Supplementary Information:

`twa`: The World Avatar Python package for dynamic knowledge graphs and its application in reticular chemistry

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A Supplementary Information

A.1 OGM algorithms and code examples

Algorithm 1: Pull nodes from the knowledge graph (triplestore)

Input: List of *iris* of nodes to pull, SPARQL *client*, recursion depth *recursion*, force overwrite flag *overwrite*, knowledge graph in Python memory G

Result: List of Python objects pulled from the triplestore

```
/* This is a @classmethod for all classes extending ogm.BaseClass                    */
Function pull_from_kg(iris, client, recursion, overwrite):
    instances, opf, dpf ← [], {}, {};
    /* Iterate over copy to avoid modifying iris list during iteration               */
    for iri in copy(iris) do
        if iri ∈ G.loading() then
            iris.remove(iri) ;                              /* prevent duplicated operations */
        else
            G.add_to_loading(iri) ;                                 /* track in-progress IRIs */
    flag_pull ← |recursion| > 0 ;                                          /* depth control */
    if recursion > −1 then
        recursion ← max(recursion − 1, 0) ;                  /* decrement finite recursion */
    else
        recursion ← −1 ;                                      /* remain infinite recursion */
    nodes ← client.query(iris) ;                             /* batch fetch triples from KG */
    for iri, props in nodes do
        /* Resolve class from the intersection of rdf:type and Python MRO            */
        if rdf_type ∉ props or props[rdf_type] ∉ cls.mro then
            G.remove_loading(iri) ;                                  /* wrong calling class */
            raise No suitable (sub)class identified for iri;
        node_cls ← G.get_cls(props[rdf_type]) ;                      /* get actual subclass */
        /* Process object properties recursively                                     */
        for op in cls.object_properties() do
            if op ∈ props then
                if flag_pull then
                    op_cls ← G.get_cls(op);
                    opf[op] ← op_cls.pull_from_kg(props[op], client, recursion, overwrite) ;
        /* Process data properties (non-recursive)                                   */
        for dp in cls.data_properties() do
            if dp ∈ props then
                dp_cls ← G.get_cls(dp);
                dpf[dp] ← props[dp];
        /* Process rdfs properties (omitted here for brevity...)                     */
        /* Update existing instance or create new                                    */
        if iri ∈ G then
            instance ← G.get(iri);
            instance.update_cache(**opf, **dpf, overwrite) ;      /* update with fetched values */
        else
            instance ← cls(**opf, **dpf) ;                   /* construct with resolved class */
        instances.add(instance);
        G.remove_loading(iri) ;                                          /* mark completion */
    return instances;
```

Algorithm 2: Push local changes of the objects to the knowledge graph (triplestore)

Input: SPARQL *client*, recursion depth *recursion*, pull latest triples flag *pull*, force overwrite flag if pulling *overwrite*, knowledge graph in Python memory G

Result: Two localised graphs containing triples to remove and add

```
/* Both functions below are member functions of the calling class                    */
Function push_to_kg(client, recursion, pull, overwrite):
    if pull then
        /* Pull the latest state from remote to avoid conflicts                      */
        cls.pull_from_kg([self.instance_iri], client, recursion, overwrite);
    g_remove, g_add ← ∅, ∅ ;                                  /* initialising diff graphs */
    /* Recursively collect triples to add/remove across linked objects               */
    g_remove, g_add ← collect_diff(g_remove, g_add, recursion, traversed ← ∅) ;
    client.update(g_remove, g_add) ;                          /* apply changes to triplestore */
    /* Retry upon failure (omitted here for brevity...)                              */
    return g_remove, g_add;

Function collect_diff(g_remove, g_add, recursion, traversed):
    if self.instance_iri ∈ traversed then
        return g_remove, g_add ;                              /* avoid duplicate or cyclic traversals */
    traversed.add(self.instance_iri) ;                        /* mark this IRI as processed */
    /* Process all fields (object/data properties) of the instance                   */
    for f, field_info in self.model_fields do
        predicate_cls ← field_info.type_annotation ;          /* get property class */
        if issubclass(predicate_cls, BaseProperty) then
            flag_collect ← |recursion| > 0 ;                  /* depth control */
            if recursion > −1 then
                recursion ← max(recursion − 1, 0) ;           /* decrement finite recursion */
            else
                recursion ← −1 ;                              /* remain infinite recursion */
            /* Compute diff between cached and local values; fetched values have already been
               dealt with in function pull_from_kg                                   */
            cache ← self.cache[f] ;                           /* last known KG state */
            local ← getattr(self, f) ;                        /* current local state */
            remove ← cache − local ;                          /* triples to delete */
            add ← local − cache ;                             /* triples to add */
            for r in remove do
                g_remove.add_triple(self.instance_iri, predicate_cls.iri, r);
            for a in add do
                g_add.add_triple(self.instance_iri, predicate_cls.iri, a);
            /* Recurse into linked objects (if recursion allowed)                    */
            if flag_collect and issubclass(predicate_cls, ObjectProperty) then
                for o in cache ∪ local do
                    /* Existing Python object, perform recursion                     */
                    if o ∈ G then
                        g_remove, g_add ← o.collect_diff(g_remove, g_add, recursion, traversed);
                    /* If the object does not exist in Python then skip as they are never
                       modified locally                                              */
        /* Process rdfs properties (omitted here for brevity...)                     */
    return g_remove, g_add;
```

Listing S1: *Minimal example on recursive push and pull. Definitions of class and relationships are omitted for brevity.*

```
# Initially (t = 0), the knowledge graph contains the following triples:
#     <i1> a <I1>.
#     <i2> a <I2>.
#     <i3> a <I3>.
#     <i1> :has <i2>, <i3>.

# At t = 1, pull the instance <i1> from the graph, retrieving all connected instances
    recursively:
i1 = I1.pull_from_kg(
    iris='https://iri_i1',
    sparql_client=sparql_client,
    recursive_depth=-1, # -1 enables full recursion, retrieving all transitive connections
)[0] # Results are stored in a list as multiple instances of the same class can be pulled
    at once if a list of IRIs is passed in for the field `iris`

# At t = 2, an external update is made directly to the knowledge graph via SPARQL:
# """INSERT DATA { <i4> a <I4> . <i2> :has <i4> . <i3> :has <i4> . }"""
# At this point, the graph contains new triples that are not yet reflected in the Python
    environment.

# At t = 2, modify the local Python object by removing the connection between `i1` and `i2
    `:
i1.has.remove('https://iri_i2')  # This change is local and not yet propagated to the
    knowledge graph

# At t = 3, push local changes to the graph while first pulling the latest remote state:
i1.push_to_kg(
    sparql_client,
    recursive_depth=-1,  # Ensures synchronisation across all transitive links
    pull_first=True  # Ensures that any external modifications are pulled before applying
        local changes
)

# At t = 4, another external update is made to the graph:
# """INSERT DATA { <i5> a <I5> . <i1> :has <i5> . }"""
# The graph now contains additional data that is not yet present in Python.

# At t = 5, create a new instance `i6` locally and establish a relationship with `i1`:
i6 = I6()  # A unique IRI is automatically assigned to `i6`
i1.has.add(i6)  # This change remains local until explicitly pushed to the graph

# At t = 6, push the local updates while first pulling any remote changes:
i1.push_to_kg(
    sparql_client,
    recursive_depth=-1,  # Ensures full synchronisation
    pull_first=True  # External modifications (e.g., `i5`) will be pulled before pushing
        local changes (e.g., `i6`)
)
# After this operation, the Python environment will contain `i5`, which was previously
    only in the graph, and the relationship involving `i6` will be pushed to the graph,
    ensuring full consistency.
```

Listing S2: *Minimal example on multi-inheritance.*

```
# Class hierarchy defining multiple inheritance:
class T(ogm.BaseClass):
    ...

class A(T):
    ...

class B(A): # Leaf subclass of `A`
    data_b: DataB[str]
    ...

class C(T): # Independent branch from `T`
    data_c: DataC[int]
    ...

class D(C): # Leaf subclass of `C`
    ...

# Knowledge graph initially contains the following triples for node <i>:
#     <i> a <T>, <A>, <B>, <C> .
#     <i> :data_c 5 .
# The instance is labelled with multiple types, requiring resolution when pulled into
    Python.

# Pull node <i> with class `A`:
i = A.pull_from_kg(
    'https://iri_i',
    sparql_client,
    recursive_depth=-1,
)[0]

# Since `B` is the most specific subclass within the pulled hierarchy, OGM resolves the
    instance as `B`:
assert type(i) is B
assert not i.data_b # No triple exists for `data_b`, so the attribute is empty

# Add a property relevant to `B` and push changes back to the graph:
i.data_b.add("my_str")
i.push_to_kg(sparql_client, -1)
# The following triple is added to the knowledge graph:
#     <i> :data_b "my_str" .

# Now pull node <i> using class `C` instead:
i = C.pull_from_kg(
    'https://iri_i',
    sparql_client,
    recursive_depth=-1,
)[0]

# The instance is now instantiated as `C`, and properties specific to `C` are retrieved:
assert type(i) is C
assert i.data_c == {5} # Retrieved from the knowledge graph

# If we create a new instance and push it to the graph:
new_i = B(data_b="new_str")
new_i.push_to_kg(sparql_client, -1)
# The following triples are added:
#     <new_i> a <B>, <A>, <T> .
#     <new_i> :data_b "new_str" .
```

Listing S3: *Minimal example on retrieval of transitive property.*

```
from typing import Optional
import twa.data_model.base_ontology as ogm
from twa.kg_operations import PySparqlClient

endpoint = '...'
sparql_client = PySparqlClient(endpoint, endpoint)

class MyOntology(ogm.BaseOntology):
    base_url = 'https://example.org/ontology/'

# We can set the ontology to development mode for testing purposes
MyOntology.set_dev_mode()

# Define transitive relationships in the knowledge graph using an OGM class structure:
Part_of = ogm.TransitiveProperty.create_from_base('Part_of', MyOntology)

# Define class hierarchies:
class Experiment(ogm.BaseClass):
    rdfs_isDefinedBy = MyOntology

class ReactionSetup(ogm.BaseClass):
    rdfs_isDefinedBy = MyOntology
    part_of: Optional[Part_of[Experiment]] = set() # Defines a transitive relationship

class Equipment(ogm.BaseClass):
    rdfs_isDefinedBy = MyOntology
    part_of: Optional[Part_of[ReactionSetup]] = set() # Equipment can be part of a
        reaction setup

class EquipmentPart(ogm.BaseClass):
    rdfs_isDefinedBy = MyOntology
    part_of: Optional[Part_of[Equipment]] = set() # Equipment part can be part of an
        equipment

# Below triples exist in the knowledge graph:
#     :beaker_A a :Equipment .
#     :clamp_B a :EquipmentPart .
#     :stand_C a :Equipment .
#     :reaction_setup_X a :ReactionSetup .
#     :experiment_Y a :Experiment .
#     :beaker_A :part_of :reaction_setup_X .
#     :reaction_setup_X :part_of :experiment_Y .
#     :clamp_B :part_of :stand_C .
#     :stand_C :part_of :reaction_setup_X .

# Pull node <beaker_A> using class `Equipment`
beaker_A = Equipment.pull_from_kg(
    'https://example.org/ontology/beaker_A',
    sparql_client,
    recursive_depth=-1,  # Fully traverse transitive properties
)[0]

# If we access `beaker_A.part_of` in normal way, we will only get the direct parent
assert beaker_A.part_of == {'https://example.org/ontology/reaction_setup_X'}

# If we access `beaker_A.part_of` using the transitive property, we will get all ancestors
assert Part_of.obtain_transitive_objects(beaker_A) == {
    'https://example.org/ontology/reaction_setup_X',
    'https://example.org/ontology/experiment_Y'
}

# Similarly, pull node <clamp_B> and verify the inferred hierarchy
clamp_B = EquipmentPart.pull_from_kg(
```

```
    'https://example.org/ontology/clamp_B',
    sparql_client,
    recursive_depth=-1,
)[0]

# If we access the transitive property in the normal way, `clamp_B` as part of `stand_C`
assert clamp_B.part_of == {'https://example.org/ontology/stand_C'}
# If we access `clamp_B` using the transitive property, we will get all ancestors
assert Part_of.obtain_transitive_objects(clamp_B) == {
    'https://example.org/ontology/stand_C',
    'https://example.org/ontology/reaction_setup_X',
    'https://example.org/ontology/experiment_Y'
}

# If we add a new equipment relationship and push it to the knowledge graph:
new_equipment = Equipment()
new_equipment.part_of.add('https://example.org/ontology/reaction_setup_X')
new_equipment.push_to_kg(sparql_client, -1)

# Below triple will be added:
#     :new_equipment :part_of :reaction_setup_X .
```

A.2 Updated OntoMOPs TBox

The description logic of the updated OntoMOPs TBox is provided below. The prefix `OntoMOPs` reads: `https://www.theworldavatar.com/kg/ontomops/`

