

Supplementary Material

Synthesis of Lanthanoid Complexes from Ln_2O_3 and Diatrizoic Acid

Guillaume Bousrez,^A Philip C. Andrews,^B Peter C. Junk,^{A,C} Dominique T. Thielemann,^B and Jun Wang^A

^ACollege of Science and Engineering, James Cook University, Townsville, Qld 4811, Australia.

^BSchool of Chemistry, Monash University, Clayton, Vic. 3800, Australia.

^CCorresponding author. Email: peter.junk@jcu.edu.au

EDS spectra for all complexes.

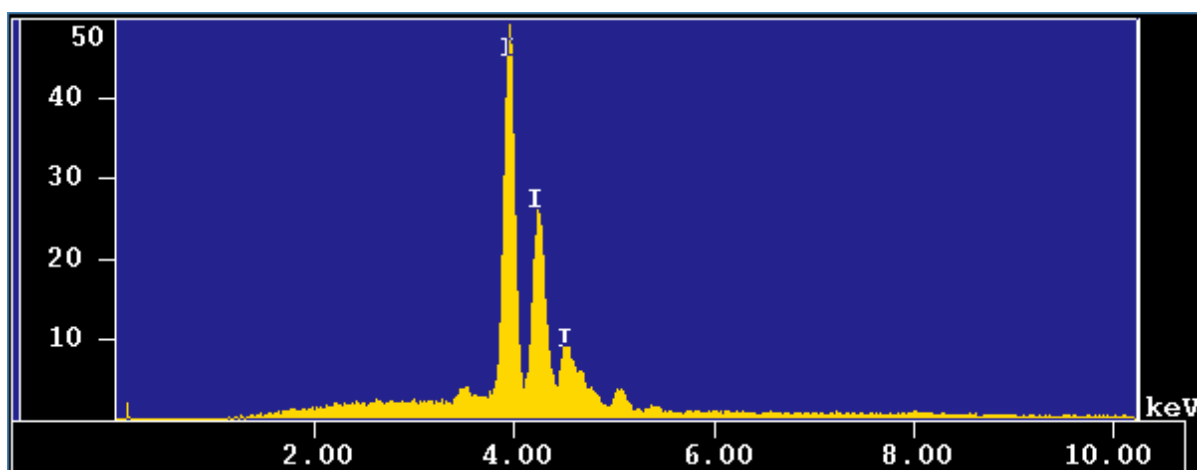


Figure S1. EDS of compound **1**, $[\text{La}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between lanthanum and iodine.

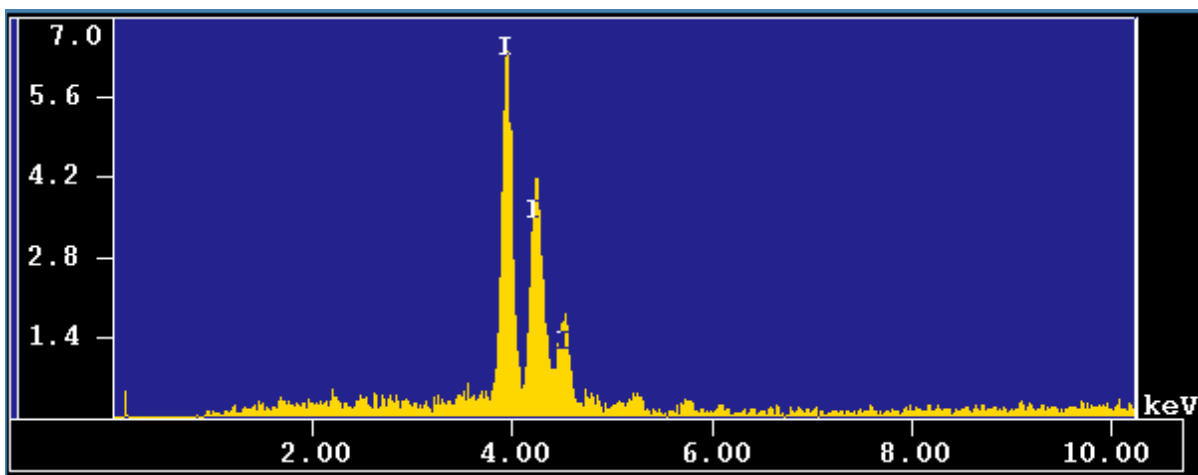


Figure S2. EDS of compound **2**, $[\text{Nd}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between neodymium and iodine.

