.0E+00
25	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_7$	1.4	3411	4.6E+06	0.0E+00	0.0E+00	4.6E+06
26	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_2$	0.0	2864	0.0E+00	0.0E+00	0.0E+00	0.0E+00
27	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_1$	0.0	2518	0.0E+00	0.0E+00	0.0E+00	0.0E+00
28	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_6$	26.3	2402	8.5E+07	0.0E+00	0.0E+00	8.5E+07
29	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_4$	0.0	2392	0.0E+00	0.0E+00	0.0E+00	0.0E+00
30	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_5$	2.4	2014	7.8E+06	0.0E+00	0.0E+00	7.8E+06
31	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_9$	0.0	827	0.0E+00	0.0E+00	0.0E+00	0.0E+00
32	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_8$	0.0	-815	0.0E+00	0.0E+00	0.0E+00	0.0E+00
33	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_5$	0.0	-1334	7.3E+02	0.0E+00	0.0E+00	7.3E+02

34	$S_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_7$	0.0	-1693	1.5E-05	0.0E+00	0.0E+00	1.5E-05
35	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_4$	0.0	21604	2.1E-01	4.9E-05	1.1E-01	1.0E-01
36	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_3$	0.0	15812	4.5E+01	2.8E-01	4.5E+01	0.0E+00
37	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_6$	0.0	15625	2.7E+03	1.5E+00	4.6E+02	2.3E+03
38	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_{10}$	0.0	15077	4.2E-01	4.2E-01	9.1E-04	0.0E+00
39	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_5$	0.0	14281	4.3E+04	5.1E+00	6.6E+01	4.3E+04
40	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_2$	0.0	13941	3.5E+00	1.8E+00	1.7E+00	0.0E+00
41	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_4$	0.0	13761	1.1E+04	3.2E+00	6.2E+02	1.0E+04
42	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_9$	0.0	13640	2.4E+01	2.3E+01	6.7E-01	0.0E+00
43	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_3$	0.0	13071	0.0E+00	0.0E+00	0.0E+00	0.0E+00
44	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_8$	0.0	12858	9.4E+01	9.0E+01	4.3E+00	0.0E+00
45	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_7$	0.0	12591	9.8E+02	3.7E+01	9.5E+02	0.0E+00
46	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_2$	0.0	12517	0.0E+00	0.0E+00	0.0E+00	0.0E+00
47	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_6$	0.0	12378	2.0E+03	0.0E+00	0.0E+00	2.0E+03
48	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_1$	0.0	11438	0.0E+00	0.0E+00	0.0E+00	0.0E+00
49	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_0$	0.0	10824	0.0E+00	0.0E+00	0.0E+00	0.0E+00
50	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_7$	0.0	10669	0.0E+00	0.0E+00	0.0E+00	0.0E+00
51	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_6$	0.1	9157	3.4E+05	0.0E+00	0.0E+00	3.4E+05
52	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_5$	2.5	8281	8.1E+06	0.0E+00	0.0E+00	8.1E+06
53	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_4$	8.5	7709	2.8E+07	0.0E+00	0.0E+00	2.8E+07
54	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_5$	7.2	7114	2.3E+07	0.0E+00	0.0E+00	2.3E+07
55	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_3$	0.0	7112	0.0E+00	0.0E+00	0.0E+00	0.0E+00
56	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_8$	0.0	6917	0.0E+00	0.0E+00	0.0E+00	0.0E+00
57	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_4$	28.4	6674	9.2E+07	0.0E+00	0.0E+00	9.2E+07
58	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_3$	0.0	5498	0.0E+00	0.0E+00	0.0E+00	0.0E+00
59	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_7$	0.0	5459	0.0E+00	0.0E+00	0.0E+00	0.0E+00
60	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_2$	0.0	4912	0.0E+00	0.0E+00	0.0E+00	0.0E+00
61	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_1$	0.0	4566	0.0E+00	0.0E+00	0.0E+00	0.0E+00
62	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_6$	2.5	4450	8.2E+06	0.0E+00	0.0E+00	8.2E+06
63	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_4$	0.0	4440	8.3E+03	0.0E+00	0.0E+00	8.3E+03
64	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_5$	0.2	4062	6.5E+05	0.0E+00	0.0E+00	6.5E+05
65	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_9$	0.0	2875	0.0E+00	0.0E+00	0.0E+00	0.0E+00
66	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_8$	0.0	1233	0.0E+00	0.0E+00	0.0E+00	0.0E+00
67	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_5$	0.1	714	3.6E+05	0.0E+00	0.0E+00	3.6E+05
68	$S_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_7$	0.0	355	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				W^S	**3.3E+08**			
69	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_4$	0.0	455	6.1E+01	1.5E-01	6.1E+01	0.0E+00
70	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_3$	0.0	-5337	6.2E-13	5.8E-13	3.8E-14	0.0E+00
71	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_6$	0.0	-5524	1.8E-04	1.8E-11	2.0E-10	1.8E-04
72	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_{10}$	0.0	-6072	5.9E-13	5.9E-13	2.5E-15	0.0E+00
73	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_5$	0.0	-6868	1.5E-08	2.6E-15	1.8E-13	1.5E-08
74	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_2$	0.0	-7208	0.0E+00	0.0E+00	0.0E+00	0.0E+00
75	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_4$	0.0	-7388	1.2E-15	1.2E-16	1.1E-15	0.0E+00
76	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_9$	0.0	-7509	3.5E-16	3.4E-16	7.1E-18	0.0E+00
77	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_3$	0.0	-8078	6.5E-19	6.1E-19	4.0E-20	0.0E+00
78	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_8$	0.0	-8291	3.2E-18	3.2E-18	1.2E-20	0.0E+00
79	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_7$	0.0	-8558	4.8E-17	4.5E-19	1.8E-17	2.9E-17
80	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5G_2$	0.0	-8632	0.0E+00	0.0E+00	0.0E+00	0.0E+00
81	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5L_6$	0.0	-8771	2.3E-13	0.0E+00	0.0E+00	2.3E-13
82	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_1$	0.0	-9711	0.0E+00	0.0E+00	0.0E+00	0.0E+00
83	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5D_0$	0.0	-10325	0.0E+00	0.0E+00	0.0E+00	0.0E+00
84	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_7$	0.0	-10480	4.0E-17	0.0E+00	0.0E+00	4.0E-17
85	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_6$	0.0	-11992	1.3E-19	0.0E+00	0.0E+00	1.3E-19
86	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_5$	0.0	-12868	1.5E-29	0.0E+00	0.0E+00	1.5E-29
87	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_4$	0.0	-13440	0.0E+00	0.0E+00	0.0E+00	0.0E+00