OntoMOPs:BindingPoint ⊑ OntoMOP:CoordinatePoint
OntoMOPs:CBUAssemblyCenter ⊑ OntoMOP:CoordinatePoint
OntoMOPs:CoordinationCage ⊑ OntoMOP:MolecularCage
OntoMOPs:DirectBinding ⊑ OntoMOP:BindingDirection
OntoMOPs:GBUConnectingPoint ⊑ OntoMOP:CoordinatePoint
OntoMOPs:GBUCoordinateCenter ⊑ OntoMOP:CoordinatePoint
OntoMOPs:MetalOrganicPolyhedron ⊑ OntoMOP:CoordinationCage
OntoMOPs:MetalOrganicPolyhedron ⊑ OntoMOP:MolecularCage
OntoMOPs:MetalSite ⊑ OntoMOP:BindingSite
OntoMOPs:OrganicSite ⊑ OntoMOP:BindingSite
OntoMOPs:SidewayBinding ⊑ OntoMOP:BindingDirection
∃ OntoMOP:alignsTo.⊤ ⊑ OntoMOP:CBUAssemblyTransformation
∃ OntoMOP:hasAssemblyModel.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasBindingDirection.⊤ ⊑ OntoMOP:ChemicalBuildingUnit
∃ OntoMOP:hasBindingPoint.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingSite ⊔ OntoMOP:MetalSite ⊔ OntoMOP:OrganicSite)
∃ OntoMOP:hasBindingSite.⊤ ⊑ OntoMOP:ChemicalBuildingUnit
∃ OntoMOP:hasCBUAssemblyCenter.⊤ ⊑ OntoMOP:ChemicalBuildingUnit
∃ OntoMOP:hasCBUAssemblyTransformation.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasCavity.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasChemicalBuildingUnit.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasGBUConnectingPoint.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/AssemblyModel ⊔ OntoMOP:GBUCoordinateCenter)
∃ OntoMOP:hasGBUCoordinateCenter.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/AssemblyModel ⊔ OntoMOP:GenericBuildingUnit)
∃ OntoMOP:hasGBUType.⊤ ⊑ OntoMOP:GenericBuildingUnit
∃ OntoMOP:hasGenericBuildingUnit.⊤ ⊑ OntoMOP:AssemblyModel
∃ OntoMOP:hasGenericBuildingUnitNumber.⊤ ⊑ OntoMOP:AssemblyModel
∃ OntoMOP:hasLargestInnerSphereDiameter.⊤ ⊑ OntoMOP:Cavity
∃ OntoMOP:hasOuterDiameter.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasPolyhedralShape.⊤ ⊑ OntoMOP:AssemblyModel
∃ OntoMOP:hasPoreDiameter.⊤ ⊑ OntoMOP:PoreSize
∃ OntoMOP:hasPoreRing.⊤ ⊑ OntoMOP:AssemblyModel
∃ OntoMOP:hasPoreSize.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasProvenance.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:isFormedBy.⊤ ⊑ OntoMOP:PoreRing
∃ OntoMOP:isFunctioningAs.⊤ ⊑ OntoMOP:ChemicalBuildingUnit
∃ OntoMOP:isNumberOf.⊤ ⊑ OntoMOP:GenericBuildingUnitNumber
∃ OntoMOP:measuresRing.⊤ ⊑ OntoMOP:PoreSize

∃ OntoMOP:transforms.⊤ ⊑ OntoMOP:CBUAssemblyTransformation
⊤ ⊑ ∀ OntoMOP:alignsTo.OntoMOPs:GBUCoordinateCenter
⊤ ⊑ ∀ OntoMOP:hasAssemblyModel.OntoMOPs:AssemblyModel
⊤ ⊑ ∀ OntoMOP:hasBindingDirection.OntoMOPs:BindingDirection
⊤ ⊑ ∀ OntoMOP:hasBindingPoint.OntoMOPs:BindingPoint
⊤ ⊑ ∀ OntoMOP:hasBindingSite.OntoMOPs:BindingSite
⊤ ⊑ ∀ OntoMOP:hasCBUAssemblyCenter.OntoMOPs:CBUAssemblyCenter
⊤ ⊑ ∀ OntoMOP:hasCBUAssemblyTransformation.OntoMOPs:CBUAssemblyTransformation
⊤ ⊑ ∀ OntoMOP:hasCavity.OntoMOPs:Cavity
⊤ ⊑ ∀ OntoMOP:hasChemicalBuildingUnit.OntoMOPs:ChemicalBuildingUnit
⊤ ⊑ ∀ OntoMOP:hasGBUConnectingPoint.OntoMOPs:GBUConnectingPoint
⊤ ⊑ ∀ OntoMOP:hasGBUCoordinateCenter.OntoMOPs:GBUCoordinateCenter
⊤ ⊑ ∀ OntoMOP:hasGBUType.OntoMOPs:GenericBuildingUnitType
⊤ ⊑ ∀ OntoMOP:hasGenericBuildingUnit.OntoMOPs:GenericBuildingUnit
⊤ ⊑ ∀ OntoMOP:hasGenericBuildingUnitNumber.OntoMOPs:GenericBuildingUnitNumber
⊤ ⊑ ∀ OntoMOP:hasLargestInnerSphereDiameter.om:Diameter
⊤ ⊑ ∀ OntoMOP:hasOuterDiameter.om:Diameter
⊤ ⊑ ∀ OntoMOP:hasPolyhedralShape.OntoMOPs:PolyhedralShape
⊤ ⊑ ∀ OntoMOP:hasPoreDiameter.om:Diameter
⊤ ⊑ ∀ OntoMOP:hasPoreRing.OntoMOPs:PoreRing
⊤ ⊑ ∀ OntoMOP:hasPoreSize.OntoMOPs:PoreSize
⊤ ⊑ ∀ OntoMOP:hasProvenance.OntoMOPs:Provenance
⊤ ⊑ ∀ OntoMOP:isFormedBy.OntoMOPs:GBUCoordinateCenter
⊤ ⊑ ∀ OntoMOP:isFunctioningAs.OntoMOPs:GenericBuildingUnit
⊤ ⊑ ∀ OntoMOP:isNumberOf.OntoMOPs:GenericBuildingUnit
⊤ ⊑ ∀ OntoMOP:measuresRing.OntoMOPs:PoreRing
⊤ ⊑ ∀ OntoMOP:transforms.OntoMOPs:ChemicalBuildingUnit
∃ OntoMOP:hasBindingFragment.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingSite ⊔ OntoMOP:MetalSite ⊔ OntoMOP:OrganicSite)
∃ OntoMOP:hasCBUFormula.⊤ ⊑ OntoMOP:ChemicalBuildingUnit
∃ OntoMOP:hasCCDCNumber.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasMOPFormula.⊤ ⊑ OntoMOP:MetalOrganicPolyhedron
∃ OntoMOP:hasModularity.⊤ ⊑ OntoMOP:GenericBuildingUnitType
∃ OntoMOP:hasOuterCoordinationNumber.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingSite ⊔ OntoMOP:MetalSite ⊔ OntoMOP:OrganicSite)
∃ OntoMOP:hasPlanarity.⊤ ⊑ OntoMOP:GenericBuildingUnitType
∃ OntoMOP:hasProbingVector.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/PoreRing ⊔ OntoMOP:PoreSize)
∃ OntoMOP:hasReferenceDOI.⊤ ⊑ OntoMOP:Provenance
∃ OntoMOP:hasSymbol.⊤ ⊑ OntoMOP:PolyhedralShape
∃ OntoMOP:hasSymmetryPointGroup.⊤ ⊑ OntoMOP:AssemblyModel
∃ OntoMOP:hasUnitNumberValue.⊤ ⊑ OntoMOP:GenericBuildingUnitNumber
∃ OntoMOP:hasX.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingPoint ⊔

OntoMOP:CBUAssemblyCenter ⊔ OntoMOP:CoordinatePoint ⊔ OntoMOP:GBUConnectingPoint ⊔ OntoMOP:GBUCoordinateCenter)
∃ OntoMOP:hasY.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingPoint ⊔ OntoMOP:CBUAssemblyCenter ⊔ OntoMOP:CoordinatePoint ⊔ OntoMOP:GBUConnectingPoint ⊔ OntoMOP:GBUCoordinateCenter)
∃ OntoMOP:hasZ.⊤ ⊑ (https://www.theworldavatar.com/kg/ontomops/BindingPoint ⊔ OntoMOP:CBUAssemblyCenter ⊔ OntoMOP:CoordinatePoint ⊔ OntoMOP:GBUConnectingPoint ⊔ OntoMOP:GBUCoordinateCenter)
∃ OntoMOP:quaternionToRotate.⊤ ⊑ OntoMOP:CBUAssemblyTransformation
∃ OntoMOP:scaleFactorToAlignCoordinateCenter.⊤ ⊑ OntoMOP:CBUAssemblyTransformation
∃ OntoMOP:translationVectorToAlignOrigin.⊤ ⊑ OntoMOP:CBUAssemblyTransformation
⊤ ⊑ ∀ OntoMOP:hasBindingFragment.xsd:string
⊤ ⊑ ∀ OntoMOP:hasCBUFormula.xsd:string
⊤ ⊑ ∀ OntoMOP:hasCCDCNumber.xsd:string
⊤ ⊑ ∀ OntoMOP:hasMOPFormula.xsd:string
⊤ ⊑ ∀ OntoMOP:hasModularity.xsd:integer
⊤ ⊑ ∀ OntoMOP:hasOuterCoordinationNumber.xsd:integer
⊤ ⊑ ∀ OntoMOP:hasPlanarity.xsd:string
⊤ ⊑ ∀ OntoMOP:hasProbingVector.xsd:string
⊤ ⊑ ∀ OntoMOP:hasReferenceDOI.xsd:string
⊤ ⊑ ∀ OntoMOP:hasSymbol.xsd:string
⊤ ⊑ ∀ OntoMOP:hasSymmetryPointGroup.xsd:string
⊤ ⊑ ∀ OntoMOP:hasUnitNumberValue.xsd:integer
⊤ ⊑ ∀ OntoMOP:hasX.xsd:double
⊤ ⊑ ∀ OntoMOP:hasY.xsd:double
⊤ ⊑ ∀ OntoMOP:hasZ.xsd:double
⊤ ⊑ ∀ OntoMOP:quaternionToRotate.xsd:string
⊤ ⊑ ∀ OntoMOP:scaleFactorToAlignCoordinateCenter.xsd:double
⊤ ⊑ ∀ OntoMOP:translationVectorToAlignOrigin.xsd:string

A.3 Ontologised algorithms for the rational design of MOPs

The two algorithms developed in our previous work [1] to expand the chemical space of MOPs were ontologised herein as SPARQL queries. The first algorithm (Listing S4) constructs MOPs using chemically complementary CBUs restricted to a single AM without allowing CBU exchanges between different AMs, whereas the second algorithm (Listing S5) expands MOP construction by enabling CBU exchanges between different AMs, increasing versatility and the number of possible structures.

Listing S4: *SPARQL query to identify the possible new metal-organic polyhedron by combining metallic and organic chemical building units that could function as different general building units within the same assembly model.*

```
prefix os: <http://www.theworldavatar.com/ontology/ontospecies/OntoSpecies.owl#>
prefix om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>
prefix mops: <https://www.theworldavatar.com/kg/ontomops/>
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#>
select distinct ?mop_formula ?mop_mw ?mop_charge ?am ?metal ?organic ?metal_gbu ?
    organic_gbu
where {
  {
    select distinct ?metal_formula ?metal_mw ?metal_charge ?metal_gbu_label ?am_label ?
        metal_gbu_number ?am ?metal_gbu ?metal ?metal_binding ?metal_ocn
    where {
      ?metal a mops:ChemicalBuildingUnit; mops:hasBindingSite ?metal_site; mops:
          hasBindingDirection/rdf:type ?metal_binding.
      ?metal_site rdf:type mops:MetalSite; mops:hasOuterCoordinationNumber ?metal_ocn.
      ?metal mops:isFunctioningAs ?metal_gbu; mops:hasCBUFormula ?metal_formula.
      ?metal ^mops:hasChemicalBuildingUnit ?existing_mop.
      ?existing_mop mops:hasAssemblyModel ?am; mops:hasMOPFormula ?existing_mop_formula.
      ?am a mops:AssemblyModel; rdfs:label ?am_label; mops:hasSymmetryPointGroup ?
          am_symmetry.
      ?metal_gbu ^mops:hasGenericBuildingUnit ?am; mops:hasGBUType/rdfs:label ?
          metal_gbu_label.
      ?metal_gbu_n mops:isNumberOf ?metal_gbu; mops:hasUnitNumberValue ?metal_gbu_number.
      ?metal os:hasMolecularWeight/om:hasValue/om:hasNumericalValue ?metal_mw; os:
          hasCharge/om:hasValue/om:hasNumericalValue ?metal_charge.
    }
  }
  {
    select distinct ?organic_formula ?organic_mw ?organic_charge ?organic_gbu_label ?
        organic_gbu_number ?am ?organic_gbu ?organic ?organic_binding ?organic_ocn
    where {
      ?organic a mops:ChemicalBuildingUnit; mops:hasBindingSite ?organic_site; mops:
          hasBindingDirection/rdf:type ?organic_binding.
      ?organic_site rdf:type mops:OrganicSite; mops:hasOuterCoordinationNumber ?
          organic_ocn.
      ?organic mops:isFunctioningAs ?organic_gbu; mops:hasCBUFormula ?organic_formula.
      ?organic ^mops:hasChemicalBuildingUnit ?_existing_mop.
      ?_existing_mop mops:hasAssemblyModel ?am; mops:hasMOPFormula ?_existing_mop_formula.
      ?am a mops:AssemblyModel; rdfs:label ?am_label; mops:hasSymmetryPointGroup ?
          am_symmetry.
      ?organic_gbu ^mops:hasGenericBuildingUnit ?am; mops:hasGBUType/rdfs:label ?
          organic_gbu_label.
      ?organic_gbu_n mops:isNumberOf ?organic_gbu; mops:hasUnitNumberValue ?
          organic_gbu_number.
      ?organic os:hasMolecularWeight/om:hasValue/om:hasNumericalValue ?organic_mw; os:
          hasCharge/om:hasValue/om:hasNumericalValue ?organic_charge.
    }
  }
```

```
  filter (?metal_gbu != ?organic_gbu)
  filter (?metal_ocn = ?organic_ocn)
  filter (?metal_binding = ?organic_binding)
  bind (?organic_mw*?organic_gbu_number+?metal_mw*?metal_gbu_number as ?mop_mw)
  bind (?organic_charge*?organic_gbu_number+?metal_charge*?metal_gbu_number as ?mop_charge
      )
  bind (concat(?metal_formula, str(?metal_gbu_number), ?organic_formula, str(?
      organic_gbu_number)) as ?mop_formula)
  filter not exists {
    ?_mop mops:hasAssemblyModel ?am; mops:hasChemicalBuildingUnit ?metal, ?organic.
  }
}
```

