Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Bright Neodymium Complexes for Efficient Near Infra-Red Organic Light Emitting Diodes

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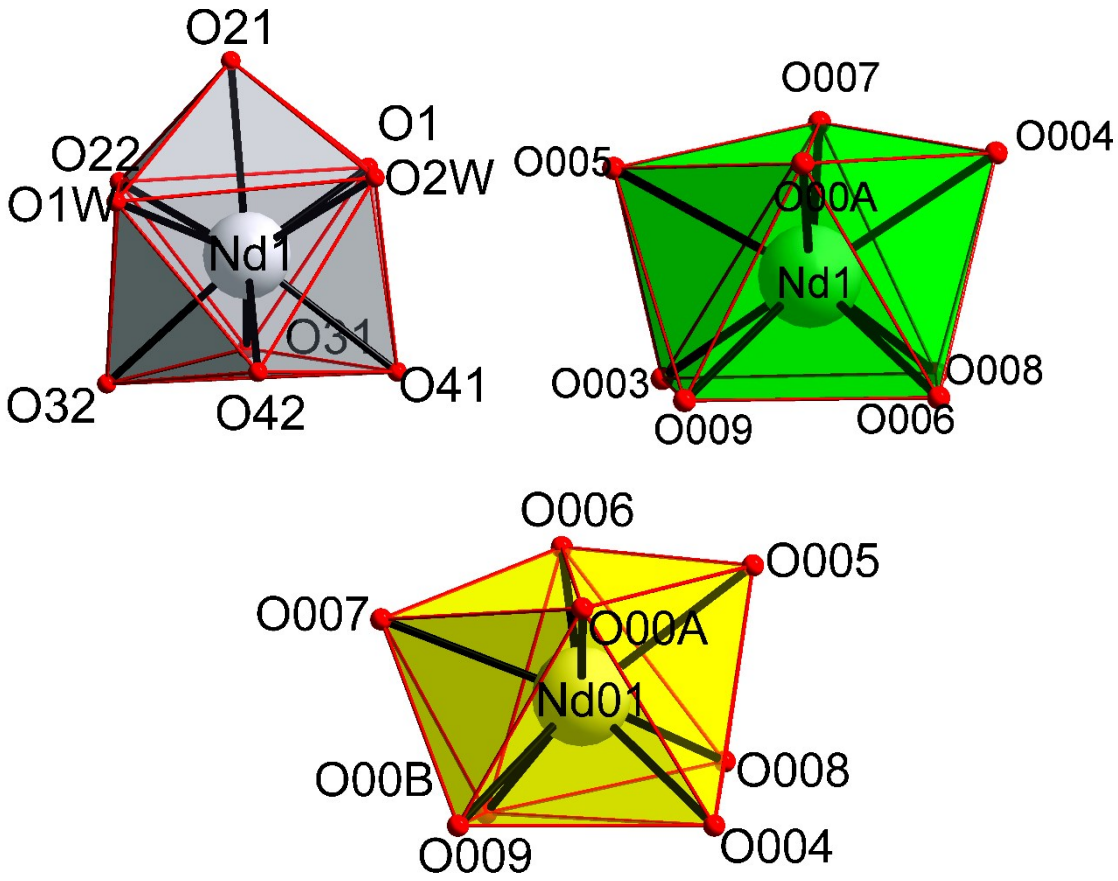

Figure S1. Coordination polyhedra of the complexes **1-3**.

