

CrystalNets vs. TopCryst

No.	CSD Refcode	Name/Formula	Topology	TopCryst	CrystalNets
1	FAVKAP	MIL-88	acs	acs	acs
2	JEJWEB	Zn ₄ O(D ₂ -tcppda) _{1.5}	act	act	AllNodes: Unknown, SingleNodes: iac
3	HUHVUD	aea-MOF-1	aea	Unknown	Unknown
4	PIVBEC	UMCM-150	agw	agw	two substructures both with kgm
5	NEJJIY	In-alb-MOF-1	alb	Unknown	Unknown
6	RAZXIA	UTSA-16	ant	Unknown	Unknown
7	BOHXED	MOF-802	bct	bct	bct
8	FIJDOS	MOF-74	bnn	4,8T1	Unknown
9	XICYOZ	DUT-68	bon	TimeoutError	Unknown
10	ALECEC	NU-1351	cml	cml	2 substructures, both 3-fold catenated, both Unknown
11	ICITEU	MOF-500	crs	crs	crs
12	QEFWUV	MOF-545	csq	csq	AllNodes: Unknown, SingleNodes: csq
13	PEJNOJ	MOAAF-1	ctn	ctn	ctn
14	LIMNUR	Zn(dmbd)	dmd	dmd	dmd
15	RIDCAJ	soc-MOF	edq	6,9T9	Unknown
16	RUBTAK	UiO-66	fcu	fcu	fcu
17	OLOPUC	UTSA-74	fgl	SingleNodes: fgl	AllNodes: Unknown, SingleNodes: fgl
18	BEWCUD	UNLPF-1	fjh	fjh	AllNodes: Unknown, SingleNodes: scu
19	BOHWIG	MOF-841	flu	flu	flu
20	ANUGEW	UMCM-151	fmj	fmj	fmj
21	JEHBAC	[Me ₂ NH ₂][Mn ₂ (H ₅ L) ₃](H ₂ O) ₂	fns	3,6T252	AllNodes: Unknown, SingleNodes: fns
22	CESFIQ	NOTT-100	fof	fof	fof (Bonding = Input necessary)
23	RIXPOF	MOF-519	fon	fon	fon
24	HANWAW	UTSA-34	frf	frf	frf
25	JIZLEL	PCN-94	ftw	ftw	AllNodes: Unknown, SingleNodes: ftw (Bonding = Input necessary)
26	VEJZAM	ZIF-5	gar	gar	gar
27	WONJUG	gea-MOF-1	gea	Unknown	gea (Bonding = Input necessary)
28	KOZQEX	DUT-75	gee	gee	gee
29	CAXTUS	DUT-42	gra	gra	gra

30	SOKXOH	NU-152	hbk	hbk	hbk
31	SEMMIJ	DUT-126	hbr	hbr	hbr
32	FIJDEI	MOF-72	hex	4,4,5,6T3	Unknown
33	ZIJSAO	UTSA-61	hey	hey	hey
34	OFOJEB	MOF-893	hfp	hfp	hfp
35	AZAVUU	MOF-890	htp	3,3,4,6T148	htp
36	IXETEM	pbz-MOF-1	hxg(-b)	hxg	hxg
37	ACODUT	UTSA-30	hyb	tsa	tsa
38	KEFBII	IZE-3	hyx	hyx	hyx
39	UGEMOK	DUT-109	iab	3,4,6T130	iab
40	BOHWOM	MOF-812	ith	ith	ith
41	SUKXUS	DUT-6	ith-d	4,4,4,6T42	pto (Bonding = Input)
42	SUKXUS ⁰¹	MOF-205	ith-d	ith-d	ith-d
43	OMULAL	TPMOF-6	jea	hcb	Unknown
44	BICPUA	UTSA-62	jjt	jjt	jjt
45	DABQQQ	Y-kce-MOF-1	kce	Unknown	Non-Periodic
46	DABQUW	Y-kex-MOF-1	kex	Unknown	Non-Periodic
47	AZAVII	MOF-888	kgd	kgd	kgd
48	PACFOP	Cu ₂ (py) ₂ (1,3-bdc) ₂	kgm	kgm	kgm
49	XANLOP	UMCM-3	koh	koh	koh (Bonding = Input necessary)
50	FINMUN	NU-1400	lim	lim	lim
51	GAZCUI	DUT-98	llj	llj	llj
52	CUSJAE	FJU-6-TATB	llz	3,9,12T3	llz
53	XANKOO	CMOF-1	lqm	pcu	pcu
54	WORREC	UTSA-60	lvt	lvt	lvt
55	FIBKEI	PCN-305	mfj	mfj	mfj
56	NAQKUM	USF-3	mmm	mmm	mmm
57	OCUNAC	MIL-101	mtn-e	TimeoutError	mtn-e
58	YIXBIQ	MOF-101	nbo	nso	nso (Bonding = Input)
59	MAPMOI	[CoCl ₄] _{0.25} [Co ₃ (μ ³ -OH)(CPT) _{4.5}]	ncb	ncb	ncb (Bonding = Input necessary)
60	MIJRIJ	MOF-907	nha	nha	rhr
61	TOVKIA	PCN-280	nht	3,3,6T99	nht
62	QUSBIP	MODF-1	mod	mod	mod