Listing S5: *SPARQL query to identify the possible new metal-organic polyhedron by combining metallic and organic chemical building units that could function as different general building units across different assembly models that they are each identified as to be compatible with.*

```
prefix os: <http://www.theworldavatar.com/ontology/ontospecies/OntoSpecies.owl#>
prefix om: <http://www.ontology-of-units-of-measure.org/resource/om-2/>
prefix mops: <https://www.theworldavatar.com/kg/ontomops/>
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix rdfs: <http://www.w3.org/2000/01/rdf-schema#>
select distinct ?mop_formula ?mop_mw ?mop_charge ?am ?metal ?organic ?metal_gbu ?
    organic_gbu ?metal_formula ?organic_formula ?am_label ?am_symmetry ?metal_gbu_label ?
    organic_gbu_label ?metal_gbu_number ?organic_gbu_number
where {
  {
    select distinct ?metal_formula ?metal_mw ?metal_charge ?metal_gbu_label ?am_label ?
        am_symmetry ?metal_gbu_number ?am ?metal_gbu ?metal ?metal_binding ?metal_ocn
    where {
      ?metal a mops:ChemicalBuildingUnit; mops:hasBindingSite ?metal_site; mops:
          hasBindingDirection/rdf:type ?metal_binding.
      ?metal_site rdf:type mops:MetalSite; mops:hasOuterCoordinationNumber ?metal_ocn.
      ?metal mops:isFunctioningAs ?_metal_gbu; mops:hasCBUFormula ?metal_formula.
      filter exists {?metal ^mops:hasChemicalBuildingUnit/mops:hasAssemblyModel/mops:
          hasGenericBuildingUnit ?_metal_gbu.}
      ?_metal_gbu mops:hasGBUType/mops:hasModularity ?_metal_gbu_modularity.
      ?_metal_gbu ^mops:isFunctioningAs/mops:isFunctioningAs ?metal_gbu.
      ?metal_gbu mops:hasGBUType/mops:hasModularity ?metal_gbu_modularity.
      ?metal_gbu ^mops:hasGenericBuildingUnit ?am; mops:hasGBUType/rdfs:label ?
          metal_gbu_label.
      ?am a mops:AssemblyModel; rdfs:label ?am_label; mops:hasSymmetryPointGroup ?
          am_symmetry.
      ?metal_gbu_n mops:isNumberOf ?metal_gbu; mops:hasUnitNumberValue ?metal_gbu_number.
      ?metal os:hasMolecularWeight/om:hasValue/om:hasNumericalValue ?metal_mw; os:
          hasCharge/om:hasValue/om:hasNumericalValue ?metal_charge.
      filter (?_metal_gbu_modularity = ?metal_gbu_modularity)
    }
  }
  {
    select distinct ?organic_formula ?organic_mw ?organic_charge ?organic_gbu_label ?
        organic_gbu_number ?am ?organic_gbu ?organic ?organic_binding ?organic_ocn #?
        equiv_cbu
    where {
      ?organic a mops:ChemicalBuildingUnit; mops:hasBindingSite ?organic_site; mops:
          hasBindingDirection/rdf:type ?organic_binding.
      ?organic_site rdf:type mops:OrganicSite; mops:hasOuterCoordinationNumber ?
          organic_ocn.
      ?organic mops:isFunctioningAs ?_organic_gbu; mops:hasCBUFormula ?organic_formula.
      filter exists {?organic ^mops:hasChemicalBuildingUnit/mops:hasAssemblyModel/mops:
          hasGenericBuildingUnit ?_organic_gbu.}
      ?_organic_gbu mops:hasGBUType/mops:hasModularity ?_organic_gbu_modularity.
```

```
      ?_organic_gbu ^mops:isFunctioningAs ?equiv_cbu. ?equiv_cbu mops:isFunctioningAs ?
          organic_gbu.
      ?organic_gbu mops:hasGBUType/mops:hasModularity ?organic_gbu_modularity.
      ?organic_gbu ^mops:hasGenericBuildingUnit ?am; mops:hasGBUType/rdfs:label ?
          organic_gbu_label.
      ?am a mops:AssemblyModel; rdfs:label ?am_label; mops:hasSymmetryPointGroup ?
          am_symmetry.
      ?organic_gbu_n mops:isNumberOf ?organic_gbu; mops:hasUnitNumberValue ?
          organic_gbu_number.
      ?organic os:hasMolecularWeight/om:hasValue/om:hasNumericalValue ?organic_mw; os:
          hasCharge/om:hasValue/om:hasNumericalValue ?organic_charge.
      filter (?_organic_gbu_modularity = ?organic_gbu_modularity)
    }
  }
  filter (?metal_gbu != ?organic_gbu)
  filter (?metal_ocn = ?organic_ocn)
  filter (?metal_binding = ?organic_binding)
  bind (?organic_mw*?organic_gbu_number+?metal_mw*?metal_gbu_number as ?mop_mw)
  bind (?organic_charge*?organic_gbu_number+?metal_charge*?metal_gbu_number as ?mop_charge
      )
  bind (concat(?metal_formula, str(?metal_gbu_number), ?organic_formula, str(?
      organic_gbu_number)) as ?mop_formula)
  filter not exists {
    ?_mop mops:hasAssemblyModel ?am; mops:hasChemicalBuildingUnit ?metal, ?organic.
  }
}
```

A.4 OGM-based algorithm for automated MOP construction

Mathematical expression definition

The generic expression of assembly model can be derived by abstracting the existing notions, *e.g.*, (4–planar)$_6$(3–pyramidal)$_8$_T$_\mathrm{h}$ and (3–planar)$_4$(3–pyramidal)$_4$_T$_\mathrm{d}$, where an AM consists of two types of GBU that each can be described by its modularity m, planarity p, and number of appearances n_i, *i.e.*, $(m_i\text{–}p_i)_{n_i}$. The GBUs can be assembled in various ways that may result in different symmetry point group for the overall AM topology. To make the generic expression beyond merely two types of GBUs:

$$\mathscr{A} = \left(\prod_{i=1}^{N} (m_i\text{–}p_i)_{n_i}\right)\text{\_sym}$$

The centre coordinates of all appearances of GBUs can represented as:

$$\mathbf{G} = \bigcup_{i=1}^{N}\bigcup_{j=1}^{n_i} \mathbf{G}_{i,j} = \bigcup_{i=1}^{N}\bigcup_{j=1}^{n_i} \{\mathbf{r}_{i,j} \mid \mathbf{r}_{i,j} = (x_{i,j}, y_{i,j}, z_{i,j})\}$$

The coordinates of the connecting points between different types of GBUs can be computed as the centroid of the centre coordinates of the involved GBUs. For AMs consisting of two types of GBUs, the set of connecting points iterates through the centre coordinates of the first type of GBU and the set of the other type of GBU that it is connected with:

$$\mathbf{P} = \bigcup_{j=1}^{n_1} \bigcup_{k \in \mathscr{K}_{1,j}} \left\{ \mathbf{c}_{j,k} \;\middle|\; \mathbf{c}_{j,k} = \frac{\mathbf{r}_{1,j} + \mathbf{r}_{2,k}}{2} \right\}, \text{where } \mathscr{K}_{1,j} \subseteq \{1, \ldots, n_2\}, \text{and } |\mathscr{K}_{1,j}| = m_1$$

The centroid of each CBU is averaged over the coordinates of its atoms, where we use M_i to express the number of atoms for the i-th CBU. In the simplest scenario, where CBUs are 1-to-1 mapped to function as GBUs, such correspondence can be expressed using the same index i, resulting in a collection of the centroids:

$$\mathbf{R} = \bigcup_{i=1}^{N} \mathbf{R}_i = \bigcup_{i=1}^{N} \left\{ \frac{1}{M_i} \sum_{\alpha=1}^{M_i} \mathbf{a}_{i,\alpha} \right\}$$

Analogous to the connecting points between different types of GBUs, binding sites are used to identify the connectivity between the CBUs where the chemical bonds are formed. The coordinates of each binding site can be approximated as the centroid of the binding atoms. Notably, the number of binding sites of a CBU should match the modularity of its corresponding GBU (m_i):

$$\mathbf{B} = \bigcup_{i=1}^{N} \bigcup_{b=1}^{m_i} \left\{ \mathbf{B}_{i,b} \;\middle|\; \mathbf{B}_{i,b} = \frac{1}{|\mathscr{B}_{i,b}|} \sum_{\alpha \in \mathscr{B}_{i,b}} \mathbf{a}_{i,\alpha} \right\}, \text{where } \mathscr{B}_{1,b} \subseteq \{1, \ldots, M_i\}$$

Fingerprint vector calculation

Here, we provide the fingerprint vector calculation for a CBU as an example. The calculation for a GBU follows the same logic, as both share the same abstraction of a set of points.

For each CBU, the centroid of binding sites can be calculated as:

$$\mathbf{c}_i^{\text{binding}} = \frac{1}{m_i} \sum_{b=1}^{m_i} \mathbf{B}_{i,b}$$

Define the centred data matrix $\mathbf{A}_i$:

$$\mathbf{A}_i = \begin{bmatrix} \mathbf{B}_{i,1} - \mathbf{c}_i^{\text{binding}} \\ \mathbf{B}_{i,2} - \mathbf{c}_i^{\text{binding}} \\ \vdots \\ \mathbf{B}_{i,m_i} - \mathbf{c}_i^{\text{binding}} \end{bmatrix} \in \mathbb{R}^{m_i \times 3}$$

Compute the Singular Value Decomposition (SVD):

$$\mathbf{A}_i = \mathbf{U}_i \mathbf{\Sigma}_i \mathbf{V}_i^\top$$

where $\mathbf{U}_i \in \mathbb{R}^{m_i \times m_i}$ contains the left singular vectors, $\mathbf{\Sigma}_i \in \mathbb{R}^{m_i \times 3}$ is the diagonal matrix of singular values,

$$\mathbf{\Sigma}_i = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \end{bmatrix}, \quad \sigma_1 \geq \sigma_2 \geq \sigma_3$$

and $\mathbf{V}_i \in \mathbb{R}^{3 \times 3}$ contains the right singular vectors:

$$\mathbf{V}_i = \begin{bmatrix} \mathbf{v}_{i,1} & \mathbf{v}_{i,2} & \mathbf{v}_{i,3} \end{bmatrix}$$

The normal vector to the best-fit plane is given by the last column of $\mathbf{V}_i$:

$$\mathbf{n}_i = \mathbf{v}_{i,3}$$

where $\mathbf{v}_{i,3}$ is the eigenvector corresponding to the smallest singular value σ_3.

We first assign the fingerprint vector as the normal vector:

$$\mathbf{v}_i^{\text{raw}} = \mathbf{n}_i$$

The next step is to compute the second vector to refine the fingerprint vector, where we need the projection of the assembly centre to the normal vector:

$$\mathbf{c}_i^{\text{assembly}} = \text{Proj}_{\mathbf{n}_i}(\mathbf{R}_i)$$

For a CBU that functions as any GBU type other than 4–planar, we take the second vector as the vector to the nearest binding site:

$$b^* = \arg\min_b \|\mathbf{B}_{i,b} - \mathbf{c}_i^{\text{binding}}\|$$
$$\mathbf{v}_i^{\text{secondary}} = \mathbf{c}_i^{\text{assembly}} - \mathbf{B}_{i,b^*}$$

For a CBU that functions as 4–planar GBU, we take the second vector as the vector to the closest pair of binding sites. This adjustment supports the newly introduced AM (4–planar)$_6$(3–pyramidal)$_8$_T$_h$, where the 4–planar GBU exhibits D_{2h} symmetry, and its dihedral angles are not evenly distributed at 90°. Simply taking the nearest binding site will cause problems with the orientation of CBUs in the assembled MOPs. We define the plane passing through $\mathbf{c}_i^{\text{assembly}}$ with normal vector $\mathbf{n}_i$:

$$\pi_i = \{\mathbf{x} \in \mathbb{R}^3 \mid (\mathbf{x} - \mathbf{c}_i^{\text{assembly}}) \cdot \mathbf{n}_i = 0\}$$

Each binding site is projected onto the plane π_i:

$$\mathbf{B}_{i,k}^{\perp} = \mathrm{Proj}_{\pi_i}(\mathbf{B}_{i,k})$$

where $\mathrm{Proj}_{\pi_i}(\mathbf{B}_{i,k})$ denotes the orthogonal projection onto the plane.

Next, we find the closest pair of projected points:

$$(\mathbf{B}_{i,a}^{\perp}, \mathbf{B}_{i,b}^{\perp}) = \arg\min_{\mathbf{B}_{i,j}^{\perp}, \mathbf{B}_{i,k}^{\perp}} \|\mathbf{B}_{i,j}^{\perp} - \mathbf{B}_{i,k}^{\perp}\|$$

The line passing through these two points is:

$$\ell_i = \{\mathbf{x} \in \mathbb{R}^3 \mid \mathbf{x} = \mathbf{B}_{i,a}^{\perp} + \lambda(\mathbf{B}_{i,b}^{\perp} - \mathbf{B}_{i,a}^{\perp}), \quad \lambda \in \mathbb{R}\}$$

where the direction vector of the line is:

$$\mathbf{d}_i = \mathbf{B}_{i,b}^{\perp} - \mathbf{B}_{i,a}^{\perp}$$

Finally, the vector from $\mathbf{c}_i^{\text{assembly}}$ to the closest line ℓ_i is considered as the secondary vector and it can be calculated as:

$$\mathbf{v}_i^{\text{secondary}} = \left(\mathbf{B}_{i,a}^{\perp} + \frac{(\mathbf{c}_i^{\text{assembly}} - \mathbf{B}_{i,a}^{\perp})^{\top} \mathbf{d}_i}{\mathbf{d}_i^{\top} \mathbf{d}_i} \mathbf{d}_i \right) - \mathbf{c}_i^{\text{assembly}}$$

The final fingerprint for the CBU can be refined as:

$$\mathbf{v}_i^{\text{CBU}} = \mathbf{n}_i \times \frac{\mathbf{v}_i^{\text{secondary}}}{\|\mathbf{v}_i^{\text{secondary}}\|}$$

The fingerprint vector for the GBU can be calculated in the same manner, and this calculation should be repeated for all occurrences of the CBUs, *i.e.*, $\mathbf{v}_{i,j}^{\text{GBU}}$.