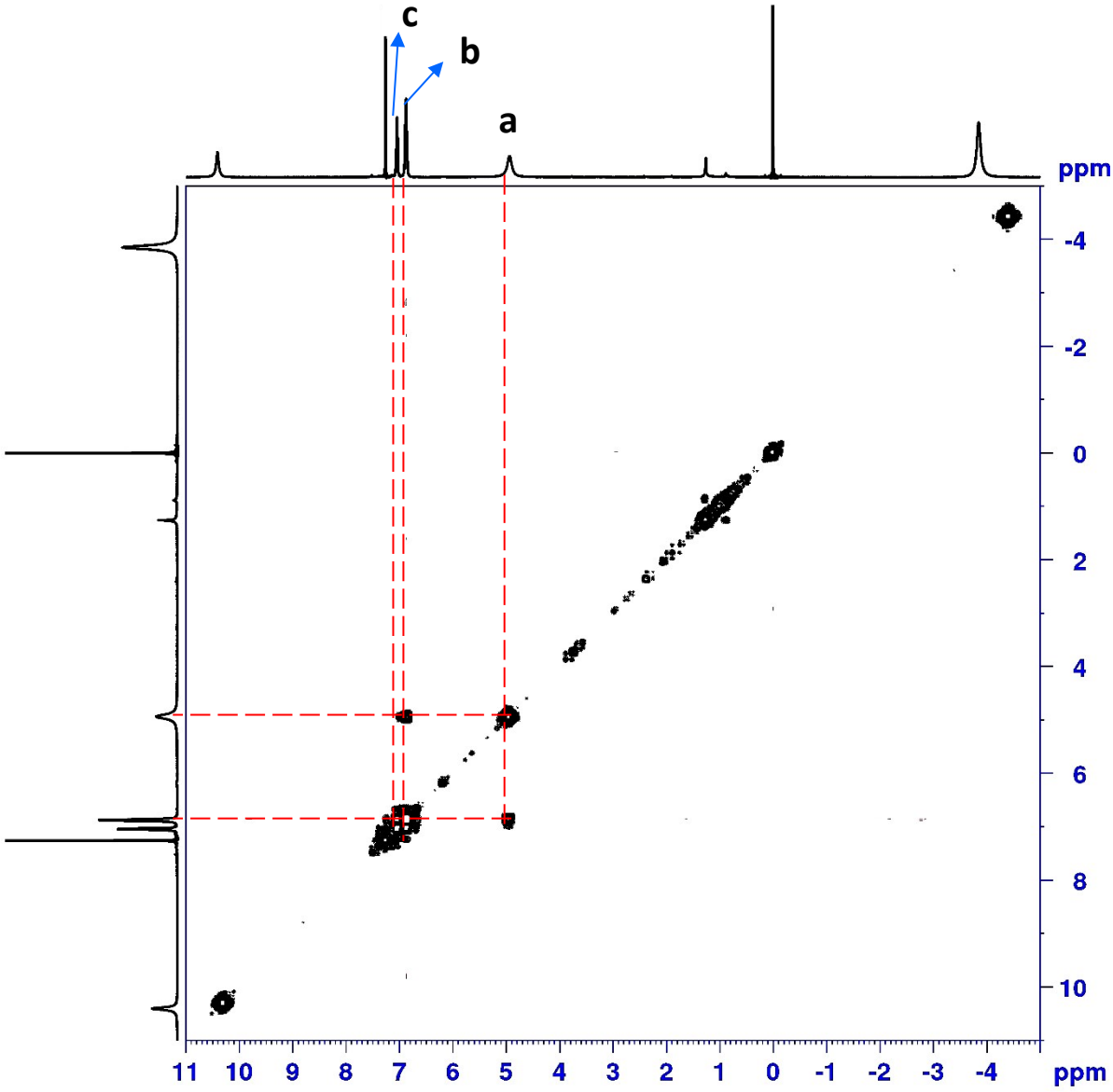

Figure S2. COSY spectrum of the complex **1**.

