

CrystalNets vs. TopCryst (v2)

| 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 | AllNodes: Unknown, SingleNodes: cml (Structure type = MOF necessary) |
| 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 |
| 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 |
| 28 | KOZQEX | DUT-75 | gee | gee | gee |

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|----|----------------------|--|---------|--------------|---------------------------------|
| 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 |
| 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 | DABQOQ | Y-kce-MOF-1 | kce | Unknown | pcu |
| 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 |
| 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 | nbo |
| 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 | nha |
| 61 | TOVKIA | PCN-280 | nht | 3,3,6T99 | nht |

| | | | | mod | mod |
|----|----------|---|---------|--------------|---|
| 62 | QUSBIP | MODF-1 | | mod | mod |
| 63 | XUDNUH | DUT-71 | nou | nou | AllNodes: Unknown, SingleNodes: nou |
| 64 | ALECY | NU-1350 | nuc | 3,6T22 | AllNodes: Unknown, SingleNodes: nuc (Structure type = MOF necessary) |
| 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 |
| 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 | qom (Structure type = MOF necessary) |
| 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 |

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|--------------|--------|---------|-----|---------------|---------------|
| 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 | 80/100 |