63	XUDNUH	DUT-71	nou	nou	AllNodes: Unknown, SingleNodes: nou
64	ALECA Y	NU-1350	nuc	3,6T22	TimeOutError
65	MAPHET	NU-1301	nun	TimeOutError	TimeOutError
66	SEMNIJ	NU-110	ntt	ntt	ntt
67	BUYBOO	FDM-3	ott	TimeOutError	ott
68	SAHYOQ	MOF-5	pcu	pcu	pcu
69	HUHWAK	pek-MOF-1	pek	Error	pek (Bonding = Input necessary)
70	TEYZAB	MOF-1210	pfm	pfm	pfm
71	QOWQUO	MOF-14	pto	pto	pto
72	BIMDIL	MOF-11	pts	pts	AllNodes: Unknown, SingleNodes: bcu
73	UKOLOV	MOF-150	pyr	pyr	pyr
74	ERIRIG	MOF-177	qom	qom	Unknown
75	XICNOO01	DUT-67	reo	reo	reo
76	CUSQEP	CTH-6	rtl	rtl	rtl
77	EPISOM	NOTT-140	scu	mmm/scu	AllNodes: mmm , SingleNodes: scu
78	DOGBEI	PCN-224	she	Error	AllNodes: sqc13549, SingleNodes: she
79	TUTWUC	PCN-223	shp	Error	AllNodes: Unknown, SingleNodes: shp
80	LIDDUB	PCN-250	edq/soc	edq/soc	AllNodes: edq , SingleNodes: soc
81	RIDCEN	In-soc-MOF-1a	edq/soc	edq/soc	AllNodes: edq , SingleNodes: soc
82	UFOROZ	Tb-sph-MOF-1	sph	TimeOutError	AllNodes: Unknown, SingleNodes: sph (Bonding = Input necessary)
83	BOHWUS	MOF-808	spn	spn	spn (Bonding = Input necessary)
84	DODBUV	PCN-225	sqc	sqc7923/sqc	AllNodes: sqc7923, SingleNodes: sqc
85	GECXUH	MOF-2	sql	sql	sql
86	KEVWIU	(Zn ₂) ₃ (tpt) ₂	srs	srs	srs
87	LAYRAH	ZJNU-74	ssa	ssa	AllNodes: sty , SingleNodes: ssa
88	OFOJAX	MOF-892	stp	stp	stp
89	SOKXIB	NU-151	sty	sty	sty
90	DAYMAS	Zn(acdc)	sur	sur	sur
91	FIQCEN	HKUST-1	tbo	tbo	tbo
92	ACOCOM	DUT-49	tfb	tfb	tfb (Bonding = Input necessary)
93	EBUCOT	[Zn ₂ (btc)] ₈ [Zn ₂ (btc) _{4/3}] ₃	tfe	tbo	tbo
94	UNEJEE	BUT-12	the	the	the
95	CUSYAR	MOF-210	toz	Error	toz

96	OVOKOB	MOF-910	tto	3,4,11T2	Unknown
97	ZECRAC	DUT-25	ttz	ttz	ttz
98	TAKKIC	UHM-25	ucp	ucp	ucp
99	TIZQOK	DUT-32	umt	umt	umt
100	HOGLEV	PCN-12	zhc	zhc	zhc
Score				69/100	75/100