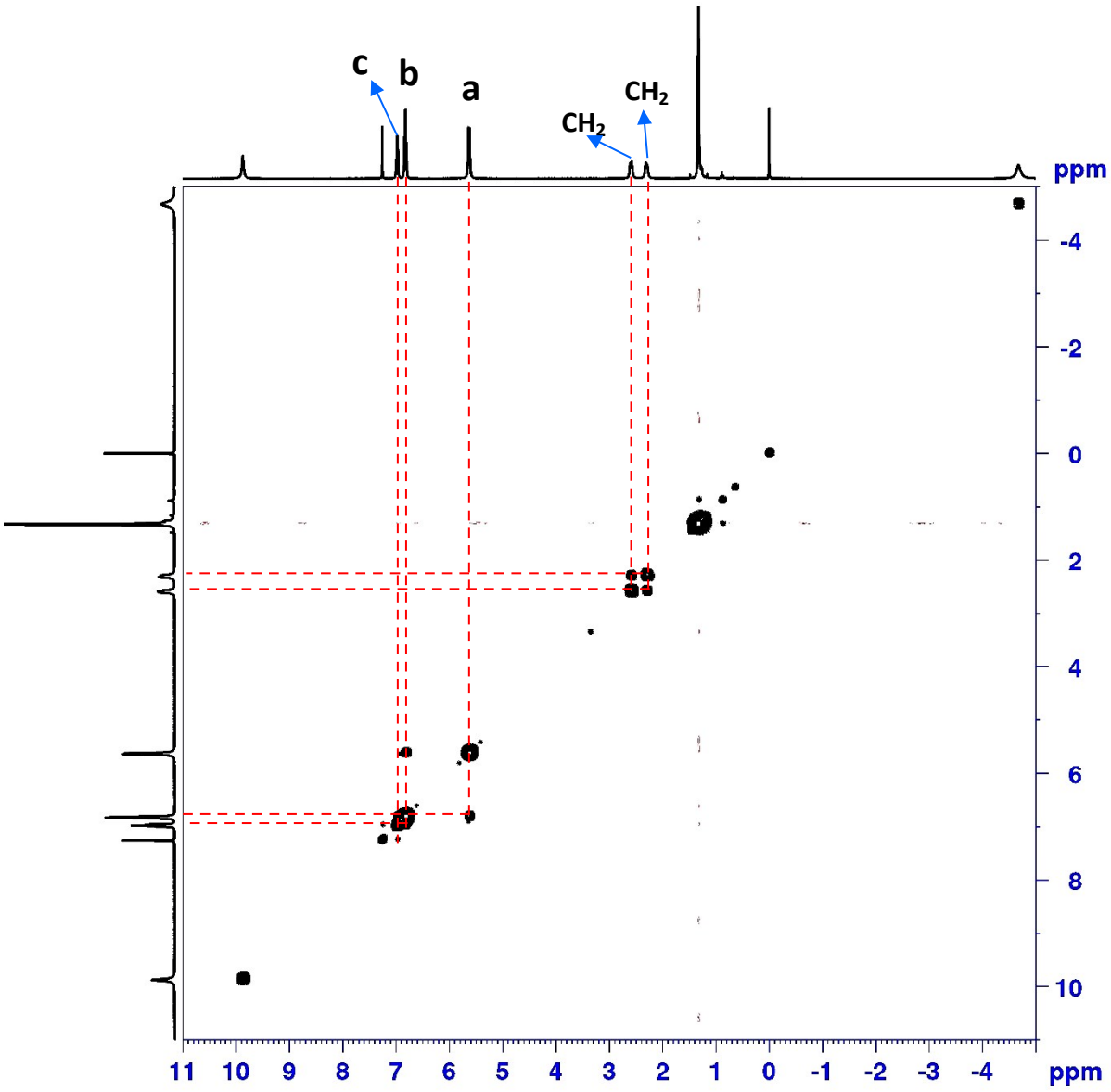

Figure S3. COSY spectrum of the complex **2**.