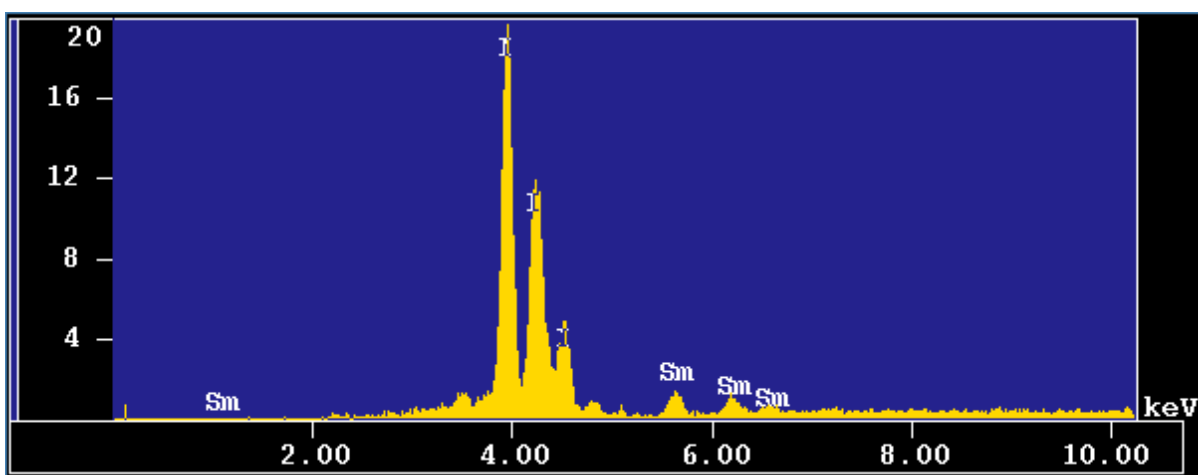


Figure S3. EDS of compound **3**, $[\text{Sm}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between samarium and iodine.

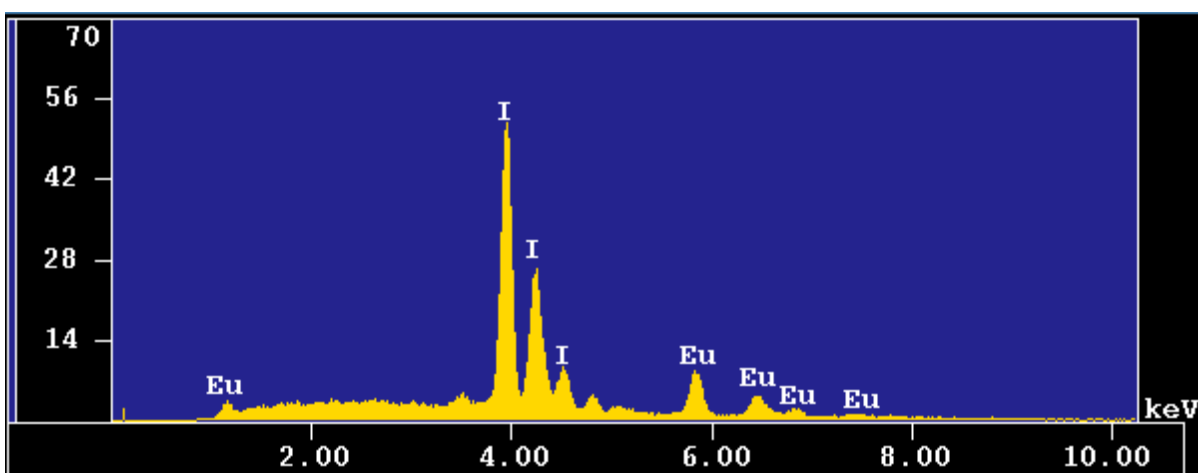


Figure S4. EDS of compound **4**, $[\text{Eu}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between europium and iodine.