Fingerprint vectors rotation

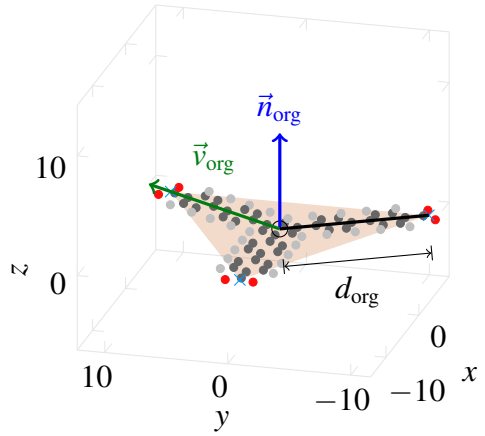
The rotation required to align CBU with its corresponding GBU appearances can be achieved by calculating the rotation quaternion between the two vectors:

$$\mathbf{q}_{i,j} = \mathrm{Quat}\left(\mathbf{v}_i^{\text{CBU}}, \mathbf{v}_{i,j}^{\text{GBU}}\right) \quad \text{(Rotation quaternion)}$$

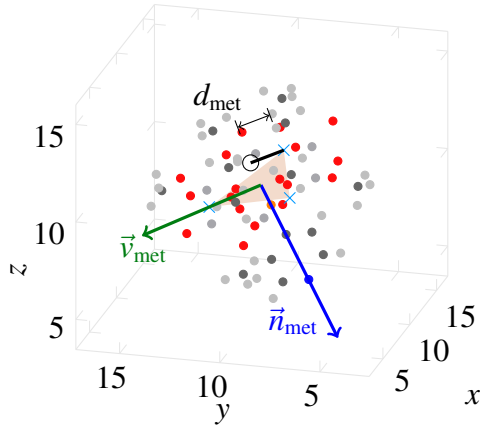
The quaternion should then be applied to rotate all atoms of the CBU and their binding sites accordingly:

$$\mathbf{R}_i^{\text{rot}} = \mathbf{q}_{i,j} \otimes \mathbf{R}_i \otimes \mathbf{q}_{i,j}^{-1},$$
$$\mathbf{B}_{i,b}^{\text{rot}} = \mathbf{q}_{i,j} \otimes \mathbf{B}_{i,b} \otimes \mathbf{q}_{i,j}^{-1},$$

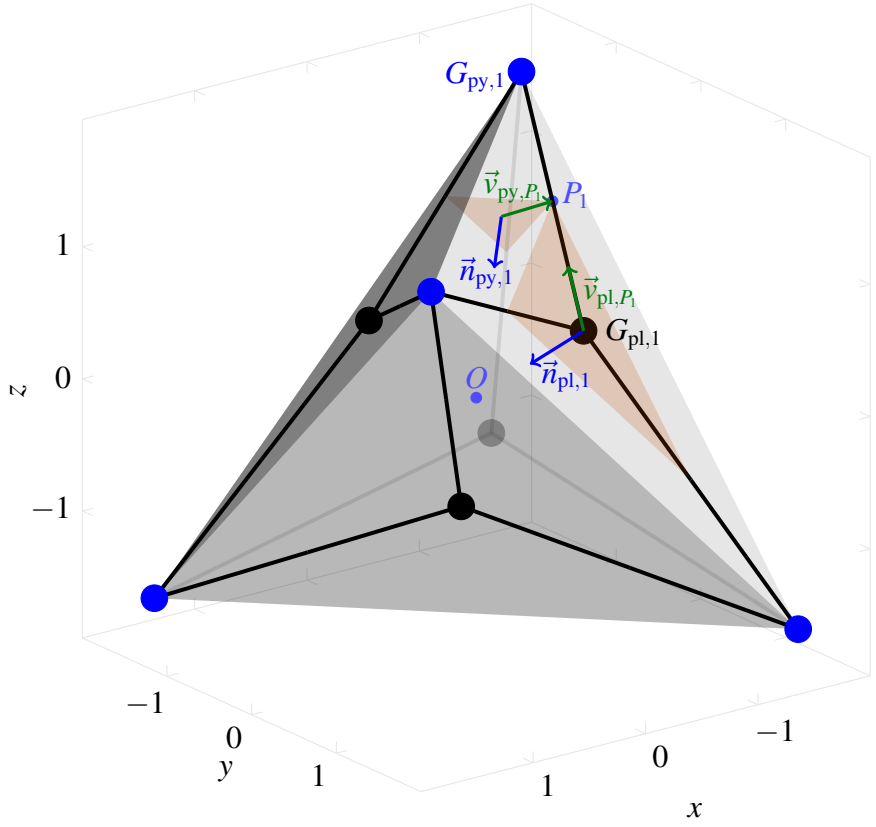
where $\otimes$ denotes quaternion rotation.



(a) *[(C6H3)((C6H4)2)3(CO2)3]*$^{3-}$



(b) *[V6O6(C5H4NPO3)(CH3O)9]*$^{1+}$



(c) *(3–planar)*$_4$*(3–pyramidal)*$_4$_$\mathrm{T_d}$

Figure S1: *Visualisation for fingerprint vector rotation in the geometry stitching algorithm using OGM to align CBUs (organic/metal - (a)/(b)) and their corresponding GBUs (3–planar/3–pyramidal).*

Figure S1 illustrates the rotation of CBUs to align with the orientation of GBUs, where

the fingerprint vector is computed using the cross-product of the two vectors shown for both CBUs and GBUs, respectively.

Scaling factor calculation

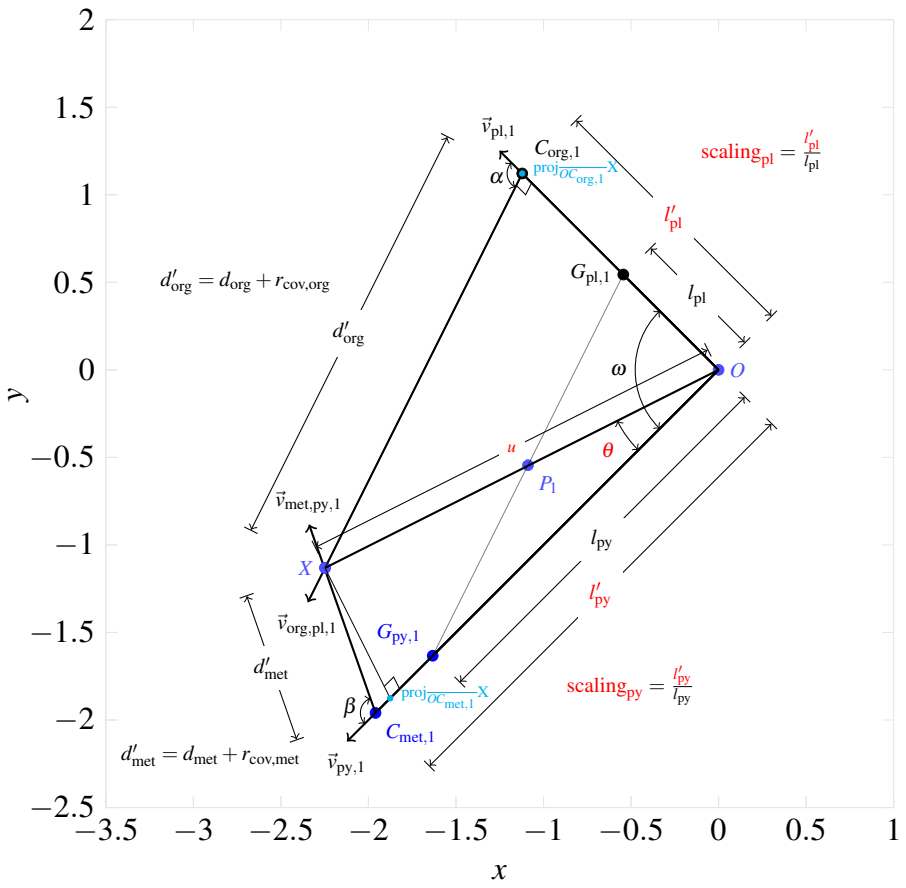


Figure S2: *The scaling factor calculation per GBU Type for the MOP shown in Fig. S1 using the OGM-based MOP geometry stitching algorithm. The geometry to be solved is projected on the X-Y plane. Note that the scaling factors (*$\mathrm{scaling}_{\mathrm{py}}$ *and* $\mathrm{scaling}_{\mathrm{pl}}$*) are only for illustrative purposes and do not reflect the actual scale of this MOP.*

Figure S2 illustrates the key parameters involved in shifting the CBUs to the correct position in 3D space, ensuring their binding sites are equidistant from the origin of the MOP. Known quantities in black include base distances, covalent radii, and directional vectors associated with planar ("pl") and pyramidal ("py") GBUs. Red annotations highlight the unknowns to be calculated: angular parameters, scaling factors, and the resulting scaled distances.

Define the plane constructed by the two directional vectors for the GBUs, $\vec{v}_{\mathrm{py},1}$ and $\vec{v}_{\mathrm{pl},1}$; the parametric equation of the plane is:

$$\Pi_{1,1} : \mathbf{r}(s,t) = \mathbf{r}_0 + s \cdot \vec{v}_{\text{py},1} + t \cdot \vec{v}_{\text{pl},1}, \quad s,t \in \mathbb{R}$$

where $\mathbf{r}_0 = (0,0,0)$ represents the origin, and s,t are scalar parameters that span the plane. The governing equation for the unknown angle θ to be solved is:

$$\frac{\sin(\theta)}{\text{Proj}_{\Pi_{1,1}}(d'_{\text{met}}) \cdot \sin(\beta)} = \frac{\sin(\omega - \theta)}{\text{Proj}_{\Pi_{1,1}}(d'_{\text{org}}) \cdot \sin(\alpha)}$$

Once θ is obtained, the shared side u can be calculated as:

$$u = \frac{\text{Proj}_{\Pi_{1,1}}(d'_{\text{met}}) \cdot \sin(\beta)}{\sin(\theta)}$$

The scaled length can then be calculated using the law of cosines:

$$l'_{\text{py}} = \sqrt{\left(\text{Proj}_{\Pi_{1,1}}(d'_{\text{met}})\right)^2 + u^2 - 2 \cdot \text{Proj}_{\Pi_{1,1}}(d'_{\text{met}}) \cdot u \cdot \cos(\beta - \theta)}$$

$$l'_{\text{pl}} = \sqrt{\left(\text{Proj}_{\Pi_{1,1}}(d'_{\text{org}})\right)^2 + u^2 - 2 \cdot \text{Proj}_{\Pi_{1,1}}(d'_{\text{org}}) \cdot u \cdot \cos(\alpha - (\omega - \theta))}$$

Finally, the scaling factor is computed by dividing the scaled length by the length of the corresponding GBU type. This factor drives the transformation vector that shifts the projected assembly centre of the CBUs to the correct spatial positions, *e.g.*, $C_{\text{met},1}$ and $C_{\text{org},1}$ for the metal and organic CBUs, respectively, based on the pair of directional vectors for the GBUs, $\vec{v}_{\text{py},1}$ and $\vec{v}_{\text{pl},1}$. The transformation vector calculation is repeated for each pair of GBU connections within the AM and applied to the corresponding rotated CBUs.

Structural properties calculation

Given a MOP with N atoms centred at the origin $(0,0,0)$:

$$\textbf{MOP} = \bigcup_{a=1}^{N} \{\mathbf{r}_a \mid \mathbf{r}_a = (x_a, y_a, z_a)\}, \text{ where } \frac{1}{N}\sum_{a=1}^{N} \mathbf{r}_a = (0,0,0)$$

The largest inner sphere diameter, ϕ_{inner}, can be calculated as:

$$\phi_{\text{inner}} = 2 \cdot \min_{1 \le a \le N} (\|\mathbf{r}_a\| - r_a)$$

where $\|\mathbf{r}_a\| = \sqrt{x_a^2 + y_a^2 + z_a^2}$ is the Euclidean distance from the origin to atom a, and r_a is the covalent radius of atom a. The minimum value represents the tightest atomic constraint on the cavity size.

The outer diameter identifies the atom farthest from the origin:

$$\phi_{\text{outer}} = 2 \cdot \max_{1 \le a \le N} \|\mathbf{r}_a\|$$

Given a direction vector $\mathbf{v}$ defining the pore axis, which is the vector from the origin to the centroid of the connecting points of ring-forming GBUs, the pore size diameter $\phi_{\text{pore}}(\mathbf{v})$ can be calculated as:

$$\phi_{\text{pore}}(\mathbf{v}) = 2 \cdot \min_{1 \le a \le N} \left(\frac{\|\mathbf{r}_a \times \mathbf{v}\|}{\|\mathbf{v}\|} - r_a \right)$$

where $\|\mathbf{r}_a \times \mathbf{v}\| / \|\mathbf{v}\|$ calculates the perpendicular distance from atom a to the pore axis. This formula ensures that the pore size is constrained by the closest atoms to the pore axis when adjusted by their covalent radii. For concrete MOPs, the pore axis might be slightly shifted from the idealised AM due to the size of the CBUs used in construction. Therefore, the centroid of the connecting points of ring-forming CBUs is used as the actual pore axis.