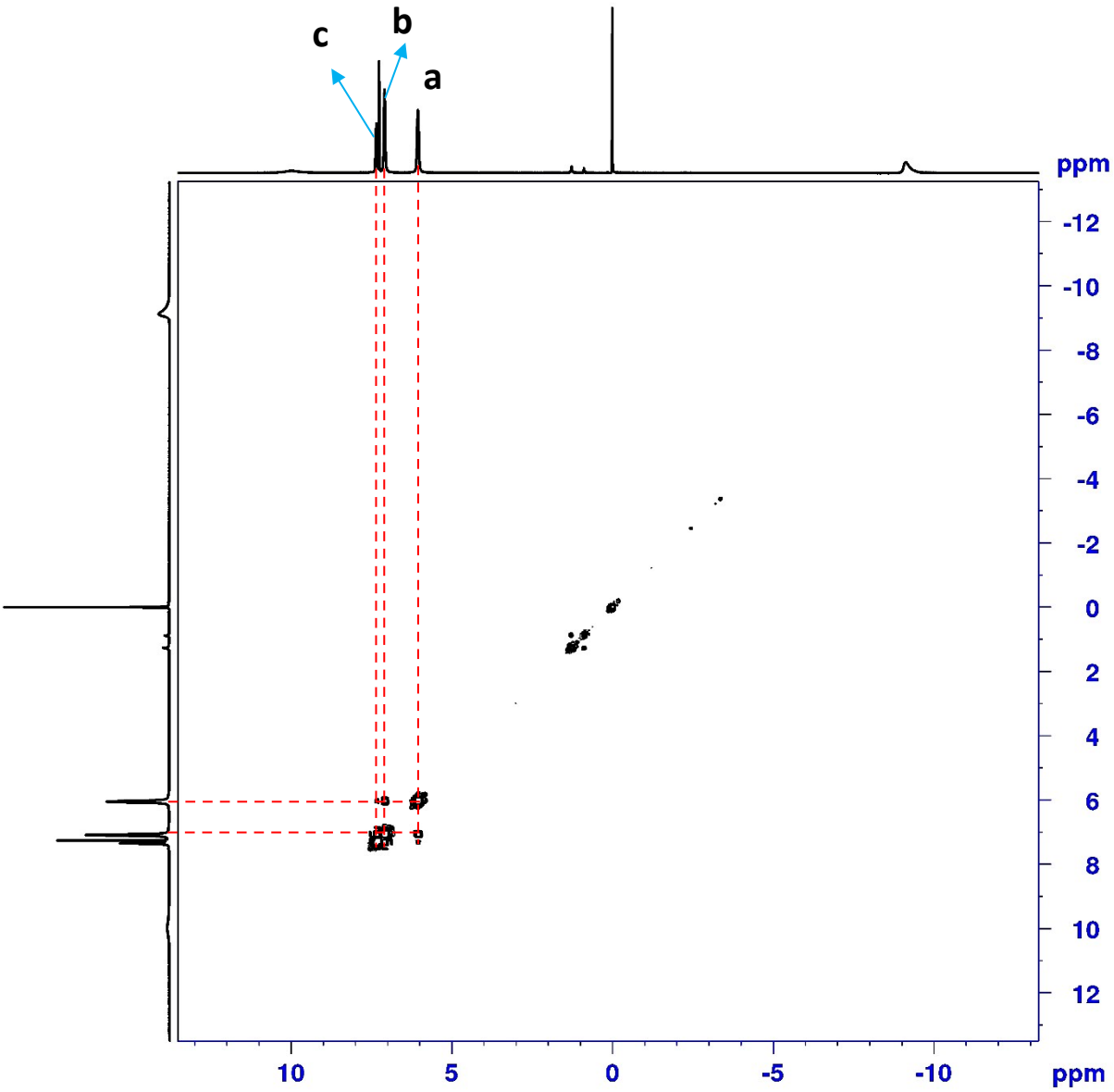

Figure S4. COSY spectrum of the complex **3**.