88	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_5$	0.0	-14035	6.1E-24	0.0E+00	0.0E+00	6.1E-24
89	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5H_3$	0.0	-14037	0.0E+00	0.0E+00	0.0E+00	0.0E+00
90	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_8$	0.0	-14232	0.0E+00	0.0E+00	0.0E+00	0.0E+00
91	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_4$	0.0	-14475	0.0E+00	0.0E+00	0.0E+00	0.0E+00
92	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_3$	0.0	-15651	0.0E+00	0.0E+00	0.0E+00	0.0E+00
93	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_7$	0.0	-15690	4.2E-29	0.0E+00	0.0E+00	4.2E-29
94	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_2$	0.0	-16237	0.0E+00	0.0E+00	0.0E+00	0.0E+00
95	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5F_1$	0.0	-16583	0.0E+00	0.0E+00	0.0E+00	0.0E+00
96	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_6$	0.0	-16699	2.8E-30	0.0E+00	0.0E+00	2.8E-30
97	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_4$	0.0	-16709	0.0E+00	0.0E+00	0.0E+00	0.0E+00
98	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5I_5$	0.0	-17087	2.9E-32	0.0E+00	0.0E+00	2.9E-32
99	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_9$	0.0	-18274	0.0E+00	0.0E+00	0.0E+00	0.0E+00
100	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_8$	0.0	-19916	0.0E+00	0.0E+00	0.0E+00	0.0E+00
101	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_5$	0.0	-20435	1.9E-41	0.0E+00	0.0E+00	1.9E-41
102	$T_1 \rightarrow S_0$	$^7F_6 \rightarrow {}^5K_7$	0.0	-20794	3.1E-49	0.0E+00	0.0E+00	3.1E-49
103	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_4$	100.0	2503	9.4E+06	4.9E-01	1.0E+03	9.4E+06
104	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_3$	0.0	-3289	4.8E-06	3.1E-08	4.8E-06	0.0E+00
105	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_6$	0.0	-3476	7.0E-01	5.1E-08	1.5E-05	7.0E-01
106	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_{10}$	0.0	-4024	4.7E-10	4.7E-10	8.3E-13	0.0E+00
107	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_5$	0.0	-4820	3.1E-03	4.0E-11	5.0E-10	3.1E-03
108	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_2$	0.0	-5160	3.1E-12	1.7E-12	1.4E-12	0.0E+00
109	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_4$	0.0	-5340	2.9E-05	1.0E-12	1.9E-10	2.9E-05
110	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_9$	0.0	-5461	3.6E-12	3.5E-12	8.8E-14	0.0E+00
111	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_3$	0.0	-6030	0.0E+00	0.0E+00	0.0E+00	0.0E+00
112	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_8$	0.0	-6243	1.1E-13	1.1E-13	4.7E-15	0.0E+00
113	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_7$	0.0	-6510	2.3E-13	9.0E-15	2.2E-13	0.0E+00
114	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5G_2$	0.0	-6584	0.0E+00	0.0E+00	0.0E+00	0.0E+00
115	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5L_6$	0.0	-6723	1.2E-09	0.0E+00	0.0E+00	1.2E-09
116	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_1$	0.0	-7663	0.0E+00	0.0E+00	0.0E+00	0.0E+00
117	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5D_0$	0.0	-8277	0.0E+00	0.0E+00	0.0E+00	0.0E+00
118	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_7$	0.0	-8432	0.0E+00	0.0E+00	0.0E+00	0.0E+00
119	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_6$	0.0	-9944	7.8E-16	0.0E+00	0.0E+00	7.8E-16
120	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_5$	0.0	-10820	1.1E-16	0.0E+00	0.0E+00	1.1E-16
121	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_4$	0.0	-11392	1.3E-17	0.0E+00	0.0E+00	1.3E-17
122	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_5$	0.0	-11987	3.4E-19	0.0E+00	0.0E+00	3.4E-19
123	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5H_3$	0.0	-11989	0.0E+00	0.0E+00	0.0E+00	0.0E+00
124	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_8$	0.0	-12184	0.0E+00	0.0E+00	0.0E+00	0.0E+00
125	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_4$	0.0	-12427	1.0E-19	0.0E+00	0.0E+00	1.0E-19
126	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_3$	0.0	-13603	0.0E+00	0.0E+00	0.0E+00	0.0E+00
127	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_7$	0.0	-13642	0.0E+00	0.0E+00	0.0E+00	0.0E+00
128	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_2$	0.0	-14189	0.0E+00	0.0E+00	0.0E+00	0.0E+00
129	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5F_1$	0.0	-14535	0.0E+00	0.0E+00	0.0E+00	0.0E+00
130	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_6$	0.0	-14651	2.7E-26	0.0E+00	0.0E+00	2.7E-26
131	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_4$	0.0	-14661	2.5E-29	0.0E+00	0.0E+00	2.5E-29
132	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5I_5$	0.0	-15039	2.3E-28	0.0E+00	0.0E+00	2.3E-28
133	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_9$	0.0	-16226	0.0E+00	0.0E+00	0.0E+00	0.0E+00
134	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_8$	0.0	-17868	0.0E+00	0.0E+00	0.0E+00	0.0E+00
135	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_5$	0.0	-18387	1.1E-36	0.0E+00	0.0E+00	1.1E-36
136	$T_1 \rightarrow S_0$	$^7F_5 \rightarrow {}^5K_7$	0.0	-18746	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				$\boldsymbol{W^T}$	**9.4E+06**			