A.5 New AMs and MOPs added to base

Table S1: *New AMs (in boldface) and MOPs added to the original OntoMOPs knowledge graph as the foundation for the subsequent expansion with Listing S5. The CCDC No. refers to the Cambridge Crystallographic Data Centre number identifier.*

Assembly Model	MOP Formula	Charge (e^-)	Molar Mass (g/mol)	CCDC No.	Ref.
$(3\text{–pyramidal})_4(2\text{–linear})_6\_T_d$	$[Zr_3O(OH)_3(C_5H_5)_3]_4[(C_8H_8)(C_6H_4)_2(CO_2)_2]_6$	4	4210.29	1955211	[2]
	$[V_6O_6(OCH_3)_9(SO_4)]_4[(C_6H_4N)_2(CO_2)_2]_6$	-8	4717.49	2259643	[3]
	$[V_6O_6(OCH_3)_9(SO_4)]_4[(C_{10}H_6)(C_6H_4)_2(CO_2)_2]_6$	-8	5306.45	2359340	[4]
	$[V_6O_6(OCH_3)_9(SO_4)]_4[(C_{14}H_8)(C_6H_4)_2(CO_2)_2]_6$	-8	5606.45	2359341	[4]
$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	$[V_5O_9]_6[(C_{14}H_8)(CO_2)_2]_{12}$	-6	5563.22	2024518	[5]
	$[Co_4C_{40}H_{44}O_{12}S_4]_6$ $[(C_{14}N_2H_{10})Co(OH_2)_4(C_6H_4)_2(CO_2)_2]_{12}$	0	13414.08	2176774	[6]
$(3\text{–planar})_8(2\text{–bent})_{12}\_O_h$	$[(C_3N_3)(C_6H_4)_3(CO_2)_3]_8[VO]_{12}$	0	4310.24	1864118	[7]
$(4\text{–pyramidal})_4(2\text{–bent})_8$ $\_D_{4h}$	$[V_5O_9]_4[(C_6H_4)(CO_2)_2]_8$	-4	2907.73	1435110	[8]
$(4\text{–planar})_6(3\text{–pyramidal})_8$ $\_T_h$	$[(C_6H_3)_2(CO_2)_4]_6[V_6O_6(OCH_3)_9(SO_4)]_8$	-16	8173.54	1583722	[9]
	$[(C_6H_3N)_2(CO_2)_4]_6[V_6O_6(OCH_3)_9(SO_4)]_8$	-16	8341.66	1985926	[9]
	$[(C_6H_3C)_2(CO_2)_4]_6[V_6O_6(OCH_3)_9(SO_4)]_8$	-16	8317.90	1985927	[9]
	$[(C_{18}H_{10})(CO_2)_4]_6[V_6O_6(OCH_3)_9(SO_4)]_8$	-16	8629.90	1985928	[9]
	$[(C_{18}H_{10})(CO_2)_4]_6[V_6O_6(C_5H_4NPO_3)(CH_3O)_9]_8$	-16	9117.88	2211525	[10]
	$[(C_{16}H_8N_2)(C_6H_4CO_2)_4]_6[V_6O_6(OCH_3)_9(SO_4)]_8$	-16	10468.30	2278526	[11]
	$[(C_{16}H_8N_2)(C_6H_4CO_2)_4]_6[V_7O_{10}(OCH_3)_9]_8$	-24	10619.31	2278527	[11]

Table S2: *New CBUs added to the original OntoMOPs knowledge graph (introduced as part of the new MOPs) as the foundation for the subsequent expansion with Listing S5. PubChem CIDs (Compound Identifications) are provided for the charge-neutral versions of the molecules, wherever available.*

CBU Formula	Binding Site	Charge (e^-)	Molar Mass (g/mol)	GBU Type	PubChem CID [or Ref.]
$[VO]$	Metal	2	66.94	2–bent	34007
$[(C_{14}H_8)(CO_2)_2]$	Organic	-2	264.25	2–linear	5219726
$[(C_8H_8)(C_6H_4)_2(CO_2)_2]$	Organic	-2	344.4	2–linear	102307057
$[(C_{14}N_2H_{10})Co(OH_2)_4(C_6H_4)_2(CO_2)_2]$	Organic	-2	577.46	2–linear	[6]
$[(C_6H_4N)_2(CO_2)_2]$	Organic	-2	268.24	2–linear	11471
$[(C_{10}H_6)(C_6H_4)_2(CO_2)_2]$	Organic	-2	366.4	2–linear	101160939
$[(C_{14}H_8)(C_6H_4)_2(CO_2)_2]$	Organic	-2	416.4	2–linear	12149442
$[V_6O_6(C_5H_4NPO_3)(CH_3O)_9]$	Metal	1	838.01	3–pyramidal	[10]
$[(C_6H_3)_2(CO_2)_4]$	Organic	-4	326.24	4–planar	15840397
$[(C_6H_3N)_2(CO_2)_4]$	Organic	-4	354.26	4–planar	15526883
$[(C_6H_3C)_2(CO_2)_4]$	Organic	-4	350.3	4–planar	91810420
$[(C_{18}H_{10})(CO_2)_4]$	Organic	-4	402.3	4–planar	46931021
$[(C_{16}H_8N_2)(C_6H_4CO_2)_4]$	Organic	-4	708.7	4–planar	132570336

Table S3: *Number of new MOPs generated using Listing S5 in comparison with the MOPs in the original OntoMOPs knowledge graph, and the new AMs/MOPs added to the base in this work.*

No.[1]	Assembly Model	Assembly Model Partial IRI[2]	In KG	Addition	Listing S5
1	$(3–pyramidal)_2(2–bent)_3\_D_{3h}$	4f695309-35ef-4b72-ac47-25d46d8e87cd	18	0	21
2	$(3–planar)_4(3–pyramidal)_4\_T_d$	793984ba-26f8-4770-aca3-e94b07f632f4	36	0	42
3	$(4–pyramidal)_3(2–bent)_6\_D_{3h}$	2fb6e7fe-95d1-400e-a9da-b6ce614935a8	11	0	15
4	$(3–pyramidal)_4(2–linear)_6\_T_d$	3d71c19a-ab54-4993-8c94-267dcfe41792	84	4	140
5	$(3–planar)_4(2–bent)_6\_T_d$	88a0302e-9b44-44ba-83bb-848315ec26d8	24	0	24
6	$(4–pyramidal)_6(3–planar)_8\_O_h$	038c423f-c7f7-48c7-8701-6441b597e6cd	102	0	102
7	$(4–pyramidal)_6(3–pyramidal)_8\_O_h$	b3922a4e-a7d0-4115-8113-64759855625e	48	0	48
8	$(4–planar)_6(3–pyramidal)_8\_O_h$	ae4c5d0c-f226-4567-8363-4af3e53da40e	40	0	40
9	$(4–planar)_6(2–bent)_{12}\_O_h$	52659f58-8e11-458e-aee9-766940004a7e	90	0	90
10	$(4–pyramidal)_6(2–bent)_{12}\_D_{3h}$	fd68c08d-8f7f-4ac9-8469-3f017c38066a	15	0	15
11	$(4–pyramidal)_6(2–linear)_{12}\_O_h$	6289a7a7-62f9-49a7-a6da-4e074b99a328	210	2	300
12	$(3–pyramidal)_8(2–bent)_{12}\_T_h$	f738bfdb-8f73-4321-9888-bb26ebad977c	39	0	40
13	$(3–planar)_8(2–bent)_{12}\_O_h$	ce490f69-fcc0-40f6-a1ac-75b8312202fa	6	1	12
14	$(3–pyramidal)_8(2–bent)_{12}\_C_s$	a4a091c4-a2c3-4320-9405-8e22836cd65b	6	0	7
15	$(5–pyramidal)_{12}(3–planar)_{20}\_I_h$	f664df33-ef4a-44f8-a76f-930234465ea5	12	0	12
16	$(4–planar)_{12}(2–bent)_{24}\_O_h$	9d9ab0eb-cec0-4dd3-aaa0-0e16d8b154f0	400	0	400
17	$(4–planar)_{12}(2–bent)_{24}\_D_{3h}$	3a3bccc5-4834-4aaf-963e-0d89df7a5242	400	0	400
18	$(5–pyramidal)_{12}(2–linear)_{30}\_I_h$	4d34c0b4-2a4b-4f16-98dd-97c5ce7349a5	28	0	40
19	$\mathbf{(4–pyramidal)_4(2–bent)_8\_D_{4h}}$	35076129-4856-4f04-a535-58e41810b4d2	0	1	600
20	$\mathbf{(4–planar)_6(3–pyramidal)_8\_T_h}$	03f32815-d43d-4fc4-94da-4157573cc668	0	7	35

[1] *The serial numbers of the existing AMs (1–18) align with those used in Kondinski et al. [1].*

[2] *The complete IRI for all of the AMs starts with* `https://www.theworldavatar.com/kg/ontomops/AssemblyModel_`.

A.6 Algorithmic output for new assemblies

Table S4: *Summary of the new metal-organic polyhedron proposed in this work using Listing S5.*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
9a0ec222-93b7-46e5-b83f-7906cce7ad5e	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C6H3)((C6H4)2)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5398.04	16.64	38.04	10.53
fc30d610-2fe7-4c83-8739-6f22291f8daa	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C6H3)(C2C6H4)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5381.91	14.79	34.13	10.08
d3afef6d-7a63-4a39-a3f5-c4c379732d67	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C3N3)(C6H4)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5105.52	9.15	28.66	7.18
92b6e0be-7eb9-4d69-b303-7bd0af6dc043	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C6H3)(C6H4)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5093.65	9.06	28.57	7.1
648e3939-fbb1-4f52-a782-616f15db6c75	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C5NH3)2(CO2)2]4[V6O6(C5H4NPO3)(CH3O)9]4	-4	4320.79	2.26	22.22	1.55
f2a4d626-8276-4732-aa5e-e39444c7a74d	(3–planar)$_4$(3–pyramidal)$_4$_T$_d$	[(C6H3)(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	4180.51	0.13	20.23	0
ecd84f2e-9490-4e89-b334-f3d39407310e	(3–planar)$_8$(2–bent)$_{12}$_O$_h$	[(C6H3)((C6H4)2)3(CO2)3]8[VO]12	0	4895.28	39.23	53.76	28.18
713c0a1f-95a3-414b-b158-f489c238ffc0	(3–planar)$_8$(2–bent)$_{12}$_O$_h$	[(C6H3)(C2C6H4)3(CO2)3]8[VO]12	0	4863.02	33.94	47.26	24.04
f2221d7e-d560-4e80-97be-bd95375fb4e6	(3–planar)$_8$(2–bent)$_{12}$_O$_h$	[(C6H3)(C6H4)3(CO2)3]8[VO]12	0	4286.51	26.33	37.91	18.21
1a372119-3600-4df9-9026-20f0565f583b	(3–planar)$_8$(2–bent)$_{12}$_O$_h$	[(C5NH3)2(CO2)2]8[VO]12	8	2740.77	17.16	26.9	9.71
96d0d5b8-ed80-423c-a5bd-447d360842a0	(3–planar)$_8$(2–bent)$_{12}$_O$_h$	[(C6H3)(CO2)3]8[VO]12	0	2460.21	14.53	23.32	9.42
02672e2a-5068-4217-b5fc-a7c97c50b4b0	(3–pyramidal)$_2$(2–bent)$_3$_D$_{3h}$	[V6O6(C5H4NPO3)(CH3O)9]2[C2H4O2(C6H3SO3)2(CO2)2]3	-10	3051.14	4.95	24.68	3.98
ac83c99d-11c6-48c7-9c82-25bffa430711	(3–pyramidal)$_2$(2–bent)$_3$_D$_{3h}$	[V6O6(C5H4NPO3)(CH3O)9]2[SO2(C6H4)2(CO2)2]3	-10	2588.84	0.29	20.37	0.29
c246e22b-d984-467c-9f2d-6819d1a18886	(3–pyramidal)$_2$(2–bent)$_3$_D$_{3h}$	[V6O6(C5H4NPO3)(CH3O)9]2[CH2(C6H4)2(CO2)2]3	-4	2438.73	0	20.03	0
eb315405-5fb9-48f6-ba1e-9b8a9f7dac7b	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(OCH3)9(SO4)]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	-8	6572.81	17.94	39.38	13.87
a49ce19b-2c14-49a2-8812-270b60f69e4b	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4)3(CO2)2]6	-8	5249.88	15.09	34.46	13.69
1fbad378-b578-4a77-a370-b0fe44931d9a	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	-8	6816.8	17.68	39.02	13.63
cb4f6f02-4df2-418d-a299-87d71733d9df	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V7O10(OCH3)9]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	-12	6648.31	17.38	39.18	13.38
a8eabdbc-1b22-4e15-8fef-d790503c036d	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V7O10(OCH3)9]4[(C6H4N)2(CO2)2]6	-12	4792.99	17.47	32.11	13
1d4c9fc3-f175-4b71-b7b8-5ffcabe95810	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4C)2(CO2)2]6	-8	4937.43	12.89	32.31	12.07
bbc59d07-f9be-4c1a-be9a-e30a0d2ac7e8	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(OCH3)9(SO4)]4[(C8H8)(C6H4)2(CO2)2]6	-8	5174.45	14.8	34.37	11.88
3eecd9c7-8fd9-4996-b75d-361e4ce52674	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C8H8)(C6H4)2(CO2)2]6	-8	5418.44	14.53	34.03	11.67
dc160d7c-b518-44f3-a16d-69223929b8f8	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4N)2(CO2)2]6	-8	4961.48	12.44	31.87	11.65
abc223cd-f227-4411-b289-1ba116c4a8e4	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V7O10(OCH3)9]4[(C8H8)(C6H4)2(CO2)2]6	-12	5249.95	14.24	34.24	11.42
f92017a5-09d2-4a84-b5e4-a9ae66b0af54	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Pd3PO(C3H7N)3]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	0	5614.82	14.05	38.27	10.67
eddff055-6bbe-4d21-9a1a-6bc06d96e7b5	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Pd3PO(C3H7N)3]4[(C6H4N)2(CO2)2]6	0	3759.5	15.16	31.07	10.44
f655bf17-f8f6-484b-b9ec-d4d8c85cb327	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Zr3O(OH)3(C5H5)3]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	4	5608.65	12.6	37.11	9.49
91fd9d00-96a6-48db-a4c5-463e7a3e9d2d	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Zr3O(OH)3(C5H5)3]4[(C6H4N)2(CO2)2]6	4	3753.33	13.69	29.96	9.36
38b6d084-8086-430f-bc71-237577732936	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V3O2(OH)2(HCO2)3]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	0	4880.32	12.33	35.78	9.28
efb5342c-064c-4930-9c90-a0c188e16986	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V3O2(OH)2(HCO2)3]4[(C6H4N)2(CO2)2]6	0	3025	13.42	28.64	9.16
032c1cf7-2172-41a4-9514-28a63824eca0	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4)2(CO2)2]6	-8	4793.3	9.79	29.31	9.15
d414b9d0-54a3-4425-b8e8-d781ac0a034a	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Fe3O(SO4)3(C5H5N)3]4[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]6	4	6300.85	12.16	36.63	9.14
d773af08-4a5e-469b-bdb7-d4ba9b17fce2	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C16H12)(CO2)2]6	-8	5105.75	9.74	29.25	9.1
143afe2f-d9f4-4ea0-8935-e761483b0bba	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C5H3N)2(CO2)2]6	-8	4805.16	9.67	29.19	9.04
576b56ed-1a82-40a0-85ab-87c131ddefe1	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Fe3O(SO4)3(C5H5N)3]4[(C6H4N)2(CO2)2]6	4	4445.53	13.23	29.5	9.03
f37d4beb-c916-46a5-8498-6106f82c80d5	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C14H8)(C6H4)2(CO2)2]6	-8	5850.44	12.71	34.18	8.75
328e7558-0551-40b2-a2ba-3f45b3555396	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[CuCl2(C5H3N)2(CO2)2]6	-8	5611.87	9.54	29.08	8.7
79aba6fb-6211-4635-a381-ef76492ad40a	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Pd3PO(C3H7N)3]4[(C8H8)(C6H4)2(CO2)2]6	0	4216.46	10.87	33.25	8.7
82d09d02-2a48-415a-8f10-1d8c3297affc	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[PdCl2(C5H3N)2(CO2)2]6	-8	5869.12	9.54	29.08	8.67
54261324-501e-4d91-b4f8-19e4c0bb2298	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V7O10(OCH3)9]4[(C14H8)(C6H4)2(CO2)2]6	-12	5681.95	12.43	34.39	8.51
c983c445-9a14-4e48-938d-b3ab2e06c551	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4)(C3H2N2)2]6	4	4601.36	8.59	28.18	8.04
9d7a5a9e-d9c6-47f7-acae-7b92683998b5	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C10H6)(C6H4)2(CO2)2]6	-8	5550.44	14.71	34.26	7.6
fe954955-b400-4b43-8df7-3187b8dd753a	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V7O10(OCH3)9]4[(C10H6)(C6H4)2(CO2)2]6	-12	5381.95	14.65	34.45	7.36
0b61b16f-27db-40a7-ab15-1ce6c3be8611	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V3O2(OH)2(HCO2)3]4[(C8H8)(C6H4)2(CO2)2]6	0	3481.96	9.13	30.81	7.27
23e842b5-0b0f-4335-9382-f2462222cc91	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Fe3O(SO4)3(C5H5N)3]4[(C8H8)(C6H4)2(CO2)2]6	4	4902.49	8.95	31.66	7.14
2195acae-785c-479e-af26-c413ab852899	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C10H6)(CO2)2]6	-8	4637.08	7.16	26.81	6.67
fe5709c5-d9d7-45f8-be72-c5df2fcb9b90	(3–pyramidal)$_4$(2–linear)$_6$_T$_d$	[Pd3PO(C3H7N)3]4[(C14H8)(C6H4)2(CO2)2]6	0	4648.46	9.19	33.4	5.86

