Table 9. 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.

mi (achorca	fil) with roar racher	our II group
Identifier	formula	framework
ADAMANU8	C10 H16	adamantane
BASAUI	C24 H12 Seb Sn4	adamantane
CAMBON	C16 H26 NA C-4	other cubane
CANFIC	C4 H24 P4 H1	MX <sub>4</sub>
CANFOM	C4 H24 B4 U1	MX <sub>4</sub>
CARPON	C1 C14	MX <sub>4</sub>
CARDIC	C1 C14	MX <sub>4</sub>
CARDICUI	C1 C14	MX <sub>4</sub>
CHCZUV	C20 H26	tetrahedrane
DEOBAO	C26 H100 P4 N12 Np4	other
DILWIE01	C16 H48 P+4 S4	cubane
DOCNIS	C8 H12 S6	adamantane
FOHCUA	C12 Ni4 O18 P4	adamantane
FO IBUB02	C4 Ni1 O4	MX <sub>4</sub>
FUZLUH	C12 Co4 O12 Sb4	cubane
FUZTEZ	H16 B4 Np1	$MX_4$
FUZVOL	H16 B4 Hf1	MX <sub>4</sub>
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	adamantane tetrahedrane cubane
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
LUFYEO	C12 H12 Si1	$MX_4$
MECKIO	C16 H36 Cl4 In4 N4	cubane cubane 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	cubane 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	Formula C10 H16 C4 H12 Se6 Sn4 C24 H48 C16 Cu4 N16 O1 C16 H36 N4 Sn4 C4 H24 B4 U1 C4 H24 B4 U1 C4 H24 B4 U1 C1 C14 C1 C14 C1 C14 C1 C18 C36 H100 B4 N12 Na4 C6 H38 P4 S4 C8 H12 S6 C12 Ni4 O18 P4 C4 Ni1 O4 C12 Co4 O12 Sb4 H16 B4 Np1 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 H36 G4 Na Si4 C16 H36 C14 P44 C4 H12 B6 Si6 C16 H48 Si4 C5 N4 C17 H36 C14 P4 C4 H12 S6 Si6 C16 H36 Si4 C16 H36 C14 P4 C4 H12 S6 Si6 C16 H36 Si4 C16 H36 C14 P4 C4 H12 S6 Si6 C16 H36 Si4 C16 H36 C14 P4 C4 H12 S6 Si6 C16 H36 Si4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4 C16 H36 C14 P4 C4 H12 B6 C16 H36 F4	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
AAGAAE	C20 H48 M-4 O4	adamantane
VEMBIR	C20 f148 Mg4 U4	cubane
VEVOAII	C12 C12 Pn4 So4	adamantane
VIMMEM	C10 H16 O4	cubane adamantane
7 EV H H W	C20 H48 C44 O4	adamantane cubane
717H17	C12 H4 Mp4 O16	cubane cubane
ZNOXACOI	C12 BH3 C4 C12 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	other
277KDW01	C1 14	
	U1 14	$MX_4$