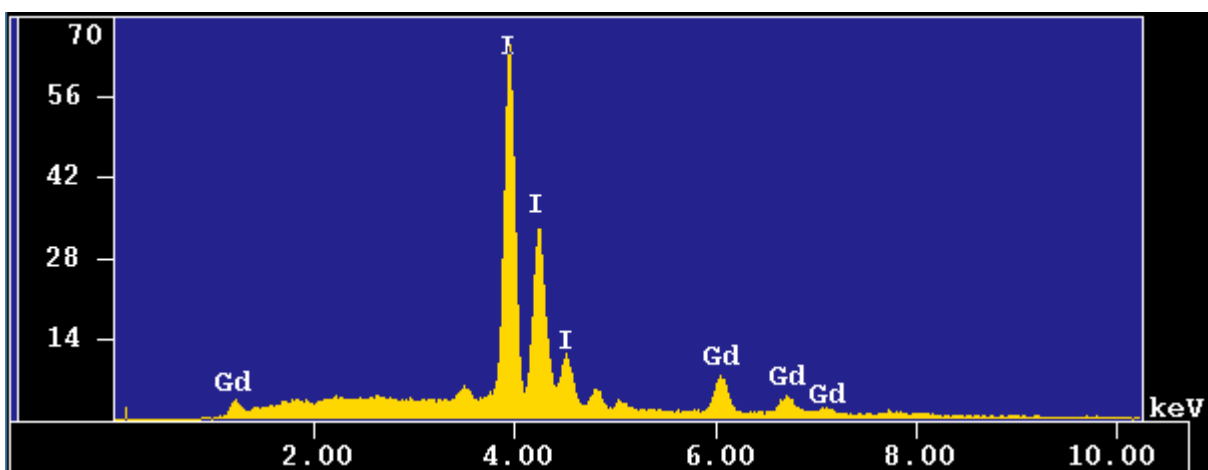


Figure S5. EDS of compound **5**, $[\text{Gd}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between gadolinium and iodine.

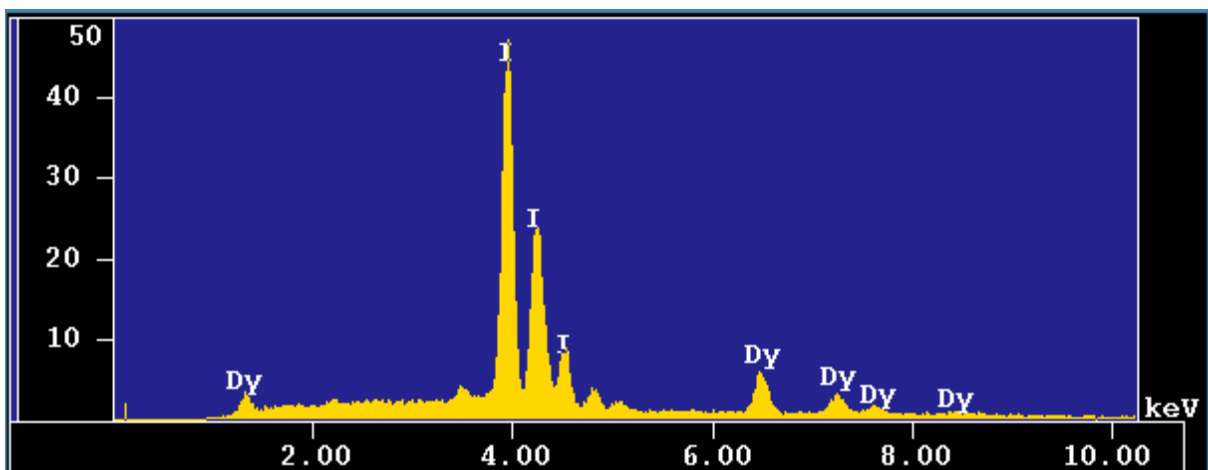


Figure S6. EDS of compound **6**, $[\text{Dy}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between dysprosium and iodine.