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
bf5377ee-3431-4cd6-9f34-27f9cd1c1622	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(OCH3)9(SO4)]4[(C14H8)(CO2)2]6	-8	4693.55	7.12	25.23	4.99
ca97dac7-ba50-41a7-9b21-5839eb3cdbd7	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C28H34N2O2)Mn(CO2)2]6	-8	6793.28	14.12	33.53	4.96
821c6957-1205-434d-840c-e36cb6cd3834	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Pd3PO(C3H7N)3]4[(C10H6)(C6H4)2(CO2)2]6	0	4348.46	11.5	33.47	4.77
6793a6bd-2371-42c0-8522-0fac64593dc7	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Zr3O(OH)3(C5H5)3]4[(C14H8)(C6H4)2(CO2)2]6	4	4642.29	7.82	32.29	4.75
830fa69b-ee4b-4094-91b8-b842ea454e1e	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V7O10(OCH3)9]4[(C14H8)(CO2)2]6	-12	4769.05	6.67	24.53	4.57
956c5a38-e619-475c-8e57-8c91088a4e4c	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V3O2(OH)2(HCO2)3]4[(C14H8)(C6H4)2(CO2)2]6	0	3913.96	7.56	30.98	4.54
68fef464-aa0c-4ae3-9633-39be9c946a07	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Fe3O(SO4)3(C5H5N)3]4[(C14H8)(C6H4)2(CO2)2]6	4	5334.49	7.41	31.82	4.42
8ed6c120-5650-461f-a3e5-6e05ed6eb4e8	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H3Br)(CO2)2]6	-8	4810.11	4.45	24.3	4.16
e0797eb4-f7c2-43e5-98d8-41f6a700dad9	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H3NH2)(CO2)2]6	-8	4426.82	4.44	24.3	4.13
48737363-25a9-42b9-a583-5272454868d5	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4)(CO2)2]6	-8	4336.73	4.44	24.25	4.11
86e06ab7-109f-4ba1-b55a-a761db54f471	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[(C14H8)(CO2)2]6	-8	4937.54	4.31	24.84	3.97
96cd57a2-c06f-4cd3-a3fd-ce13fed0a517	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Zr3O(OH)3(C5H5)3]4[(C10H6)(C6H4)2(CO2)2]6	4	4342.29	10.19	32.38	3.68
8e0480d1-55b0-4f1e-9d7b-e7c3102b8c9e	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V3O2(OH)2(HCO2)3]4[(C10H6)(C6H4)2(CO2)2]6	0	3613.96	9.92	31.09	3.49
638379fc-df62-4175-b5ef-09558e23d8f5	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Fe3O(SO4)3(C5H5N)3]4[(C10H6)(C6H4)2(CO2)2]6	4	5034.49	9.81	31.91	3.37
c646da30-cd6e-4beb-9523-0d052aa5070e	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Pd3PO(C3H7N)3]4[(C14H8)(CO2)2]6	0	3735.56	3.72	23.1	2.12
5cfed265-192f-496e-a807-49df82727a25	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Zr3O(OH)3(C5H5)3]4[(C14H8)(CO2)2]6	4	3729.39	2.44	22.11	1.03
f3bbf3fe-fe25-4126-99e9-28a490493947	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V3O2(OH)2(HCO2)3]4[(C14H8)(CO2)2]6	0	3001.06	2.19	20.82	0.84
a70317bb-927e-4811-907e-e9dc2644b958	$(3–pyramidal)_4(2–linear)_6\_T_d$	[Fe3O(SO4)3(C5H5N)3]4[(C14H8)(CO2)2]6	4	4421.59	2.05	21.65	0.72
2e7e6f25-3e49-4877-a28b-961fa569c231	$(3–pyramidal)_4(2–linear)_6\_T_d$	[V6O6(C5H4NPO3)(CH3O)9]4[C2O4]6	-8	3880.16	0	19.41	0
549f6f31-6f10-4a05-b165-087c433f50f9	$(3–pyramidal)_8(2–bent)_{12}\_C_s$	[V6O6(C5H4NPO3)(CH3O)9]8[(C5H5)(CH3)3(CO2)2]12	-16	9082.65	12.54	32.29	10
792aef56-9301-42cb-8fc7-2e10fdf2ccee	$(3–pyramidal)_8(2–bent)_{12}\_T_h$	[PW9O37Ni6NH2C4H3]8[(C6H3)(OCH3)(CO2)2]12	-24	23903.77	13.07	38.24	3.06
ae2a61be-ace3-4db8-a2ba-cb74716828f0	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C16H8N2)(C6H4CO2)4]6[V6O6(C5H4NPO3)(CH3O)9]8	-16	10956.28	21.46	40.73	8.9
793015c2-1cd8-498a-b4ab-1057c9fc290d	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C16H8N2)(C6H4CO2)4]6[Pd3PO(C3H7N)3]8	0	8552.31	21.22	40.03	6.9
f8264e64-3f47-42b9-8e39-37633388a01a	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C16H8N2)(C6H4CO2)4]6[Zr3O(OH)3(C5H5)3]8	8	8539.97	19.76	38.88	5.94
87e2e882-3141-413a-83b8-cd69c553d1f2	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C16H8N2)(C6H4CO2)4]6[V3O2(OH)2(HCO2)3]8	0	7083.33	19.49	37.54	5.74
87d4d1bc-2b24-4563-ab00-2dc81c4eca94	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C16H8N2)(C6H4CO2)4]6[Fe3O(SO4)3(C5H5N)3]8	8	9924.37	19.31	38.41	4.64
fd190880-50c4-4901-9033-973a30baeffe	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[Pd3PO(C3H7N)3]8	0	6257.55	13.14	26.47	4.16
dc95add3-e84d-4df5-8084-3fd27c576331	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[Pd3PO(C3H7N)3]8	0	6401.91	13.9	28.59	3.36
533fd923-e03c-418f-89a3-304aa13810a0	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[Pd3PO(C3H7N)3]8	0	6425.67	13.95	28.84	3.06
3c25529e-f5e7-44d0-980a-0ede147001e1	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C18H10)(CO2)4]6[V7O10(OCH3)9]8	-24	8780.91	16.28	30.96	2.92
c82fbf6e-4fb6-4410-af0d-cc7389ad7b08	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C18H10)(CO2)4]6[Pd3PO(C3H7N)3]8	0	6713.91	13.84	29.91	2.5
cdb3483f-ef06-4c19-85ec-18e0ec174d86	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[V6O6(C5H4NPO3)(CH3O)9]8	-16	8829.64	10.12	29.64	2.32
b0ea5526-0388-44b0-aae3-00518d9831c9	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[V3O2(OH)2(HCO2)3]8	0	4788.57	11.41	24.11	2.32
91b0d0ca-c8b1-4dcc-8a4e-954899070a60	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[Zr3O(OH)3(C5H5)3]8	8	6389.57	12.43	27.52	2.28
77d8425b-2d7c-4f23-90df-18ce38869d10	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[V7O10(OCH3)9]8	-24	8468.91	14.91	29.68	2.18
16008ec9-edce-46ea-8e91-d6cc84816a11	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[V6O6(C5H4NPO3)(CH3O)9]8	-16	8805.88	9.84	29.38	2.13
0184f14f-7ace-430d-860f-59306c36cb15	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[V3O2(OH)2(HCO2)3]8	0	4932.93	12.15	26.22	2.05
343cd95b-c2da-4946-9ef4-2a9d38a98802	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[Zr3O(OH)3(C5H5)3]8	8	6413.33	12.48	27.76	2
e0b3b107-a465-4c58-b929-53a322993028	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[V7O10(OCH3)9]8	-24	8492.67	15.19	29.92	1.96
8d7752c5-021e-4f49-ba92-10554e5264cf	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[V3O2(OH)2(HCO2)3]8	0	4956.69	12.22	26.44	1.78
28bd2b28-f73c-4d25-8313-8a536150174b	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[Zr3O(OH)3(C5H5)3]8	8	6245.21	11.67	25.41	1.57
9e9b68ea-ebde-4c8d-af91-a2f6a5b1fa25	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C18H10)(CO2)4]6[Zr3O(OH)3(C5H5)3]8	8	6701.57	12.38	28.82	1.42
10f93be1-e9e8-485e-91ee-81b5039ca273	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C18H10)(CO2)4]6[V3O2(OH)2(HCO2)3]8	0	5244.93	12.11	27.5	1.18
9ad11f5d-3235-4a78-b3dd-698874d06883	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[V6O6(C5H4NPO3)(CH3O)9]8	-16	8661.52	7.7	27.33	1.03
3fff4b8c-39f7-451c-ba07-248a9cb34bd4	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[V7O10(OCH3)9]8	-24	8324.55	12.77	27.61	0.77
11baa47a-8c1a-45ff-b2be-cf0317515a99	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3)2(CO2)4]6[Fe3O(SO4)3(C5H5N)3]8	8	7629.61	11.21	24.99	0
1bb55cab-b74f-4908-be8f-3d5b7141fe35	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3C)2(CO2)4]6[Fe3O(SO4)3(C5H5N)3]8	8	7773.97	11.98	27.07	0
106ee8ab-6f3b-4261-9959-28d8f758e608	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C18H10)(CO2)4]6[Fe3O(SO4)3(C5H5N)3]8	8	8085.97	11.93	28.38	0
6be143e1-6429-4899-af6a-068de7397d7f	$(4–planar)_6(3–pyramidal)_8\_T_h$	[(C6H3N)2(CO2)4]6[Fe3O(SO4)3(C5H5N)3]8	8	7797.73	12.02	27.33	0
252c890b-1bf9-4f13-b132-d33568bd1c55	$(4–pyramidal)_3(2–bent)_6\_D_{3h}$	[Mg4C56H76O12S4]3[(C4H2S)(CO2)2]6	0	4520.86	6.99	30.38	4.34
f91e6889-1f98-4d11-8a9b-f75aa94e715f	$(4–pyramidal)_3(2–bent)_6\_D_{3h}$	[Co4C56H76O12S4]3[(C4H2S)(CO2)2]6	0	4936.43	6.87	30.07	4.24
bf98c36a-d48a-4e1c-a571-73344545edd5	$(4–pyramidal)_3(2–bent)_6\_D_{3h}$	[Ni4C56H76O12S4]3[(C4H2S)(CO2)2]6	0	4933.52	6.85	30.03	4.22