Table S18. Backward IET rates (in units of s^{-1}) for $[Tb(OPAd_2Bz)_2(H_2O)_4Cl]$ (**2**). The Δ is the donor-acceptor energy difference. W_b^S and W_b^T are the total energy transfer to the S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$^5D_4 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-19556	5.9E-42	1.4E-44	5.9E-42	0.0E+00
2	$^5D_3 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-13764	7.7E-29	7.2E-29	5.3E-30	0.0E+00
3	$^5G_6 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-13577	1.0E-23	9.5E-27	1.1E-25	1.0E-23
4	$^5L_{10} \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-13029	7.6E-26	7.6E-26	3.7E-28	0.0E+00
5	$^5G_5 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-12233	2.6E-21	3.8E-24	2.8E-22	2.4E-21
6	$^5D_2 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-11893	0.0E+00	0.0E+00	0.0E+00	0.0E+00
7	$^5G_4 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-11713	6.5E-22	6.1E-23	5.9E-22	0.0E+00
8	$^5L_9 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-11592	3.1E-22	3.0E-22	7.2E-24	0.0E+00
9	$^5G_3 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-11023	7.5E-22	7.0E-22	5.2E-23	0.0E+00
10	$^5L_8 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-10810	1.5E-20	1.5E-20	6.8E-23	0.0E+00
11	$^5L_7 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-10543	1.8E-18	4.3E-20	1.8E-18	3.1E-22
12	$^5G_2 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-10469	0.0E+00	0.0E+00	0.0E+00	0.0E+00
13	$^5L_6 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-10330	2.8E-17	0.0E+00	0.0E+00	2.8E-17
14	$^5D_1 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-9390	0.0E+00	0.0E+00	0.0E+00	0.0E+00
15	$^5D_0 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-8776	0.0E+00	0.0E+00	0.0E+00	0.0E+00
16	$^5H_7 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-8621	4.0E-13	0.0E+00	0.0E+00	4.0E-13
17	$^5H_6 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-7109	1.5E-08	0.0E+00	0.0E+00	1.5E-08
18	$^5H_5 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-6233	2.1E-14	0.0E+00	0.0E+00	2.1E-14
19	$^5H_4 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-5661	0.0E+00	0.0E+00	0.0E+00	0.0E+00
20	$^5F_5 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-5066	1.9E-03	0.0E+00	0.0E+00	1.9E-03
21	$^5H_3 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-5064	0.0E+00	0.0E+00	0.0E+00	0.0E+00
22	$^5I_8 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-4869	0.0E+00	0.0E+00	0.0E+00	0.0E+00
23	$^5F_4 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-4626	0.0E+00	0.0E+00	0.0E+00	0.0E+00
24	$^5F_3 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-3450	0.0E+00	0.0E+00	0.0E+00	0.0E+00
25	$^5I_7 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-3411	3.1E-01	0.0E+00	0.0E+00	3.1E-01
26	$^5F_2 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-2864	0.0E+00	0.0E+00	0.0E+00	0.0E+00
27	$^5F_1 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-2518	0.0E+00	0.0E+00	0.0E+00	0.0E+00
28	$^5I_6 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.2	-2402	8.5E+02	0.0E+00	0.0E+00	8.5E+02
29	$^5I_4 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-2392	0.0E+00	0.0E+00	0.0E+00	0.0E+00
30	$^5I_5 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.1	-2014	5.8E+02	0.0E+00	0.0E+00	5.8E+02
31	$^5K_9 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	-827	0.0E+00	0.0E+00	0.0E+00	0.0E+00
32	$^5K_8 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	815	0.0E+00	0.0E+00	0.0E+00	0.0E+00
33	$^5K_5 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	97.5	1334	5.2E+05	0.0E+00	0.0E+00	5.2E+05
34	$^5K_7 \rightarrow {}^7F_6$	$S_0 \rightarrow S_1$	0.0	1693	4.3E-02	0.0E+00	0.0E+00	4.3E-02
35	$^5D_4 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-21604	2.6E-46	6.0E-50	1.3E-46	1.3E-46
36	$^5D_3 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-15812	8.3E-32	5.1E-34	8.2E-32	0.0E+00
37	$^5G_6 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-15625	6.6E-30	3.6E-33	1.1E-30	5.5E-30
38	$^5L_{10} \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-15077	8.8E-33	8.8E-33	1.9E-35	0.0E+00
39	$^5G_5 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-14281	7.8E-26	9.2E-30	1.2E-28	7.8E-26
40	$^5D_2 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-13941	7.0E-29	3.6E-29	3.4E-29	0.0E+00
41	$^5G_4 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-13761	2.9E-25	8.6E-29	1.7E-26	2.7E-25
42	$^5L_9 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-13640	5.4E-28	5.3E-28	1.5E-29	0.0E+00
43	$^5G_3 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-13071	0.0E+00	0.0E+00	0.0E+00	0.0E+00
44	$^5L_8 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-12858	1.0E-25	9.6E-26	4.6E-27	0.0E+00
45	$^5L_7 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-12591	4.3E-24	1.6E-25	4.1E-24	0.0E+00
46	$^5G_2 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-12517	0.0E+00	0.0E+00	0.0E+00	0.0E+00
47	$^5L_6 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-12378	2.7E-23	0.0E+00	0.0E+00	2.7E-23
48	$^5D_1 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-11438	0.0E+00	0.0E+00	0.0E+00	0.0E+00
49	$^5D_0 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-10824	0.0E+00	0.0E+00	0.0E+00	0.0E+00
50	$^5H_7 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-10669	0.0E+00	0.0E+00	0.0E+00	0.0E+00
51	$^5H_6 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-9157	2.4E-14	0.0E+00	0.0E+00	2.4E-14

