

Electronic supplementary information:

Table 1. G_{vac}^i and ΔG_s^i computed for all the reactants and products.

	$G_{\text{vac}}(\text{Hartree})$	ΔG_s (kcal/mol)
H_2O	-76,41668	-2,30
H_3O^+	-76,69037	-111,62
$\text{Al}(\text{H}_2\text{O})_6^{3+}$	-699,97786	-468,37
AP	-953,58944	-15,22
LU	-1028,80805	-17,28
$\text{Al}_1\text{B}^{45}\text{Ap}_2^+$	-2301,28296	-62,38
$\text{Al}_1\text{B}^{45}\text{Ap}_1^{2+}$	-1500,75987	-179,62
$\text{Al}_1\text{M}^4\text{Ap}_1^{3+}$	-1577,31296	-355,49
$\text{Al}_1\text{M}^5\text{Ap}_1^{2+}$	-----	-194,12
$\text{Al}_1\text{M}^7\text{Ap}_1^{2+}$	-1577,11304	-211,56
$\text{Al}_1\text{M}^{4'}\text{Ap}_1^{2+}$	-1577,09248	-229,24
$\text{Al}_1\text{B}^{45}\text{Lu}_2^+$	-2451,72178	-67,31
$\text{Al}_1\text{B}^{45}\text{Lu}_1^{2+}$	-1575,97794	-181,600
$\text{Al}_1\text{B}^{3'4'}\text{Lu}_2^-$	-2450,82345	-63,22
$\text{Al}_1\text{B}^{3'4'}\text{Lu}_1^+$	-1575,66716	-99,53
$\text{Al}_1\text{B}^{45-3'4'}\text{Lu}_2$	-2451,30011	-48,34
$\text{Al}_2\text{B}^{45-3'4'}\text{Lu}_1^{3+}$	-2122,75006	-312,95
$\text{Al}_1\text{M}^4\text{Lu}_1^{3+}$	-1652,53512	-357,85
$\text{Al}_1\text{M}^5\text{Lu}_1^{2+}$	-----	-197,2
$\text{Al}_1\text{M}^7\text{Lu}_1^{2+}$	-1652,32797	-215,26
$\text{Al}_1\text{M}^{3'}\text{Lu}_1^{2+}$	-1652,33066	-211,3
$\text{Al}_1\text{M}^{4'}\text{Lu}_1^{2+}$	-1652,33202	-217,85

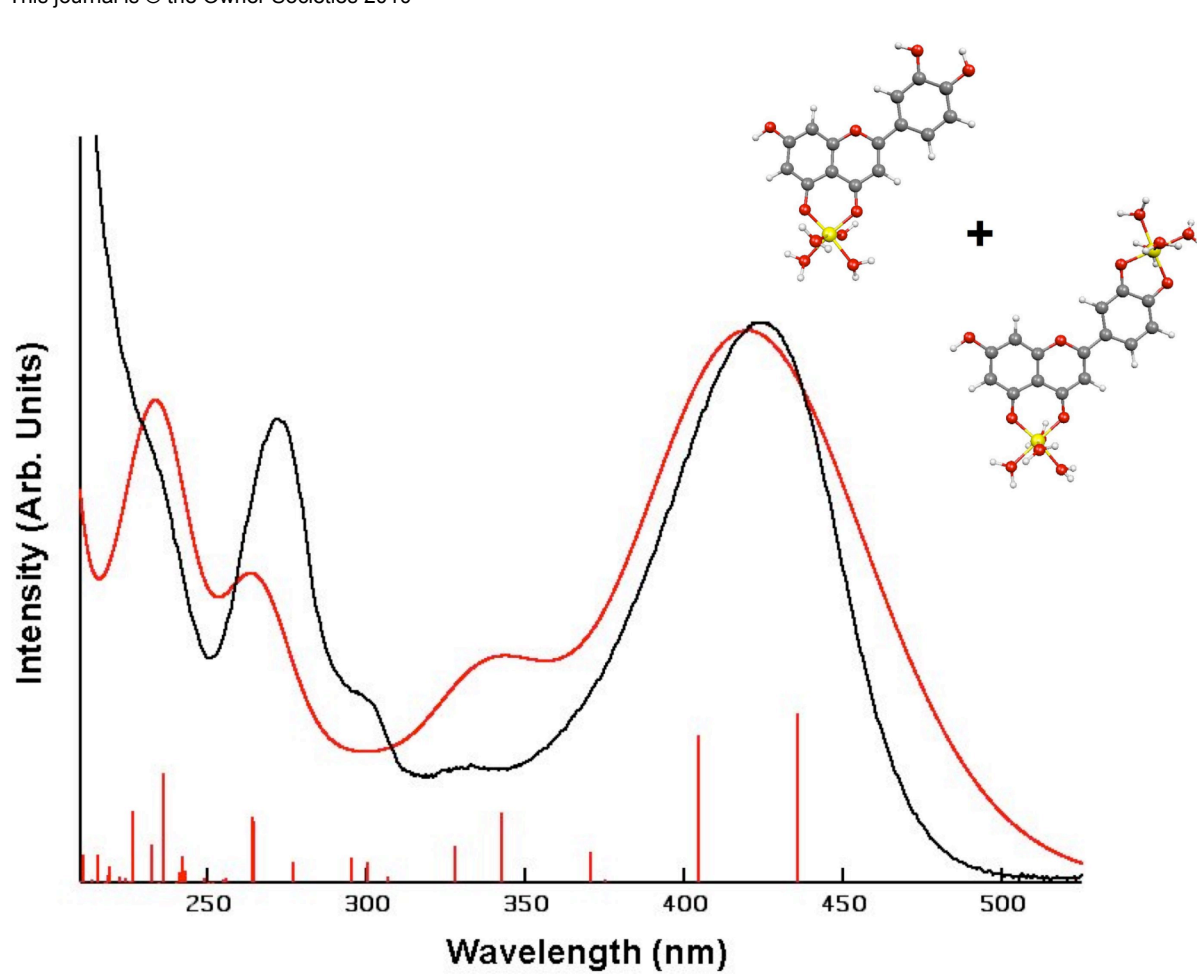


Figure 1. Experimental spectra at $[Al^{3+}] = 3 \cdot 10^{-4}$ and $[Lu] = 2.7 \cdot 10^{-5}$ mol/dm³ (black line). Theoretical spectra (red line) of $Al_1B^{3',4'}Lu_1^{3+} + Al_2B^{4,5-3',4'}Lu_1^{3+}$ (50%-50%) complexes.