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
3b86d708-0036-481d-973a-ee032a8ee4c4	$(4\text{–pyramidal})_3(2\text{–bent})_6\_D_{3h}$	[Zn4C40H44O12S4]3[(C4H2S)(CO2)2]6	0	4340.62	6.52	30.01	2.94
c975a140-2f44-4da9-954b-bfa0eaf7098a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)2(CO2)2]8	-4	3500.33	13.33	24.8	9.31
846d20cc-3dbb-4548-a309-fa679105494e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)2(CO2)2]8	0	3232.57	12.87	21.97	8.91
6ba1f2c6-8147-4956-b587-0251b07a65da	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)2(CO2)2]8	0	6036.44	11.83	39.75	8.39
ba5f8318-5d17-46f0-92ab-89e208a0c992	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C56H76O12S4]4[(C6H3)2(CO2)2]8	0	6572.19	11.96	36.52	8.39
05d6f468-69cb-4b43-a8a8-95aa73f61598	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)2(CO2)2]8	0	5667.16	11.99	36.17	8.37
6e7c1f7b-e6bf-457c-92a6-97408bcd767d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)2(CO2)2]8	0	5716.6	11.93	36.04	8.34
009fc610-69d0-4203-b5f4-3bdc0901e143	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)2(CO2)2]8	0	7126.28	11.83	36.18	8.31
7aa54b76-c139-4cf3-b1e3-2b2e20cb0a23	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)2(CO2)2]8	0	7122.41	11.81	36.13	8.3
057d132f-866b-4075-8a4e-730e01cb1138	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C6H3)2(CO2)2]8	0	5330.88	11.87	31.45	8.28
23f2d5ad-3c19-45d6-9ba5-bcf5962d4649	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C24H12O12S4]4[(C6H3)2(CO2)2]8	0	5327.03	11.84	31.4	8.27
fd5698be-7c17-419d-b853-a772bf3b504a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C40H44O12S4]4[(C6H3)2(CO2)2]8	0	5674.51	11.76	36.89	8.2
bbea90f3-d2e1-4d26-952f-f2ec9e003e0b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H8O24S8]4[(C6H3)2(CO2)2]8	-16	6595.76	11.68	34.52	8.16
03e6a62e-56f7-4038-a2d1-09fdff212ce5	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C10H6)(CO2)2]8	-4	3308.2	12.3	23.18	8.1
07d04db5-4415-477e-bf28-4169a3f663e1	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)2(CO2)2]8	0	6224.72	11.46	35.93	8.1
4f5f007f-af1d-4f05-8b24-3a83c55ce88d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)2(CO2)2]8	0	6331.87	11.44	35.89	8.09
39d20859-2035-49dc-8e8b-1a0dc6a3030c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C10H6)(CO2)2]8	0	3040.43	11.86	20.45	7.67
056b2bb2-5287-4f23-8ee8-5d3b08b63c4a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)2(CO2)2]8	0	6228.56	10.71	35.86	7.62
c4ab94d7-ac74-4ec8-a072-e5ebb475af75	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C10H6)(CO2)2]8	0	5844.31	10.86	38.24	7.14
16131400-e991-4db0-8b20-6835c240bcb1	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C56H76O12S4]4[(C10H6)(CO2)2]8	0	6380.06	10.99	34.96	7.12
8b433046-80f9-4a93-9ef0-56f47545c636	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C10H6)(CO2)2]8	0	5475.03	11.01	34.64	7.11
3d42506a-0ca0-4da4-bd1d-e3aa6d80fbc9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C10H6)(CO2)2]8	0	5524.47	10.96	34.51	7.07
9ebbf082-9916-4251-ad06-af4d13feac3e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C10H6)(CO2)2]8	0	6934.15	10.87	34.62	7.03
2da94335-7e07-47be-a238-d38966cd7fdd	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C10H6)(CO2)2]8	0	5138.75	10.89	29.91	7.02
7c14ab97-432e-41b8-a988-d7f4edadbe18	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C10H6)(CO2)2]8	0	6930.27	10.85	34.57	7.02
a491afd9-22f3-4800-91fb-b02a0771100a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C24H12O12S4]4[(C10H6)(CO2)2]8	0	5134.9	10.87	29.86	7.01
808c5596-104b-4895-bc11-72d8bae5cba3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C40H44O12S4]4[(C10H6)(CO2)2]8	0	5482.37	10.79	35.32	6.93
5f018c78-110d-4020-bae6-1d156f83de80	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H8O24S8]4[(C10H6)(CO2)2]8	-16	6403.63	10.7	32.95	6.9
5531ba7a-90aa-43c6-a046-b99c0d89fb56	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C10H6)(CO2)2]8	0	6032.59	10.49	34.42	6.85
64116819-068d-446f-9185-f8c27468d5ac	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C10H6)(CO2)2]8	0	6139.73	10.48	34.38	6.84
21301c3f-9e47-44d0-9ff1-b77fafb9f091	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C10H6)(CO2)2]8	0	6036.43	9.78	34.34	6.35
7e33daa6-ebf3-49df-a39a-e11da157f670	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H4)(CO2)2]8	0	2639.97	9.96	17.54	5.47
69d240d4-72f4-4cac-9996-67f8c819ef76	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3OH)(CO2)2]8	-4	3035.73	10.42	20.02	5.02
9e96f6cb-d73c-40cb-8184-af6f834f0150	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H4)(CO2)2]8	0	5443.84	8.9	35.32	4.95
ead2cc02-d1cd-41c3-89fb-a1fcb955894d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OCH3)(CO2)2]8	-4	3147.94	10.42	20.02	4.85
e97fb070-106a-4832-89c5-5c528cead283	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H4)(CO2)2]8	0	5074.56	9.06	31.69	4.83
6bad4023-6513-4baf-8dd8-10f8267fcb3e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H4)(CO2)2]8	0	5124	9.01	31.56	4.79
dd635530-bb04-44d7-8e6a-6725bc467571	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C6H4)(CO2)2]8	0	4738.28	8.95	26.92	4.79
041ca318-264c-400a-95ea-04d576b273b0	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C24H12O12S4]4[(C6H4)(CO2)2]8	0	4734.43	8.93	26.88	4.78
f9718b5c-6471-430c-8f36-12838aa09bae	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C56H76O12S4]4[(C6H4)(CO2)2]8	0	5979.59	9.02	31.94	4.78
683a0591-9610-49a5-bc57-b4f3d781a315	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H4)(CO2)2]8	0	6533.68	8.89	31.6	4.69
442db98e-6a8a-47bb-ae6d-c48d2b1c9495	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(CO2)3]8	-12	3251.75	10.41	20.01	4.69
e60b7d67-7a41-4225-a976-87effcf75cc6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H4)(CO2)2]8	0	6529.81	8.87	31.56	4.68
aa6e1b64-39a4-4baa-bad2-452a0e8b4157	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H4)(CO2)2]8	0	5632.12	8.54	31.49	4.66
f7dcda4f-2604-4072-9057-8028f856f8c3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H8O24S8]4[(C6H4)(CO2)2]8	-16	6003.16	8.76	29.92	4.66
758c317a-350b-45a1-b567-bcccb55c2c00	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C40H44O12S4]4[(C6H4)(CO2)2]8	0	5081.9	8.84	32.26	4.65
c147bdcb-facd-4f9e-9846-915e03268126	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H4)(CO2)2]8	0	5739.26	8.53	31.45	4.65
57004130-f0bc-4053-9d90-565b9deb6809	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3OH)(CO2)2]8	0	2767.96	9.96	17.54	4.5
e28033ce-5684-4853-96e6-04f66e6a1370	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)(OCH3)(CO2)2]8	0	2880.17	9.96	17.8	4.46
5b78e7f9-4dff-434a-a28f-c098cbfe6890	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)(CO2)3]8	-8	2983.98	9.96	17.53	4.17
59b035b7-071f-4926-a619-18995159137a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H4)(CO2)2]8	0	5635.96	7.8	31.42	4.15
582e979c-8d8e-4ccd-b203-576f97ff118f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3OH)(CO2)2]8	0	5571.84	8.9	35.32	4.01

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
7fba42d0-227c-4289-b345-6df0ab3b981b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OCH3)(CO2)2]8	0	5684.05	8.91	35.31	3.97
8be40509-2738-4add-9e48-e7a8a2d66861	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V5O9]4[(C6H3(CH3))(CO2)2]8	-4	3019.94	10.42	20.02	3.91
6aa7305f-5ff1-4d98-863b-552386a806c4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V5O9]4[(C6H3NH2)(CO2)2]8	-4	3027.85	10.42	20.02	3.91
82625b08-8b1a-4921-b3aa-f5edac65fa52	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OCH3)(CO2)2]8	0	5314.77	9.07	31.68	3.86
6f65bb2e-3af3-45a9-9cc3-74462b0aa169	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3OH)(CO2)2]8	0	5202.56	9.06	31.69	3.86
ed673ebf-5caa-4528-ac36-c69ab8157ffa	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	4978.49	8.95	26.92	3.83
1111bf7a-b178-4582-969a-eba90073c2c7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3OH)(CO2)2]8	0	4866.28	8.95	26.92	3.83
97f41eca-f4e7-4f07-a4e3-6c489b97a5ce	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OCH3)(CO2)2]8	0	5364.21	9.01	31.55	3.82
c60ce960-d9ce-4060-b364-8d89df76e878	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	6219.8	9.03	31.93	3.82
476051c2-8224-4af2-a51a-bd89ade33443	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C40H44O4S4]4[(C6H3OH)(CO2)2]8	0	5252	9.01	31.56	3.82
11e33ae3-cdb8-4d1d-9fc0-c98b4a987c9c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3OH)(CO2)2]8	0	4862.43	8.93	26.88	3.81
9eda58a9-7bb7-4ec1-b490-9e9b4ed11817	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3OH)(CO2)2]8	0	6107.59	9.02	31.94	3.81
95797aeb-5471-480c-92b0-e8b7263a050e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	4974.64	8.93	26.88	3.81
13e052df-0b7a-4598-a04b-53b0b4d009fa	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V5O9]4[(C6H2O)(CH2CHCH2)(CO2)2]8	-4	3348.17	10.42	22.15	3.74
02a2eea4-0c84-4324-8f8d-b821ca428fc1	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3OH)(CO2)2]8	0	5760.12	8.54	31.49	3.73
2faea5d7-1a20-494c-bb1b-842505acd267	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	6773.89	8.9	31.59	3.72
1b50e790-7860-43d6-9f49-0a859d8942b4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[(C6H3OH)(CO2)2]8	0	6661.68	8.89	31.6	3.71
5dd1564f-ea9e-421d-8abf-d47c2bc41fd9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[(C6H3OH)(CO2)2]8	0	5867.26	8.53	31.45	3.71
5792c164-d7e0-46dc-af4e-224ec1b96f59	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	6770.01	8.89	31.55	3.71
663ed0ad-9134-46ae-bec4-19d04935f17a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C56H76O12S4]4[(C6H3OH)(CO2)2]8	0	6657.8	8.87	31.55	3.7
d25156b3-9556-49a5-b425-2cdcab7f6391	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3OH)(CO2)2]8	-16	6131.16	8.76	29.92	3.69
f3a9d849-dbec-4641-9d49-9149fe0149a0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OCH3)(CO2)2]8	-16	6243.37	8.76	29.92	3.69
f6fc6ab9-38d1-439f-95b3-84f823555a59	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3OH)(CO2)2]8	0	5209.9	8.84	32.26	3.68
584e9f6c-60a2-4b94-8660-1dd5e563183a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	5322.11	8.84	32.26	3.68
5e531cfc-6205-496f-a57c-906e0e1c1d84	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C48H28O4S4]4[(C6H3)(CO2)3]8	-8	5787.85	8.9	35.31	3.68
53a01aef-31e5-4e01-858c-783bd4a09628	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OCH3)(CO2)2]8	0	5872.33	8.54	31.49	3.68
247c049b-ee08-46f4-ba1e-e19b47a97187	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	5979.47	8.53	31.45	3.67
14d6012c-6598-4843-8322-f3ffe93596f7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(CO2)3]8	-8	5418.58	9.06	31.67	3.53
8264f8e9-d9de-4257-aa23-6e1f503d9822	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3SO3)(CO2)2]8	0	3272.41	9.96	18.67	3.52
224c82fc-24cc-4af8-93e0-029df96ee93d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3Br)(CO2)2]8	0	3271.14	9.96	17.54	3.52
4fb2b1d3-9339-4014-b5db-f56f426c4ebe	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3(CH3))(CO2)2]8	0	2752.18	9.96	17.54	3.52
39c345ef-fef8-44b2-9640-d9dea72a21d5	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	4114.49	9.95	40.72	3.52
f68039f1-b9c7-45eb-87ef-efe4eee288b3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	4722.24	9.91	40.49	3.52
1c5e64fd-a911-4c7b-8e24-ec63eaf9a04e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	3104.6	9.96	21.9	3.52
0fa6b0f8-2c2b-46ef-93d9-9a657bb311fb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	3080.41	9.96	21.78	3.52
e1248bc8-8791-443c-ae6f-4d81906e47f8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(OCH2CH3)(CO2)2]8	0	2992.38	9.96	20.17	3.52
7cf33184-6895-4d00-815c-3e611b26d7e9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	3825.22	9.94	34.64	3.52
ef7cb2fa-4db5-4d88-8614-8e8248bc651e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	3585.05	9.96	27.84	3.52
71a385fc-c00a-4844-b550-c6fac178a1d3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3(NO2))(CO2)2]8	0	2999.95	9.96	17.94	3.52
dd313c87-542e-4fab-b9e5-f148072105f9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3NH2)(CO2)2]8	0	2760.08	9.96	17.54	3.52
03f970ae-e3af-4dc8-8831-51d8083df256	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	9018.89	9.96	61.36	3.52
0b2e88eb-4c2d-4f9b-a2fa-ec2db15c774b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(OC2H4OH)(CO2)2]8	0	3120.38	9.96	22.34	3.52
f9fabfb6-349a-4ef8-9838-3312f279dffb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	4385.6	9.94	34.89	3.52
6216bda7-1dff-4c71-8775-c27dbc24454c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[((C6H3)C(CH3)3)(CO2)2]8	0	3088.81	9.96	19.91	3.52
f6312165-e2a1-4c96-8e21-dcc20632f493	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(OCH2C2H)(CO2)2]8	0	3072.34	9.96	22.4	3.52
01ba9ad7-32e5-441e-ad43-e42ab563ccb9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	3744.96	9.95	25.79	3.52
ac8aa2bd-08a5-46bf-9af6-be43716bc1c2	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	3697.26	9.94	28.07	3.52
bf677a77-92ee-402c-8404-93278861fe57	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	4073.34	9.94	32.98	3.52
84da0017-1443-4fde-9c35-7d98a9ed778a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[C6H3C2Si(C3H7)3(CO2)2]8	0	4082.85	9.94	26.99	3.51
b351c0c4-8447-4f6a-a612-6f76b692d15b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	3793.91	9.93	27.93	3.51
2959fe81-57e3-4369-9861-69fecaa3c304	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V5O9]4[(C6H3Br)(CO2)2]8	-4	3538.9	10.42	20.02	3.5
834d8229-5c09-4dc2-a98b-b9b8a8b0ac43	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V4O8]4[C6H3CH2CS3C4H9(CO2)2]8	0	4066.67	9.9	30.79	3.5

