

## **Molecules and Crystals with Both Icosahedral and Cubic Symmetry**

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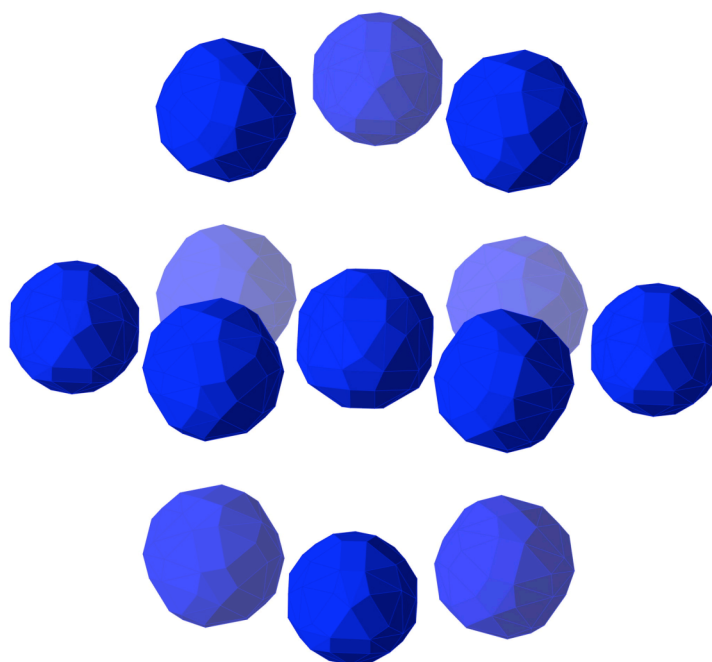
### **Supporting Information**

**Table S1.** Shape measures of the  $M_8$  and  $X_{12}$  groups relative to the cube and the icosahedron, respectively, in the family of compounds of general formula  $[M_8(AX_2)_6]$ .

Refcode	M	X	A	S(cube, $M_8$ )	S(icosahedron, $X_{12}$ )
cudtsp	Cu	C=C	S	0.03	0.04
sabsaq	Cu	P	Se	0.07	0.14
jotzoh	Cu1	P	Se	0.02	0.20
	Cu2			0.01	0.19
xubkua	Cu	P	Se	0.00	0.20
zevfah	Cu	P	Se	0.01	0.27
wutlay	Cu	P	S	0.66	0.34
arufoi	Cu	P	S	0.04	0.37
labbia	Ag	P	Se	0.14	0.57
labbog	Ag	P	Se	1.46	0.57
fibnin	Ag	P	Se	0.08	0.63
tamyel	Cu	C	Se	0.05	0.73
kefsuk	Cu	C	S	0.02	0.98
abinef	Cu	C	S	0.01	0.99
feqfox	Cu	C	S	0.02	0.99
sazzey	Cu	C	S	0.03	0.99
feqfud	Cu	C	S	0.17	1.03
feqgak	Cu	C	S	0.09	1.04
baxzuv	Cu	C	S	0.05	1.03
cudeda	Cu	C	S	0.03	1.12



**Figure S2.** Representation of one plane of the  $\text{Cs}_8\text{Sn}_{46}$  structure showing four of the six edge-sharing  $\text{Cs}_{12}$  icosahedra connected to the central one that are responsible for a primitive cubic packing.



**Figure S3.** Perspective view of the nearly perfect cuboctahedral ( $S(\text{cuboctahedron}) = 0.001$ ) arrangement of the nearest neighbour  $(\text{H}_2\text{O})_{60}$  clusters that form part of the  $(\text{H}_2\text{O})_{100}$  nanodrops in the guanidinium salt of a  $\text{Mo}_{132}$  complex.