52	$^5H_5 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-8281	4.6E-11	0.0E+00	0.0E+00	4.6E-11
53	$^5H_4 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-7709	3.0E-09	0.0E+00	0.0E+00	3.0E-09
54	$^5F_5 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-7114	3.6E-08	0.0E+00	0.0E+00	3.6E-08
55	$^5H_3 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-7112	0.0E+00	0.0E+00	0.0E+00	0.0E+00
56	$^5I_8 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-6917	0.0E+00	0.0E+00	0.0E+00	0.0E+00
57	$^5F_4 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-6674	1.4E-06	0.0E+00	0.0E+00	1.4E-06
58	$^5F_3 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-5498	0.0E+00	0.0E+00	0.0E+00	0.0E+00
59	$^5I_7 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-5459	0.0E+00	0.0E+00	0.0E+00	0.0E+00
60	$^5F_2 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-4912	0.0E+00	0.0E+00	0.0E+00	0.0E+00
61	$^5F_1 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-4566	0.0E+00	0.0E+00	0.0E+00	0.0E+00
62	$^5I_6 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-4450	3.8E-03	0.0E+00	0.0E+00	3.8E-03
63	$^5I_4 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-4440	5.8E-06	0.0E+00	0.0E+00	5.8E-06
64	$^5I_5 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-4062	2.3E-03	0.0E+00	0.0E+00	2.3E-03
65	$^5K_9 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-2875	0.0E+00	0.0E+00	0.0E+00	0.0E+00
66	$^5K_8 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-1233	0.0E+00	0.0E+00	0.0E+00	0.0E+00
67	$^5K_5 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	2.2	-714	1.2E+04	0.0E+00	0.0E+00	1.2E+04
68	$^5K_7 \rightarrow {}^7F_5$	$S_0 \rightarrow S_1$	0.0	-355	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				W_b^S	**5.3E+05**			
69	$^5D_4 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	-455	1.0E+01	2.4E-02	9.98E+00	0.00E+00
70	$^5D_3 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	5337	1.5E-01	1.4E-01	9.19E-03	0.00E+00
71	$^5G_6 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	41.6	5524	5.8E+07	5.9E+00	6.5E+01	5.75E+07
72	$^5L_{10} \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	6072	1.6E+00	1.6E+00	6.73E-03	0.00E+00
73	$^5G_5 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	2.5	6868	3.5E+06	6.2E-01	4.38E+01	3.52E+06
74	$^5D_2 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	7208	0.0E+00	0.0E+00	0.00E+00	0.00E+00
75	$^5G_4 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	7388	4.4E+00	4.2E-01	3.94E+00	0.00E+00
76	$^5L_9 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	7509	1.0E+00	1.0E+00	2.14E-02	0.00E+00
77	$^5G_3 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	8078	8.1E-02	7.6E-02	4.94E-03	0.00E+00
78	$^5L_8 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	8291	4.6E-01	4.6E-01	1.74E-03	0.00E+00
79	$^5L_7 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	8558	2.8E+01	2.6E-01	1.03E+01	1.71E+01
80	$^5G_2 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	8632	0.0E+00	0.0E+00	0.00E+00	0.00E+00
81	$^5L_6 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.3	8771	4.2E+05	0.0E+00	0.00E+00	4.24E+05
82	$^5D_1 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	9711	0.0E+00	0.0E+00	0.00E+00	0.00E+00
83	$^5D_0 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	10325	0.0E+00	0.0E+00	0.00E+00	0.00E+00
84	$^5H_7 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.2	10480	2.4E+05	0.0E+00	0.00E+00	2.35E+05
85	$^5H_6 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.9	11992	1.2E+06	0.0E+00	0.00E+00	1.24E+06
86	$^5H_5 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	12868	1.1E-02	0.0E+00	0.00E+00	1.12E-02
87	$^5H_4 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	13440	0.0E+00	0.0E+00	0.00E+00	0.00E+00
88	$^5F_5 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.9	14035	1.2E+06	0.0E+00	0.00E+00	1.22E+06
89	$^5H_3 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	14037	0.0E+00	0.0E+00	0.00E+00	0.00E+00
90	$^5I_8 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	14232	0.0E+00	0.0E+00	0.00E+00	0.00E+00
91	$^5F_4 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	14475	0.0E+00	0.0E+00	0.00E+00	0.00E+00
92	$^5F_3 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	15651	0.0E+00	0.0E+00	0.00E+00	0.00E+00
93	$^5I_7 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	15690	1.7E+04	0.0E+00	0.00E+00	1.73E+04
94	$^5F_2 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	16237	0.0E+00	0.0E+00	0.00E+00	0.00E+00
95	$^5F_1 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	16583	0.0E+00	0.0E+00	0.00E+00	0.00E+00
96	$^5I_6 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.1	16699	1.7E+05	0.0E+00	0.00E+00	1.67E+05
97	$^5I_4 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	16709	0.0E+00	0.0E+00	0.00E+00	0.00E+00
98	$^5I_5 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	17087	1.3E+04	0.0E+00	0.00E+00	1.33E+04
99	$^5K_9 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	18274	0.0E+00	0.0E+00	0.00E+00	0.00E+00
100	$^5K_8 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	19916	0.0E+00	0.0E+00	0.00E+00	0.00E+00
101	$^5K_5 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	20435	8.3E+01	0.0E+00	0.00E+00	8.27E+01
102	$^5K_7 \rightarrow {}^7F_6$	$S_0 \rightarrow T_1$	0.0	20794	5.6E-06	0.0E+00	0.00E+00	5.58E-06
103	$^5D_4 \rightarrow {}^7F_5$	$S_0 \rightarrow T_1$	0.0	-2503	7.0E+01	3.7E-06	7.7E-03	7.04E+01
104	$^5D_3 \rightarrow {}^7F_5$	$S_0 \rightarrow T_1$	0.0	3289	5.3E+01	3.4E-01	5.30E+01	0.00E+00
105	$^5G_6 \rightarrow {}^7F_5$	$S_0 \rightarrow T_1$	7.4	3476	1.0E+07	7.5E-01	2.23E+02	1.03E+07

106	$^5L_{10}\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	4024	5.9E-02	5.9E-02	1.04E-04	0.00E+00
107	$^5G_5\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	24.3	4820	3.4E+07	4.4E-01	5.5E+00	3.36E+07
108	$^5D_2\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	5160	3.9E-01	2.1E-01	1.75E-01	0.00E+00
109	$^5G_4\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	3.4	5340	4.8E+06	1.6E-01	3.05E+01	4.77E+06
110	$^5L_9\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	5461	4.9E-01	4.8E-01	1.21E-02	0.00E+00
111	$^5G_3\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	6030	0.0E+00	0.0E+00	0.00E+00	0.00E+00
112	$^5L_8\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	6243	7.5E-01	7.2E-01	3.06E-02	0.00E+00
113	$^5L_7\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	6510	6.0E+00	2.4E-01	5.80E+00	0.00E+00
114	$^5G_2\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	6584	0.0E+00	0.0E+00	0.00E+00	0.00E+00
115	$^5L_6\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.1	6723	9.9E+04	0.0E+00	0.00E+00	9.87E+04
116	$^5D_1\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	7663	0.0E+00	0.0E+00	0.00E+00	0.00E+00
117	$^5D_0\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	8277	0.0E+00	0.0E+00	0.00E+00	0.00E+00
118	$^5H_7\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	8432	0.0E+00	0.0E+00	0.00E+00	0.00E+00
119	$^5H_6\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.2	9944	3.4E+05	0.0E+00	0.00E+00	3.40E+05
120	$^5H_5\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	2.7	10820	3.7E+06	0.0E+00	0.00E+00	3.70E+06
121	$^5H_4\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	6.0	11392	8.3E+06	0.0E+00	0.00E+00	8.34E+06
122	$^5F_5\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	2.3	11987	3.1E+06	0.0E+00	0.00E+00	3.13E+06
123	$^5H_3\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	11989	0.0E+00	0.0E+00	0.00E+00	0.00E+00
124	$^5I_8\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	12184	0.0E+00	0.0E+00	0.00E+00	0.00E+00
125	$^5F_4\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	7.0	12427	9.6E+06	0.0E+00	0.00E+00	9.64E+06
126	$^5F_3\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	13603	0.0E+00	0.0E+00	0.00E+00	0.00E+00
127	$^5I_7\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	13642	0.0E+00	0.0E+00	0.00E+00	0.00E+00
128	$^5F_2\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	14189	0.0E+00	0.0E+00	0.00E+00	0.00E+00
129	$^5F_1\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	14535	0.0E+00	0.0E+00	0.00E+00	0.00E+00
130	$^5I_6\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.1	14651	7.4E+04	0.0E+00	0.00E+00	7.40E+04
131	$^5I_4\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	14661	1.1E+02	0.0E+00	0.00E+00	1.07E+02
132	$^5I_5\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	15039	4.9E+03	0.0E+00	0.00E+00	4.94E+03
133	$^5K_9\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	16226	0.0E+00	0.0E+00	0.00E+00	0.00E+00
134	$^5K_8\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	17868	0.0E+00	0.0E+00	0.00E+00	0.00E+00
135	$^5K_5\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	18387	2.1E+02	0.0E+00	0.00E+00	2.09E+02
136	$^5K_7\rightarrow{}^7F_5$	$S_0\rightarrow T_1$	0.0	18746	0.0E+00	0.0E+00	0.00E+00	0.00E+00
				$\boldsymbol{W_b^T}$	**1.4E+08**			

