## Supplementary Material

Table 1: Identifiers, chemical formulas, and assigned frameworks of the tetrahedral data set. The adamantane and cubane molecular frameworks are substituted derivatives of these molecules, while  $\mathrm{MX}_4$  molecules have a central atom (denoted M) with four identical X groups.

T1 4:0		6
Identifier	formula	framework
ADAMAN08	C10 H16 C4 H12 Se6 Sn4 C24 H48 Cl6 Cu4 N16 O1 C16 H36 N4 Sn4 C4 H24 B4 U1 C4 H24 B4 Th1 C1 Cl4	adamantane
BASXOI	C4 H12 Se6 Sn4	adamantane
BOGMEP	C24 H48 Cl6 Cu4 N16 O1	other
CAMPOV	C16 H36 N4 Sp4	cubane
CANTOV	C4 H04 D4 H1	
CANFIG	C4 H24 B4 U1	$MX_4$
CANFOM	C4 H24 B4 Th1	$MX_4$
CARBTC	C1 Cl4	$MX_4$
CARBTC07	C1 C14	$MX_4$
CTBROM	C1 Br4	$MX_4$
CHECKI	C1 B14	
CUCZUV	C20 H36	tetrahedrane
DEQPAQ	C36 H100 B4 N12 Na4	other
DILWIE01	C16 H48 Pt4 S4	cubane
DOCNIS	C8 H12 S6	adamantane
FOHCUA	C12 Ni4 O18 P4	adamantane
FOIRUBOR	C4 N:1 O4	MX <sub>4</sub>
FOJBUB02	C4 NII O4	
FUZLUH	C12 Co4 O12 Sb4	cubane
FUZTEZ	H16 B4 Np1	$MX_4$
FUZVOL	H16 B4 Hf1	$MX_4$
GERHOA	C4 H12 CH2 N4 Sb4	cubane
GLITTON	COC 1100	
GUICED	C40 H32	other
HMGETP	C12 H36 Ge6 P4	adamantane
HMSIPA	C12 H36 P4 Si6	adamantane
HXMTAM07	C6 H12 N4	adamantane
JEYSEL.	C18 H36 Ni4 O6 P4	tetrahedrane
JUFWUC	C3 124 B4 Thi C1 C14 C1 C1 C14 C1 C1 B74 C20 H36 C36 H100 B4 N12 Na4 C16 H48 Pt4 S4 C8 H12 S6 C12 Ni4 O18 P4 C4 Ni1 O4 C12 Co4 O12 Sb4 H16 B4 Np1 H16 B4 Hf1 C4 H12 C112 N4 Sb4 C26 H32 C12 H36 Ge6 P4 C12 H36 P4 Si6 C6 H12 N4 C18 H36 Ni4 O6 P4 C12 H40 Cs4 N4 Si4	cubane
ICANCUDO1	C12 H40 Cs4 N4 Si4 C10 H12 I4	
KANGUB01	C10 H12 14	adamantane
KELKEI	C12 H36 Cl4 Ti4	cubane
KOXKOX	C16 H36 Ga4 Se4	cubane
KUJSIR	C20 H48 O4 Zp4	cubane
LUFYEQ	C12 H12 Si1	$MX_4$
MECKIO	C16 H26 C14 I-4 N4	cubane
MECKIO	C12 H12 Si1 C16 H36 Cl4 In4 N4 C16 H36 Br4 In4 N4 C16 H36 I4 In4 N4 C12 H36 As4 Si6	
MECKOU	C16 H36 Br4 In4 N4	cubane
MECKUA	C16 H36 I4 In4 N4	cubane
MESIAD	C12 H36 As4 Si6	adamantane
MEZDIE01	C12 H36 Si1 Sn4	$MX_4$
MEZDOK01	C12 H36 Ge1 Sp4	$MX_4$
MEZDOROI	C12 H40 O4 D44	
MFIHOIOI	C12 H40 O4 F14	cubane
MSISUL10	C4 H12 S6 Si4	adamantane
MTRETC10	C16 H12 O12 Re4 S4	cubane
MXSNOX	C4 H12 O8 Sn6	other
MZNMOX10	C8 H24 O4 Zn4	cubane
NIMMID	C12 H26 A14 N4 C6	adamantane
NIWMIF	C12 H30 A14 N4 30	
OHABEE	C16 H36 S14	tetrahedrane
POSLOY10	C12 Cl4 O12 Tc4	cubane
QUGBOJ	C16 O16 Rh6	other
BASDOE	C16 H48 Ga4 N4 Si4	cubane
REKVIIB	C16 H36 G24 S4	cubane
DIMMOD	C16 H40 A14 N4	
DIMINIOF	C10 1140 A14 N4	cubane
RIMNAC	C10 H36 As4 S16 C12 H36 S11 Sn4 C12 H36 Ge1 Sn4 C12 H36 Ge1 Sn4 C12 H36 Ge1 Sn4 C14 H12 S6 Si4 C16 H12 O12 Re4 S4 C4 H12 O8 Sn6 C8 H24 O4 Zn4 C12 H36 Al4 N4 S6 C16 H36 Si4 C12 C14 O12 Tc4 C16 O16 Rh6 C16 H36 Ga4 S4 C16 H36 Ga4 S4 C16 H36 Ga4 S4 C16 H36 Ga4 S4 C16 H40 Al4 N4 C20 H48 Al4 N4 C20 H48 Al4 N4 C16 H36 Cu4 I4 N4 C16 H36 Cu4 I	cubane
RIMNAC RUQMEV SENLAY TCYMET	C12 H36 Cu4 I4 N4	cubane
SENLAY	C16 H36 P4 Si4	cubane
TCYMET	C5 N4	$MX_4$
TCYMET TFMETH02	C1 F4	$MX_4$
TMEDTO		
I MET I C	C12 H36 Cl4 Pt4	cubane
TMGEHS10	C4 H12 Ge4 S6	adamantane
TMSIAD	C10 H24 Si4	adamantane
TMSNHS10	C4 H12 S6 Sn4	adamantane
TOHSUE	C16 F12 O12 P4 Ru4	cubane
VADRAU	C4 H12 Pb1	MX <sub>4</sub>
VAFWAA	C12 Bi4 Co4 O12	cubane
VAVYAS	C20 H36 P4	cubane
XAGXAE	P4 S10	adamantane
XUWROW	C20 H48 Mg4 O4	cubane
VEMBIR	O6 P4 S4	adamantane
VEVOAU	C12 O12 Pu4 C-4	
i E i QAU	C12 O12 Ru4 Se4	cubane
YIMWEW	C10 H16 O4	adamantane
ZEYHIU	C20 H48 Cd4 O4	cubane
ZIZHIZ	C12 H4 Mn4 O16	cubane
ZNOX AC01	C12 H18 O13 Zn4	other
ZZZKDW01	C1 14	$MX_4$
	C20 H36 P4 P4 S10 C20 H48 Mg4 O4 O6 P4 S4 C12 O12 Ru4 Se4 C10 H16 O4 C20 H48 Cd4 O4 C12 H4 Mn4 O16 C12 H18 O13 Zn4 C1 I4	4