Supplementary Materials

Table S1. Site coordinates (*xyz*) and site multiplicities (Mult.) for MDO2 polytype of compounds with the general formula $Cs\{Al_2[TP_6O_{20}]\}$ (T = Al, B) (standard setting: a = 11.815 Å, b = 13.3160 Å, c = 10.042 Å; sp. gr.: *Pcnb*).

Cs	0.5	0.25	0.2753	4
M	0.2335	0.9682	0.7221	8
P1	0.1979	0.6105	0.5074	8
P2	0.7044	0.6749	0.4866	8
P3	0.0360	0.5892	0.7191	8
T4	0.5	0.75	0.3882	4
O1	0.4189	0.9470	0.2161	8
O2	0.3000	0.5550	0.6124	8
O3	0.7800	0.6200	0.3600	8
O4	0.7200	0.6200	0.6052	8
O5	0.6104	0	0.2744	8
O6	0.2000	0.5550	0.3830	8
O7	0.4124	0.7937	0.4785	8
O8	0.0755	0.6164	0.5690	8
O9	0.2181	0.7203	0.4582	8
O10	0.0554	0.6784	0.7916	8