Table S19. Forward IET rates (in units of s^{-1}) for $[Dy(OPAd_2Bz)_2(H_2O)_4Cl]$ (**4**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{9/2}$	0.0	18947	2.2E-02	2.1E-02	1.4E-03	0.0E+00
2	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{15/2}$	8.0	17953	1.5E+03	2.8E+00	1.5E+03	3.7E+01
3	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4G_{11/2}$	0.1	16612	9.6E+00	1.3E-01	9.5E+00	0.0E+00
4	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{21/2}$	0.1	15066	1.8E+01	1.7E+01	9.5E-01	0.0E+00
5	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{13/2}$	61.1	14381	1.2E+04	1.3E+01	1.8E+03	9.9E+03
6	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{7/2}$	0.2	14319	4.4E+01	2.7E+01	1.6E+01	0.0E+00
7	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4K_{17/2}$	28.0	14285	5.4E+03	5.2E+01	5.3E+03	0.0E+00
8	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{19/2}$	1.5	13841	2.8E+02	9.7E+01	1.9E+02	0.0E+00
9	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{3/2}$	1.0	12632	1.9E+02	1.9E+02	3.3E-01	0.0E+00
10	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{5/2}$	0.1	12551	1.1E+01	1.1E+01	1.9E-02	0.0E+00
				W^S	**1.9E+04**			
11	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{9/2}$	0.0	-154	1.1E+00	1.0E+00	6.3E-02	0.0E+00
12	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{15/2}$	100.0	-1148	2.9E+04	2.4E-01	1.2E+02	2.9E+04
13	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4G_{11/2}$	0.0	-2489	1.6E-04	2.3E-06	1.5E-04	0.0E+00
14	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{21/2}$	0.0	-4035	1.9E-08	1.8E-08	8.7E-10	0.0E+00
15	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{13/2}$	0.0	-4720	1.3E-03	1.9E-10	2.6E-08	1.3E-03
16	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{7/2}$	0.0	-4782	4.1E-10	2.7E-10	1.5E-10	0.0E+00
17	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4K_{17/2}$	0.0	-4816	4.2E-08	4.2E-10	4.1E-08	0.0E+00
18	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{19/2}$	0.0	-5260	1.4E-10	5.0E-11	9.2E-11	0.0E+00
19	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{3/2}$	0.0	-6469	6.0E-14	6.0E-14	8.4E-17	0.0E+00
20	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{5/2}$	0.0	-6550	2.0E-15	2.0E-15	2.9E-18	0.0E+00
				W^T	**2.9E+04**			

Table S20. Backward IET rates (in units of s^{-1}) for $[Dy(OPAd_2Bz)_2(H_2O)_4Cl]$ (**4**). The Δ is the donor-acceptor energy difference. W_b^S and W_b^T are the total energy transfer to the S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$^4F_{9/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-18947	1.3E-41	1.2E-41	8.1E-43	0.0E+00
2	$^4I_{15/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-17953	6.2E-35	1.1E-37	6.0E-35	1.5E-36
3	$^4G_{11/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-16612	3.3E-34	4.6E-36	3.3E-34	0.0E+00
4	$^4M_{21/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-15066	5.4E-31	5.2E-31	2.8E-32	0.0E+00
5	$^4I_{13/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.3	-14381	1.5E-26	1.7E-29	2.3E-27	1.3E-26
6	$^4F_{7/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-14319	1.4E-28	8.7E-29	5.3E-29	0.0E+00
7	$^4K_{17/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.2	-14285	8.4E-27	8.2E-29	8.3E-27	0.0E+00
8	$^4M_{19/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.1	-13841	3.3E-27	1.1E-27	2.2E-27	0.0E+00
9	$^6P_{3/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	94.8	-12632	4.7E-24	4.7E-24	8.1E-27	0.0E+00
10	$^6P_{5/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	4.7	-12551	2.3E-25	2.3E-25	4.0E-28	0.0E+00
				W_b^S	**5.0E-24**			
11	$^4F_{9/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	154	3.9E+00	3.6E+00	2.2E-01	0.0E+00
12	$^4I_{15/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	40.8	1148	7.0E+06	5.8E+01	3.0E+04	7.0E+06
13	$^4G_{11/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	2489	3.3E+01	4.7E-01	3.2E+01	0.0E+00
14	$^4M_{21/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	4035	3.4E+00	3.2E+00	1.6E-01	0.0E+00
15	$^4I_{13/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	59.2	4720	1.0E+07	1.5E+00	2.0E+02	1.0E+07
16	$^4F_{7/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	4782	8.1E+00	5.2E+00	2.8E+00	0.0E+00
17	$^4K_{17/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	4816	3.9E+02	4.0E+00	3.9E+02	0.0E+00
18	$^4M_{19/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	5260	1.0E+01	3.6E+00	6.6E+00	0.0E+00
19	$^6P_{3/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	6469	8.9E+00	8.9E+00	1.2E-02	0.0E+00
20	$^6P_{5/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	6550	2.7E-01	2.7E-01	3.8E-04	0.0E+00
				W_b^T	**1.7E+07**			

