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 MX_4 molecules have a central atom (denoted M) with four identical X groups.

Identifier	formula	framework
ADAMAN08	C10 H16	adamantane
BASXOI	C4 H12 Se6 Sn4	adamantane
BOGMEP	C24 H48 Cl6 Cu4 N16 O1	other
CAMPOV	C16 H36 N4 Sn4	cubane
CANFIG	C4 H24 B4 U1	MX_4
CANFOM	C4 H24 B4 Th1	MX_4
CARBTC	C1 Cl4	MX_4
CARBTC07	C1 Cl4	MX_4
CTBROM	C1 Br4	MX_4
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
FOJBUB02	C4 Ni1 O4	MX_4
FUZLUH	C12 Co4 O12 Sb4	cubane
FUZTEZ	H16 B4 Np1	MX_4
FUZVOL	H16 B4 Hf1	MX_4
GERHOA	C4 H12 Cl12 N4 Sb4	cubane
GUTCED	C26 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	C12 H40 Cs4 N4 Si4	cubane
KANGUB01	C10 H12 I4	adamantane
KELREY	C12 H36 Cl4 Ti4	cubane
KOXKOX	C16 H36 Ga4 Se4	cubane
KUJSIR	C20 H48 O4 Zn4	cubane
LUFYEQ	C12 H12 Si1	MX_4
MECKIO	C16 H36 Cl4 In4 N4	cubane
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 Sn4	MX_4
MPTHOT01	C12 H40 O4 Pt4	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
NIWMIP	C12 H36 Al4 N4 S6	adamantane
OHABEE	C16 H36 Si4	tetrahedrane
POSLOY10	C12 Cl4 O12 Tc4	cubane
QUGBOJ	C16 O16 Rh6	other
RASDOE	C16 H48 Ga4 N4 Si4	cubane
REKYUB	C16 H36 Ga4 S4	cubane
RIMMOP	C16 H40 Al4 N4	cubane
RIMNAC	C20 H48 Al4 N4	cubane
RUQMEV	C12 H36 Cu4 I4 N4	cubane
SENLAY	C16 H36 P4 Si4	cubane
TCYMET	C5 N4	MX_4
TFMETH02	C1 F4	MX_4
TMEPTC	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_4
VAFWAA	C12 Bi4 Co4 O12	cubane
VAVYAS	C20 H36 P4	cubane
XAGXAE	P4 S10	adamantane
XUWROW	C20 H48 Mg4 O4	cubane
YEMRIR	O6 P4 S4	adamantane
YEYQAU	C12 O12 Ru4 Se4	cubane
YIMWEW	C10 H16 O4	adamantane
ZEYHIU	C20 H48 Cd4 O4	cubane
ZIZHIZ	C12 H4 Mn4 O16	cubane
ZNOXAC01	C12 H18 O13 Zn4	other
ZZZKDW01	C1 I4	MX_4