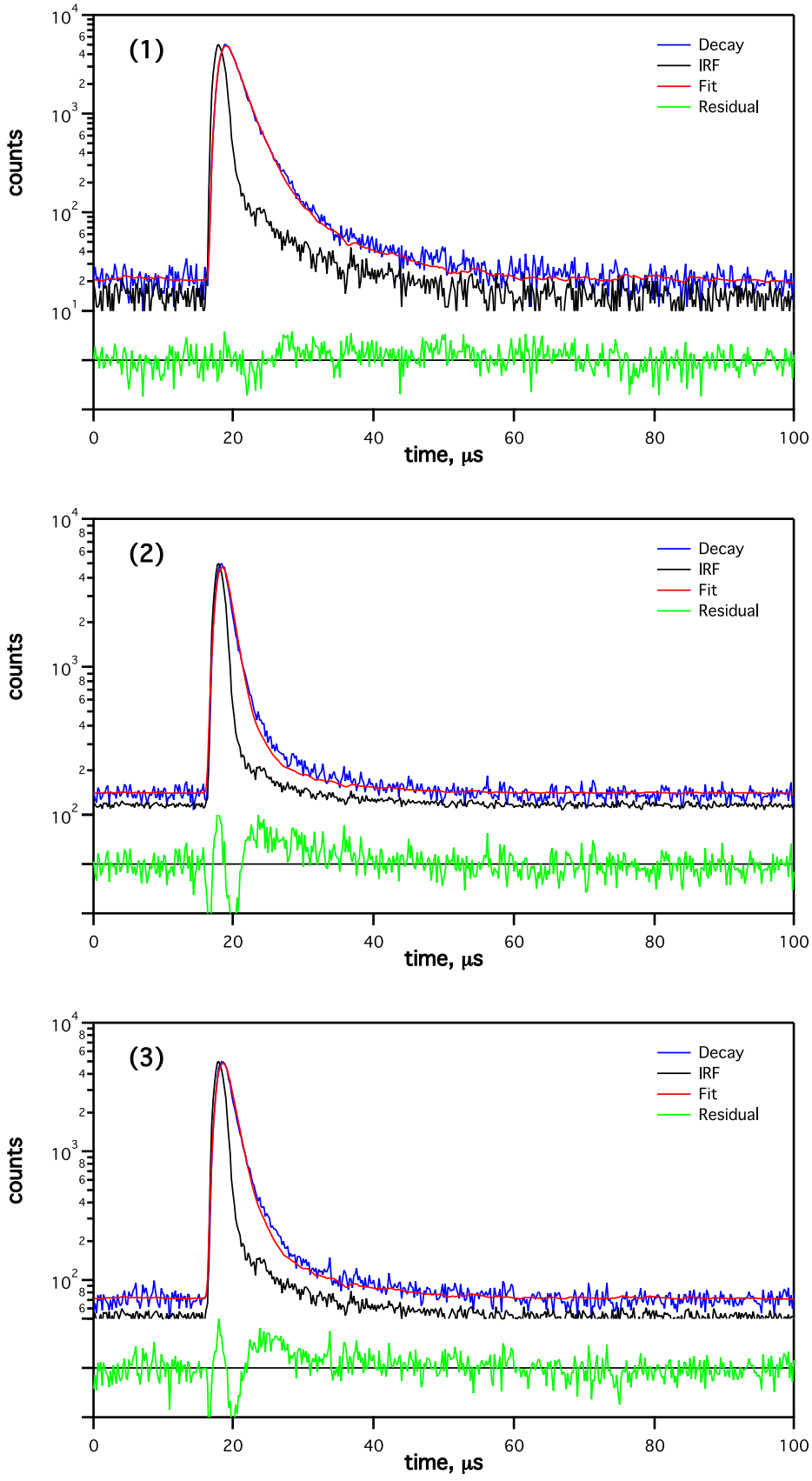

Figure S5. Emission decays for complex **1-3** in CH_2Cl_2, λ_{ex} = 305 nm.