Table S21. Forward IET rates (in units of s^{-1}) for $[Eu(OPAd_2Bz)_2(H_2O)Cl_3]$ (**5**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_0$	0.0	22707	3.6E-04	9.9E-08	3.6E-04	0.0E+00
2	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_1$	0.1	20973	6.6E-01	0.0E+00	0.0E+00	6.6E-01
3	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_2$	0.0	18517	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_3$	0.0	15645	0.0E+00	0.0E+00	0.0E+00	0.0E+00
5	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_6$	0.3	14675	3.0E+00	2.9E+00	8.5E-02	0.0E+00
6	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_7$	0.0	13643	0.0E+00	0.0E+00	0.0E+00	0.0E+00
7	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_2$	0.0	13608	0.0E+00	0.0E+00	0.0E+00	0.0E+00
8	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_3$	0.0	13378	0.0E+00	0.0E+00	0.0E+00	0.0E+00
9	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_4$	0.0	13265	0.0E+00	0.0E+00	0.0E+00	0.0E+00
10	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_6$	0.4	13248	4.1E+00	4.0E+00	1.2E-01	0.0E+00
11	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_5$	0.0	13237	0.0E+00	0.0E+00	0.0E+00	0.0E+00
12	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_8$	0.0	12756	0.0E+00	0.0E+00	0.0E+00	0.0E+00
13	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_4$	2.8	12414	2.6E+01	2.1E+00	2.4E+01	0.0E+00
14	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_9$	0.0	12040	0.0E+00	0.0E+00	0.0E+00	0.0E+00
15	$S_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_{10}$	0.0	11573	0.0E+00	0.0E+00	0.0E+00	0.0E+00
16	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_0$	0.0	23079	3.4E-03	0.0E+00	0.0E+00	3.4E-03
17	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_1$	0.0	21345	8.2E-03	2.2E-06	8.2E-03	2.3E-05
18	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_2$	0.0	18889	2.7E-01	0.0E+00	0.0E+00	2.7E-01
19	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_3$	0.8	16017	7.3E+00	3.8E-03	7.3E+00	0.0E+00
20	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_6$	0.0	15047	7.5E-02	7.3E-02	2.1E-03	0.0E+00
21	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_7$	0.1	14015	5.5E-01	5.3E-01	1.5E-02	0.0E+00
22	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_2$	88.2	13980	8.3E+02	0.0E+00	0.0E+00	8.3E+02
23	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_3$	7.2	13750	6.8E+01	5.3E-02	6.8E+01	0.0E+00
24	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_4$	0.0	13637	0.0E+00	0.0E+00	0.0E+00	0.0E+00
25	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_6$	0.0	13620	2.4E-01	2.3E-01	6.7E-03	0.0E+00
26	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_5$	0.1	13609	6.4E-01	4.8E-01	1.6E-01	0.0E+00
27	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_8$	0.0	13128	0.0E+00	0.0E+00	0.0E+00	0.0E+00
28	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_4$	0.0	12786	0.0E+00	0.0E+00	0.0E+00	0.0E+00
29	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_9$	0.0	12412	0.0E+00	0.0E+00	0.0E+00	0.0E+00
30	$S_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_{10}$	0.0	11945	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				W^S	**9.4E+02**			
31	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_0$	0.0	3606	2.7E+01	7.7E-03	2.7E+01	0.0E+00
32	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_1$	80.7	1872	2.1E+07	0.0E+00	0.0E+00	2.1E+07
33	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_2$	0.0	-584	0.0E+00	0.0E+00	0.0E+00	0.0E+00
34	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_3$	0.0	-3456	0.0E+00	0.0E+00	0.0E+00	0.0E+00
35	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_6$	0.0	-4426	2.8E-10	2.8E-10	7.0E-12	0.0E+00
36	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_7$	0.0	-5458	0.0E+00	0.0E+00	0.0E+00	0.0E+00
37	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_2$	0.0	-5493	0.0E+00	0.0E+00	0.0E+00	0.0E+00
38	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_3$	0.0	-5723	0.0E+00	0.0E+00	0.0E+00	0.0E+00
39	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_4$	0.0	-5836	0.0E+00	0.0E+00	0.0E+00	0.0E+00
40	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_6$	0.0	-5853	5.7E-14	5.6E-14	1.4E-15	0.0E+00
41	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5G_5$	0.0	-5864	0.0E+00	0.0E+00	0.0E+00	0.0E+00
42	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_8$	0.0	-6345	0.0E+00	0.0E+00	0.0E+00	0.0E+00
43	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5D_4$	0.0	-6687	2.1E-15	1.8E-16	1.9E-15	0.0E+00
44	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_9$	0.0	-7061	0.0E+00	0.0E+00	0.0E+00	0.0E+00
45	$T_1 \rightarrow S_0$	$^7F_0 \rightarrow {}^5L_{10}$	0.0	-7528	0.0E+00	0.0E+00	0.0E+00	0.0E+00
46	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_0$	18.9	3978	5.0E+06	0.0E+00	0.0E+00	5.0E+06
47	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_1$	0.0	2244	1.5E+03	1.5E-02	5.2E+01	1.4E+03
48	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_2$	0.3	-212	9.2E+04	0.0E+00	0.0E+00	9.2E+04
49	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_3$	0.0	-3084	2.9E-06	1.6E-09	2.9E-06	0.0E+00
50	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_6$	0.0	-4054	7.2E-11	7.0E-11	1.8E-12	0.0E+00

51	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_7$	0.0	-5086	8.6E-13	8.4E-13	2.1E-14	0.0E+00
52	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_2$	0.0	-5121	9.9E-06	0.0E+00	0.0E+00	9.9E-06
53	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_3$	0.0	-5351	2.0E-11	1.6E-14	2.0E-11	0.0E+00
54	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_4$	0.0	-5464	0.0E+00	0.0E+00	0.0E+00	0.0E+00
55	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_6$	0.0	-5481	3.3E-14	3.2E-14	8.1E-16	0.0E+00
56	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5G_5$	0.0	-5492	8.1E-14	6.1E-14	2.0E-14	0.0E+00
57	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_8$	0.0	-5973	0.0E+00	0.0E+00	0.0E+00	0.0E+00
58	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5D_4$	0.0	-6315	0.0E+00	0.0E+00	0.0E+00	0.0E+00
59	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_9$	0.0	-6689	0.0E+00	0.0E+00	0.0E+00	0.0E+00
60	$T_1 \rightarrow S_0$	$^7F_1 \rightarrow {}^5L_{10}$	0.0	-7156	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				W^T	**2.6E+07**			