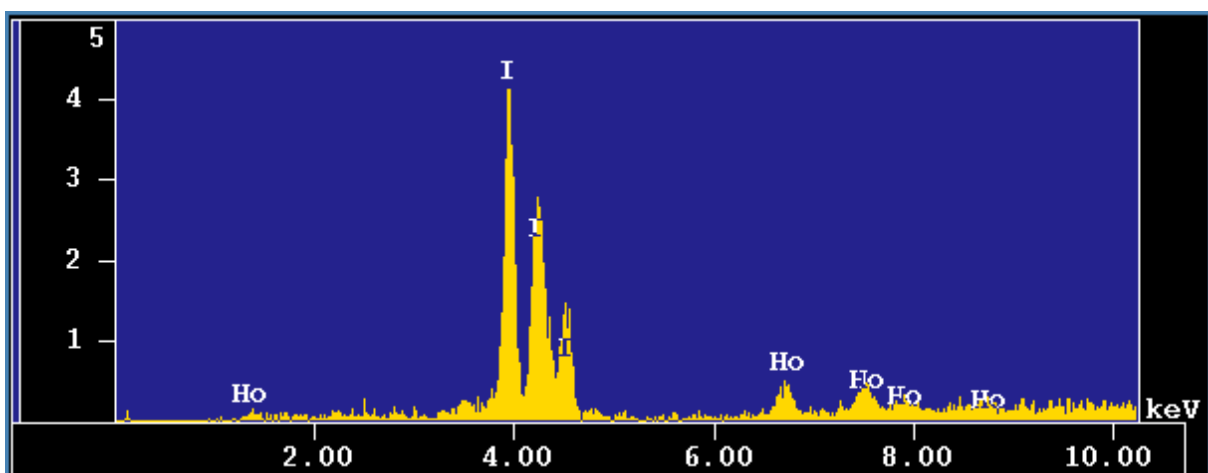


Figure S7. EDS of compound **7**, $[\text{Ho}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between holmium and iodine.

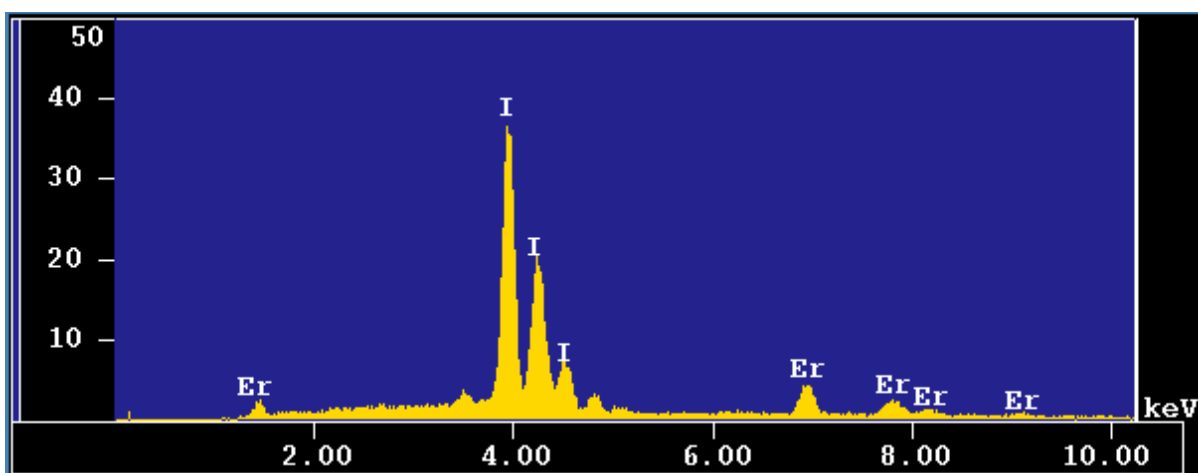


Figure S8. EDS of compound **8**, $[\text{Er}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between erbium and iodine.

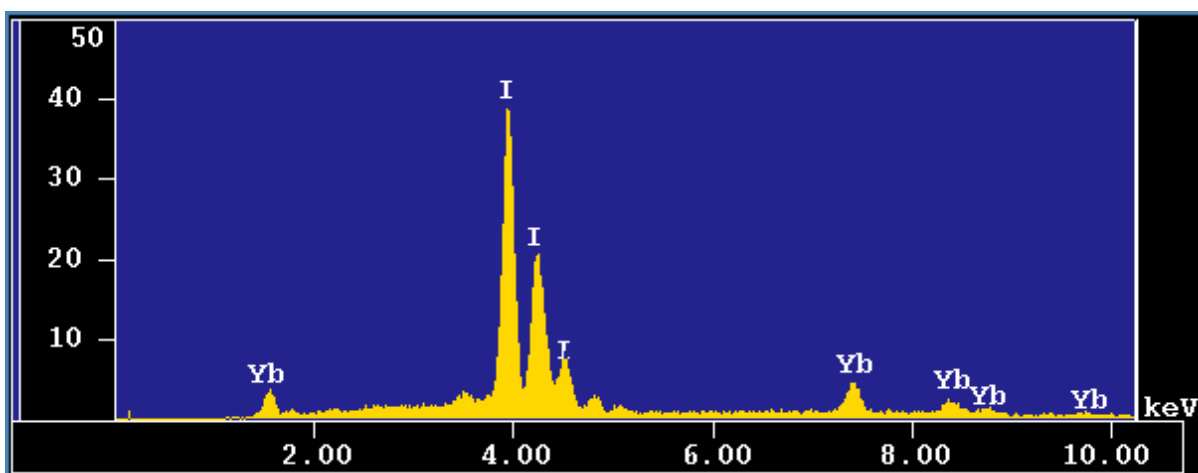


Figure S9. EDS of compound **9**, $[\text{Yb}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between ytterbium and iodine.