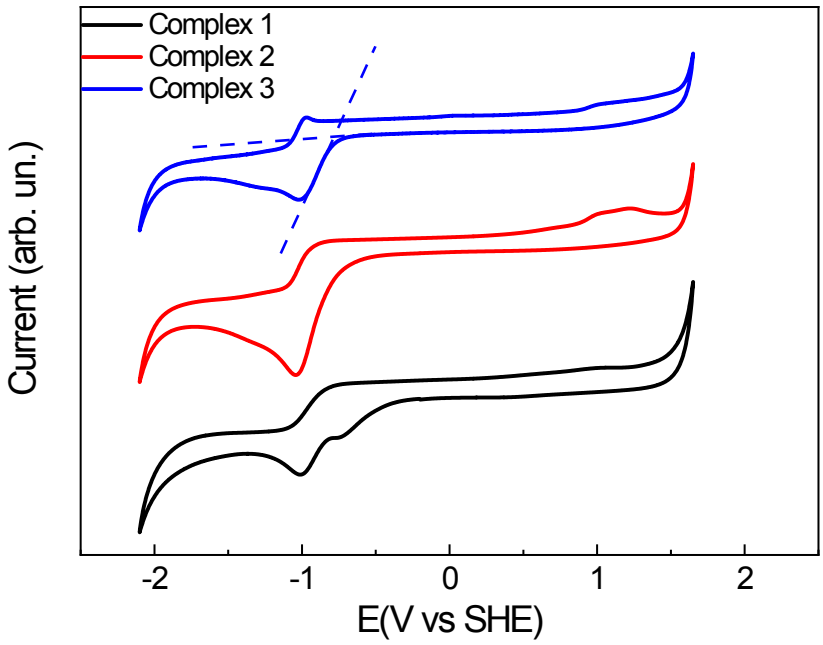

Figure S6.Cyclic Voltammetry curves of the complexes, **1-3.**

Table S1. Bond lengths (Å) of the complexes **1-3**.

	1	**2**	**3**
Nd01–O1	2.443(2)	2.373(3)	2.3634(17)
Nd01–O2	2.425(2)	2.428(3)	2.3670(17)
Nd01–O3	2.539(2)	2.395(3)	2.449(2)
Nd01–O4	2.470(2)	2.471(3)	2.4715(19)
Nd01–O5	2.454(2)	2.443(3)	2.428(2)
Nd01–O6	2.462(2)	2.447(3)	2.4574(19)
Nd01–O7	2.495(2)	2.398(3)	2.4621(18)
Nd01–O8			2.4503(19)
Nd01–O1W	2.515(3)	2.525(3)	
Nd01–O2W	2.503(3)		

Table S2. δ (deg) and φ (deg) values of the complexes **1-3**

	1		**2**		**3**	
δ_1	O2W−[O1W−O1]−O2	2.6	O3−[O2−O4]−O1	0.2	O8−[O1−O3]−O4	8.96
δ_2	O7−[O5−O6]−O4	12.4	O5−[O7−O1W]−O4	9.98	O7−[O2−O5]−O6	16.8
δ_3	O1W−[O5−O2]−O4	49.3	O3−[O5−O4]−O1W	59.4	O6−[O1−O5]−O8	49.3
δ_4	O2W−[O6−O1]−O4	54.1	O7−[O2−O6]−O1	57.3	O2−[O3−O7]−O8	56.2
δ_5	O2−[O3−O1W]−O2W	60.6	–	–	–	–
φ_1	O1W−[O4−2W]−O6	30.0	O4−[O6−O7]−O3	29.9	O1−[O7−O4]−O2	28.3
φ_2	O1−[O7−O5]−O2	32.4	O1W−[O1−O2]−O5	31.0	O3−[O6−O5]−O8	24.7
S	distorted MSAP (C_{4V})		distorted SAP (D_{4d})		distorted SAP (D_{4d})	

Table S3. δ (deg) and φ (deg) values of ideal polyhedrons

	SAP	TP	DD	MSAP	TTP
δ_1	0.0	0.0	29.5	0.0	26.4
δ_2	0.0	21.8	29.5	69.1	59.6
δ_3	52.4	48.2	29.5	53.0	59.6
δ_4	52.4	48.2	29.5	53.0	47.6
δ_5	–	–	–	59.0	59.6
φ_1	24.5	14.1	0.0	37.6	26.6
φ_2	24.5	14.1	0.0	37.6	47.6