Table S22. Backward IET rates (in units of s^{-1}) for $[Eu(OPAd_2Bz)_2(H_2O)Cl_3]$ (**5**). The Δ is the donor-acceptor energy difference. W_b^S and W_b^T are the total energy transfer to the S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$^5D_0 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-22707	2.2E-51	6.0E-55	2.2E-51	0.0E+00
2	$^5D_1 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-20973	5.5E-45	0.0E+00	0.0E+00	5.5E-45
3	$^5D_2 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-18517	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4	$^5D_3 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-15645	0.0E+00	0.0E+00	0.0E+00	0.0E+00
5	$^5L_6 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-14675	7.6E-32	7.4E-32	2.1E-33	0.0E+00
6	$^5L_7 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-13643	0.0E+00	0.0E+00	0.0E+00	0.0E+00
7	$^5G_2 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-13608	0.0E+00	0.0E+00	0.0E+00	0.0E+00
8	$^5G_3 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-13378	0.0E+00	0.0E+00	0.0E+00	0.0E+00
9	$^5G_4 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-13265	0.0E+00	0.0E+00	0.0E+00	0.0E+00
10	$^5G_6 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.1	-13248	9.7E-29	9.4E-29	2.7E-30	0.0E+00
11	$^5G_5 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-13237	0.0E+00	0.0E+00	0.0E+00	0.0E+00
12	$^5L_8 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-12756	0.0E+00	0.0E+00	0.0E+00	0.0E+00
13	$^5D_4 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	64.3	-12414	4.8E-26	4.0E-27	4.4E-26	0.0E+00
14	$^5L_9 \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-12040	0.0E+00	0.0E+00	0.0E+00	0.0E+00
15	$^5L_{10} \rightarrow {}^7F_0$	$S_0 \rightarrow S_1$	0.0	-11573	0.0E+00	0.0E+00	0.0E+00	0.0E+00
16	$^5D_0 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-23079	5.2E-50	0.0E+00	0.0E+00	5.2E-50
17	$^5D_1 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-21345	1.7E-46	4.6E-50	1.7E-46	4.8E-49
18	$^5D_2 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-18889	4.4E-40	0.0E+00	0.0E+00	4.4E-40
19	$^5D_3 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-16017	8.1E-33	4.3E-36	8.1E-33	0.0E+00
20	$^5L_6 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-15047	4.7E-33	4.6E-33	1.3E-34	0.0E+00
21	$^5L_7 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-14015	4.2E-30	4.1E-30	1.2E-31	0.0E+00
22	$^5G_2 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	30.2	-13980	2.3E-26	0.0E+00	0.0E+00	2.3E-26
23	$^5G_3 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	5.3	-13750	4.0E-27	3.1E-30	4.0E-27	0.0E+00
24	$^5G_4 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-13637	0.0E+00	0.0E+00	0.0E+00	0.0E+00
25	$^5G_6 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-13620	1.4E-29	1.4E-29	3.9E-31	0.0E+00
26	$^5G_5 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.1	-13609	4.7E-29	3.5E-29	1.2E-29	0.0E+00
27	$^5L_8 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-13128	0.0E+00	0.0E+00	0.0E+00	0.0E+00
28	$^5D_4 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-12786	0.0E+00	0.0E+00	0.0E+00	0.0E+00
29	$^5L_9 \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-12412	0.0E+00	0.0E+00	0.0E+00	0.0E+00
30	$^5L_{10} \rightarrow {}^7F_1$	$S_0 \rightarrow S_1$	0.0	-11945	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				W_b^S	**7.5E-26**			
31	$^5D_0 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	-3606	1.0E-06	2.8E-10	1.0E-06	0.0E+00
32	$^5D_1 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	-1872	1.1E+03	0.0E+00	0.0E+00	1.1E+03
33	$^5D_2 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	584	0.0E+00	0.0E+00	0.0E+00	0.0E+00
34	$^5D_3 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	3456	0.0E+00	0.0E+00	0.0E+00	0.0E+00
35	$^5L_6 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	4426	4.4E-02	4.2E-02	1.1E-03	0.0E+00
36	$^5L_7 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5458	0.0E+00	0.0E+00	0.0E+00	0.0E+00
37	$^5G_2 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5493	0.0E+00	0.0E+00	0.0E+00	0.0E+00
38	$^5G_3 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5723	0.0E+00	0.0E+00	0.0E+00	0.0E+00

39	$^5G_4 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5836	0.0E+00	0.0E+00	0.0E+00	0.0E+00
40	$^5G_6 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5853	8.2E-03	8.0E-03	2.0E-04	0.0E+00
41	$^5G_5 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	5864	0.0E+00	0.0E+00	0.0E+00	0.0E+00
42	$^5L_8 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	6345	0.0E+00	0.0E+00	0.0E+00	0.0E+00
43	$^5D_4 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	6687	2.3E-02	2.0E-03	2.1E-02	0.0E+00
44	$^5L_9 \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	7061	0.0E+00	0.0E+00	0.0E+00	0.0E+00
45	$^5L_{10} \rightarrow {}^7F_0$	$S_0 \rightarrow T_1$	0.0	7528	0.0E+00	0.0E+00	0.0E+00	0.0E+00
46	$^5D_0 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	-3978	4.6E-01	0.0E+00	0.0E+00	4.6E-01
47	$^5D_1 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	-2244	1.9E-01	1.9E-06	6.6E-03	1.8E-01
48	$^5D_2 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	35.7	212	9.1E+05	0.0E+00	0.0E+00	9.1E+05
49	$^5D_3 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	3084	2.0E+01	1.1E-02	2.0E+01	0.0E+00
50	$^5L_6 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	4054	2.7E-02	2.7E-02	6.7E-04	0.0E+00
51	$^5L_7 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5086	4.0E-02	3.9E-02	9.9E-04	0.0E+00
52	$^5G_2 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	64.2	5121	1.6E+06	0.0E+00	0.0E+00	1.6E+06
53	$^5G_3 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5351	7.2E+00	5.8E-03	7.2E+00	0.0E+00
54	$^5G_4 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5464	0.0E+00	0.0E+00	0.0E+00	0.0E+00
55	$^5G_6 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5481	1.2E-02	1.1E-02	2.9E-04	0.0E+00
56	$^5G_5 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5492	3.6E-02	2.7E-02	8.7E-03	0.0E+00
57	$^5L_8 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	5973	0.0E+00	0.0E+00	0.0E+00	0.0E+00
58	$^5D_4 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	6315	0.0E+00	0.0E+00	0.0E+00	0.0E+00
59	$^5L_9 \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	6689	0.0E+00	0.0E+00	0.0E+00	0.0E+00
60	$^5L_{10} \rightarrow {}^7F_1$	$S_0 \rightarrow T_1$	0.0	7156	0.0E+00	0.0E+00	0.0E+00	0.0E+00
				$\boldsymbol{W_b^T}$	**2.6E+06**			