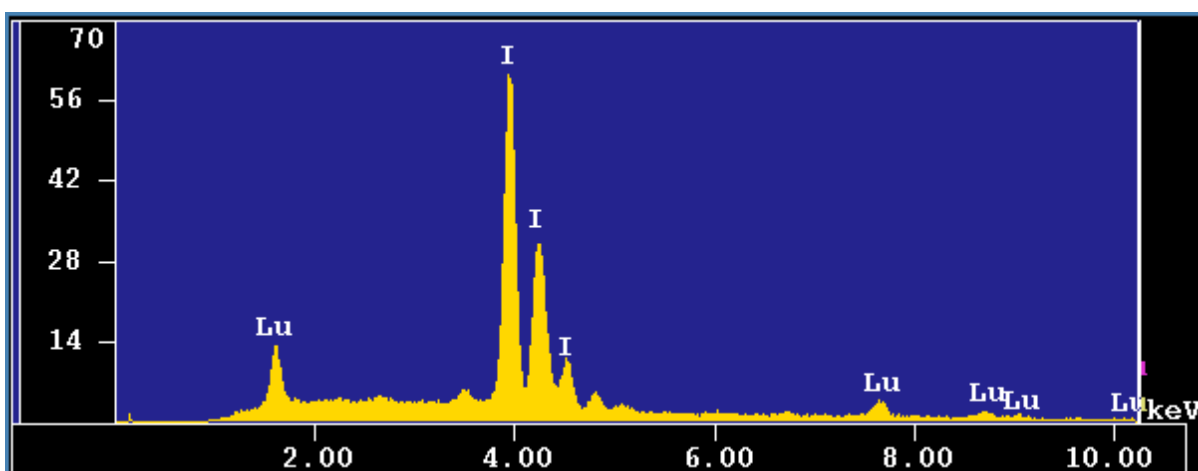


Figure S10. EDS of compound **10**, $[\text{Lu}(\text{H}_2\text{O})_8][\text{DTA}]_3$, verifying a ratio of approximately 1:9 between lutetium and iodine.

Table S1: Hydrogen bonds for complexes **1a**, **4a** and **6a**

	1a	4a	6a
Bond or angle	(Å) or (°)	(Å) or (°)	(Å) or (°)
N1-H1	1.002	0.988	0.989
H1-O5	1.815	1.860	1.861
N1-H1-O5	168.70	163.61	163.93
N2-H2	0.999	0.997	0.998
H2-O10	1.783	1.799	1.790
N2-H2-O10	173.79	170.44	171.64
O6-H3B	2.050	2.028	-
H3B-O3	0.930	0.930	-
O6-H3B-O3	129.33	131.84	-
O6-H4A	2.197	1.922	1.844
H4A-O4	0.930	0.930	0.930
O6-H4A-O4	115.6	141.17	156.31

Table S2: Hydrogen bonds for complex **6**

Bond or angle	(Å) or (°)
O15-H15A	0.903
H15A-O11	1.873
O15-H15A-O11	157.80
O16-H16A	0.752
H16A-O22	2.035
O16-H16A-O22	164.61
O17-H17A	0.888
H17A-O11	1.897
O17-H17A-O11	157.80
O17-H17B	0.881
H17B-O22	1.836
O17-H17B-O22	175.81
O18-H18A	0.870
H18A-O10	2.081
O18-H18A-O10	169.09
O19-H19A	1.014
H19A-O12	1.712
O19-H19A-O12	157.48
O21-H21B	0.896
H21B-O5	1.842
O21-H21B-O5	165.82
O22-H22D	0.719
H22D-O7	2.065
O22-H22D-O7	176.02
O23-H23B	0.894
H23B-O21	1.892
O23-H23B-O21	171.69
O24-H24A	0.979
H24A-O7	1.835
O24-H24A-O7	147.79
O24-H24B	0.694
H24B-O8	2.159
O24-H24B-O8	158.75
O25-H25A	0.909
H25A-O24	1.827
O25-H25A-O24	163.57
O26-H26A	0.854
H26A-O23	1.942
O26-H26A-O23	176.34
O27-H27B	0.884
H27B-O12	1.868
O27-H27B-O12	174.42
N2-H2	0.860
H2-O6	1.964
N2-H2-O6	174.96
N3-H3	0.860
H3-O3	1.946
N3-H3-O3	148.26