Table S23. Forward IET rates (in units of s^{-1}) for $[Dy(OPAd_2Bz)_2(THF)Cl_3]$ (**7**). The Δ is the donor-acceptor energy difference. W^S and W^T are the total energy transfer via S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{9/2}$	0.0	18947	2.0E-03	8.0E-04	1.2E-03	0.0E+00
2	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{15/2}$	7.0	17953	9.9E+02	3.4E-01	9.6E+02	3.2E+01
3	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4G_{11/2}$	0.0	16612	6.2E+00	1.2E-02	6.2E+00	0.0E+00
4	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{21/2}$	0.0	15066	1.5E+00	6.5E-01	8.1E-01	0.0E+00
5	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{13/2}$	67.9	14381	9.7E+03	7.4E-01	1.2E+03	8.5E+03
6	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{7/2}$	0.1	14319	1.6E+01	1.6E+00	1.4E+01	0.0E+00
7	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4K_{17/2}$	24.1	14285	3.4E+03	2.7E+00	3.4E+03	0.0E+00
8	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{19/2}$	0.9	13841	1.3E+02	3.7E+00	1.2E+02	0.0E+00
9	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{3/2}$	0.1	12632	7.2E+00	6.9E+00	2.7E-01	0.0E+00
10	$S_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{5/2}$	0.0	12551	4.0E-01	3.9E-01	1.5E-02	0.0E+00
				W^S	**1.4E+04**			
11	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{9/2}$	0.0	-1518	2.3E-04	9.4E-05	1.4E-04	0.0E+00
12	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{15/2}$	100.0	-2512	5.3E+01	5.8E-05	1.6E-01	5.3E+01
13	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4G_{11/2}$	0.0	-3853	1.5E-07	3.0E-10	1.5E-07	0.0E+00
14	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{21/2}$	0.0	-5399	1.3E-12	6.1E-13	7.3E-13	0.0E+00
15	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4I_{13/2}$	0.0	-6084	8.5E-07	7.5E-15	1.2E-11	8.5E-07
16	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4F_{7/2}$	0.0	-6146	1.0E-13	1.1E-14	9.2E-14	0.0E+00
17	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4K_{17/2}$	0.0	-6180	1.8E-11	1.5E-14	1.8E-11	0.0E+00
18	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^4M_{19/2}$	0.0	-6624	3.6E-14	1.1E-15	3.5E-14	0.0E+00
19	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{3/2}$	0.0	-7833	7.0E-19	6.8E-19	2.5E-20	0.0E+00
20	$T_1 \rightarrow S_0$	$^6H_{15/2} \rightarrow {}^6P_{5/2}$	0.0	-7914	2.3E-20	2.2E-20	8.2E-22	0.0E+00
				W^T	**5.3E+01**			

Table S24. Backward IET rates (in units of s^{-1}) for $[Dy(OPAd_2Bz)_2(THF)Cl_3]$ (**7**). The Δ is the donor-acceptor energy difference. W_b^S and W_b^T are the total energy transfer to the S_1 and T_1 states.

Pathway	Donor	Acceptor	W(%)	Δ	W_{total}	W_{d-d}	W_{d-m}	W_{ex}
1	$^4F_{9/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-18947	1.1E-42	4.6E-43	6.9E-43	0.0E+00
2	$^4I_{15/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-17953	4.0E-35	1.4E-38	3.9E-35	1.3E-36
3	$^4G_{11/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-16612	2.1E-34	4.1E-37	2.1E-34	0.0E+00
4	$^4M_{21/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-15066	4.3E-32	1.9E-32	2.4E-32	0.0E+00
5	$^4I_{13/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	6.1	-14381	1.2E-26	9.5E-31	1.5E-27	1.1E-26
6	$^4F_{7/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.0	-14319	5.0E-29	5.1E-30	4.5E-29	0.0E+00
7	$^4K_{17/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	2.6	-14285	5.3E-27	4.2E-30	5.3E-27	0.0E+00
8	$^4M_{19/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	0.7	-13841	1.5E-27	4.4E-29	1.4E-27	0.0E+00
9	$^6P_{3/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	86.3	-12632	1.8E-25	1.7E-25	6.5E-27	0.0E+00
10	$^6P_{5/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow S_1$	4.3	-12551	8.7E-27	8.4E-27	3.2E-28	0.0E+00
				W_b^S	**2.0E-25**			
11	$^4F_{9/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	1518	5.6E-01	2.3E-01	3.3E-01	0.0E+00
12	$^4I_{15/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	66.4	2512	9.1E+06	9.9E+00	2.8E+04	9.1E+06
13	$^4G_{11/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	3853	2.2E+01	4.3E-02	2.2E+01	0.0E+00
14	$^4M_{21/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	5399	1.7E-01	7.7E-02	9.2E-02	0.0E+00
15	$^4I_{13/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	33.6	6084	4.6E+06	4.1E-02	6.4E+01	4.6E+06
16	$^4F_{7/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	6146	1.4E+00	1.5E-01	1.3E+00	0.0E+00
17	$^4K_{17/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	6180	1.2E+02	9.5E-02	1.2E+02	0.0E+00
18	$^4M_{19/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	6624	1.8E+00	5.3E-02	1.7E+00	0.0E+00
19	$^6P_{3/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	7833	7.3E-02	7.0E-02	2.6E-03	0.0E+00
20	$^6P_{5/2} \rightarrow {}^6H_{15/2}$	$S_0 \rightarrow T_1$	0.0	7914	2.1E-03	2.0E-03	7.5E-05	0.0E+00
				W_b^T	**1.4E+07**			

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