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
1ff8754a-98d9-4e1d-8e8b-ef458ab50735	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	3970.07	9.92	25.29	3.5
37929ad8-25b2-42ba-a3db-55c4d3447852	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[C6H3CO2CH3(CO2)2]8	0	3104.26	9.93	20.85	3.5
dffa7668-1e56-44c5-a683-64a73129aebd	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[C6H3OCOCHCH2(CO2)2]8	0	3200.34	9.93	22.47	3.5
8801c583-2167-4526-92dc-d6f655837e26	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C6H3)(CO2)3]8	-8	5082.29	8.94	26.91	3.5
892bc8a2-bd65-4bc2-a5f2-cdd5d28eadf6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	3329.02	9.92	27.07	3.5
b9aaea0a-a3bb-44e8-b3a7-806498d27a37	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	3216.81	9.92	24.49	3.5
1027d8ea-ca54-4555-a0ea-9d3c1b49ff66	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	3472.8	9.91	27.9	3.49
8c72225a-ec3f-4aa6-bcc2-1923767aa7ff	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	3937.43	9.92	36.45	3.49
1e0556fc-d700-4519-bf6c-3478bb582b9d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	3561	9.91	24.39	3.49
4d9a6a09-84ce-4851-bfc3-a769c60f8f97	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	4338.92	9.92	48.76	3.49
e067a04a-7472-49b1-92dd-2e357922750d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(CO2)3]8	-8	5468.01	9	31.54	3.49
a14baf1b-cabb-4f3a-9f74-5f385cbb575f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	4273.39	9.92	32.33	3.49
cb4d1de4-9fa5-46c4-96b3-d6e84a863c58	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V4O8]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	3433.01	9.92	23.52	3.49
1b980ad2-e5f5-4357-9079-2591181065a8	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(CO2)3]8	-8	5078.45	8.92	26.87	3.48
62cc803b-2e3f-4154-9635-e5e5f1f4dfd3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(CO2)3]8	-8	6323.61	9.02	31.92	3.48
2ece2eb8-5dac-4388-8e14-c3021a866354	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(CO2)3]8	-8	5976.13	8.54	31.48	3.4
c67e05e4-21f8-4149-911f-a166edf36b69	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(CO2)3]8	-8	6083.28	8.52	31.44	3.39
fd3cc09a-af10-4c0c-b023-d46e623c3b37	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(CO2)3]8	-8	6877.69	8.89	31.58	3.38
5fefef1d-fab1-4e45-8786-b4ad37abb15e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(CO2)3]8	-8	6873.82	8.87	31.54	3.37
dd12d21c-8edf-4c8b-81a5-33a0eb0259b7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H8O24S8]4[(C6H3)(CO2)3]8	-24	6347.17	8.76	29.91	3.37
b46e96bd-accb-4fc3-88a0-6c9371799627	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(CO2)3]8	-8	5425.92	8.83	32.25	3.35
f1ae455d-d70b-44be-95bf-4446958d8105	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OCH2C2H)(CO2)2]8	-4	3340.11	10.42	22.78	3.23
ccb45327-e3c3-4ed0-abd6-a1e77591ffe6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3OH)(CO2)2]8	0	5763.96	7.8	31.42	3.21
03e1440c-702b-4705-ab5e-4667ba06f201	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OCH3)(CO2)2]8	0	5876.17	7.8	31.42	3.21
f5047b2c-4226-4480-a455-b16dc57e137c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)O(CH2)11CH3(CO2)2]8	-4	4382.26	10.4	41.08	3.11
66010140-f0a9-4e98-a793-d78eb9fca438	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	-4	3372.36	10.42	22.29	3.11
f968008c-6b08-49bc-b094-76ff954fe5d5	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	-4	3852.81	10.42	28.21	3.11
005f0468-975d-4d73-8ac5-3a03bf4cf60d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3(NO2))(CO2)2]8	-4	3267.71	10.42	20.02	3.11
72288b20-aa8d-4da0-b204-5335ca38a092	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OCH2CH3)(CO2)2]8	-4	3260.15	10.42	20.59	3.11
40a0887f-a1a1-46a0-968a-10f5a6abdd0f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	-4	4092.98	10.4	35.06	3.11
5b02d725-df8a-4cb4-9865-7732ecb1f21c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(OC2H4OH)(CO2)2]8	-4	3388.14	10.42	22.75	3.11
9d048b6c-1cf3-435f-9955-5156c3a3d68b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	-4	4653.37	10.39	35.22	3.11
9a413da2-d88e-4c31-9fbd-77dbf3fb6c43	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	-4	9286.65	10.42	61.63	3.11
cf1c0e64-8b5f-42cd-92d8-1f78c8d21633	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3)C(CH3)3)(CO2)2]8	-4	3356.57	10.42	20.34	3.11
1f8b3827-c7c5-42f0-a2a2-28c8519c5cc2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3SO3)(CO2)2]8	-4	3540.18	10.42	20.02	3.11
26c89477-1ec3-4f31-9586-7bf6fa5ff185	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	-4	4541.16	10.37	32.66	3.11
b473b78c-1086-4fe8-b7ea-44062e010f6d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3N2C6H3(CH3)2(CO2)2]8	-4	3965.02	10.4	28.43	3.11
6f966025-a8f3-4e59-a0fd-aae5a1d60d78	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	-4	4990	10.37	40.8	3.1
5ce0c201-f222-4aa0-87a0-6ac17949fc68	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3C2Si(C3H7)3(CO2)2]8	-4	4350.61	10.4	27.39	3.1
8de55fe9-0843-4592-a803-fc07f8267e7c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	-4	4012.72	10.41	26.18	3.1
a4f3ecbc-c241-486e-bca8-340582c02743	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	-4	4341.11	10.39	33.33	3.1
79217c42-a9a5-4792-8c4c-d5c21ec9623f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3CO2CH3(CO2)2]8	-4	3372.02	10.39	21.27	3.09
cbbfecc7-75c2-466a-90fd-dc0e2ab5e0eb	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3OCOCHCH2(CO2)2]8	-4	3468.1	10.39	22.85	3.09
85e28bf4-93bb-48f0-aa2d-a8427c925f3b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	-4	4061.67	10.39	28.32	3.09
9fd5582a-9041-43bb-bd68-0f1f2f402e38	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3CH2CS3C4H9(CO2)2]8	-4	4334.43	10.35	31.13	3.08
9ec3e022-e900-4a89-a405-9d727d93bc24	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3)(OC2H4)2(OH)(CO2)2]8	-4	3740.56	10.37	28.3	3.08
f311fcbc-8ae3-4b43-b66a-98cce2bd1e6a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)O(CH2)4CH3(CO2)2]8	-4	3596.78	10.37	27.42	3.08
34e1cbe4-649e-4bd7-acb1-e4a45e14db1f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	-4	4237.83	10.38	25.7	3.08
e40971d6-9fc5-475f-80cf-3396c3fc032e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3)(OC2H4)3(OCH3)(CO2)2]8	-4	4205.19	10.37	36.88	3.08
0b24ea4a-fed4-4fa1-bbbf-dddd1a0f957c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[C6H3NHCO2C(CH3)3(CO2)2]8	-4	3828.77	10.37	24.78	3.08
44e368cb-89b9-4eef-b8f3-aed4bfcb6870	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[(C6H3)O(CH2)13CH3(CO2)2]8	-4	4606.68	10.37	49.04	3.08
0db45e56-63ad-4bed-8b90-5d4601ee6ef6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[V5O9]4[((C6H3)NHCOC(CH3)3(CO2)2]8	-4	3700.77	10.37	23.93	3.08

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
d4c93151-bf7a-44af-a350-54371b733580	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[V5O9]4[(C6H3)O(CH2)3CH3(CO2)2]8	-4	3484.57	10.38	24.85	3.08
debc9359-9efe-4a3a-9d94-ccf6e3a26f6d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	8061.86	9.06	40.28	3.05
d30532ae-4e52-4c61-80ca-8ddac192d1bc	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	7406.29	9.01	31.86	3.04
b6120179-3a69-4a18-92a5-d3d5e00e35f4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	7164.84	9.06	34.29	3.04
88fa4c45-659f-4df5-8e2a-b72399f9c292	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	7036.88	9.05	31.89	3.03
9f4a8c38-aca0-45cd-96f6-1eb6ab1540a4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12358.51	9.2	61.07	3.01
66cdab96-7833-4ee5-9ed9-e5b910935261	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	7454.12	9.1	40.44	3
715faa83-82db-4fd0-9869-28797f3b69ca	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3SO3)(CO2)2]8	0	6612.04	9.03	31.93	3
e1fdbcc0-3305-426e-926e-9ed343a6a63b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3(CH3))(CO2)2]8	0	6091.8	9.03	31.93	3
ea8512c1-4501-4911-8325-9f8917ad486b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3Br)(CO2)2]8	0	6610.76	9.02	31.94	3
1a687303-13e5-476b-8896-8cf3325024b7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6444.22	9.05	31.91	3
7efda505-7f96-4ff8-b95f-d2a68dd053a1	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6924.67	9.06	31.9	3
d40984c9-d8fd-4233-8256-57c00060ef86	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6812.42	9.02	31.86	3
91afeb21-6789-4a41-a530-c917bfd6c241	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	6332.01	9.04	31.92	3
405b15a9-75bc-4908-b808-96570ece91c7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	6539.97	9.01	31.89	3
8c80550f-902a-4a7d-86dd-727999b05cac	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3CO2CH3(CO2)2]8	0	6443.88	9	31.89	3
cac45fc0-dd9f-4ab7-99ed-6b19c5381a72	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	7309.69	9.03	31.86	3
bf7e93c6-7dbd-4732-8d94-bd86172b57fb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6420.03	9.05	31.91	3
bbffb23a-27e7-40b5-abc2-4e2cf8a06375	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3(NO2))(CO2)2]8	0	6339.57	9.02	31.93	3
c00938f4-6c57-47ef-8225-6a3fa211568c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	6460.01	9.05	31.91	3
bff2c88e-6a23-4014-b878-93cdf2073dd4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6411.97	9.04	31.92	3
f796c39d-d109-4b7f-9922-d954a3035a1a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3NH2)(CO2)2]8	0	6099.71	9.02	31.93	3
b6ef5bfd-6c1b-4419-967a-f39a5c07dde1	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	6428.44	9.06	31.91	3
a95b1f13-8a6c-49b5-9b6e-b05f87ed0aab	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7412.97	9.06	32.75	3
f2e22acd-4e02-426e-a509-51d4e1a7fb5e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	7084.58	9.06	31.89	3
eb6f5064-8a54-4dda-9067-4710861f3513	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7422.47	9.08	31.85	2.99
deea5166-8a38-4c23-943a-017451368524	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	7277.05	9.04	36.1	2.99
5c90419e-0b72-4fc9-a0c0-25bc96975c22	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	7725.23	9.06	34.68	2.99
89c73608-2385-4d49-8f08-22990528858e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	6556.43	9.02	31.87	2.99
430139d2-a93f-45c4-bd07-527f25d01602	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	7678.54	9.08	48.56	2.98
c7449515-d4af-4b6a-b7f9-2bca38db424d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	7133.53	9.05	31.87	2.98
fa7d4aab-4371-4fff-96ed-18d95c606403	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6900.63	9.02	31.86	2.98
8f32a8f7-5e33-4b3d-8a8d-ea93f1e4fc7b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	6772.63	9.02	31.86	2.98
a133740a-5676-42d3-b4e3-74c0ca96b0da	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	6668.64	9.02	31.86	2.98
8fd6782d-4e0e-4e2d-abfc-f0026ef1f8ee	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7156.83	9.05	40.08	2.96
1f5916b9-8474-481e-9c32-00747876b5a2	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6259.81	9.06	34.04	2.96
93e1f1d4-ecb3-4ac6-8005-7f4ccc9c2a86	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C56H76O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	7613.02	9.04	32.12	2.96
05991b74-5980-4d4d-b7b8-88794ad48f48	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	8615.95	8.93	40.2	2.95
899840c6-f7b3-46bf-9460-108f8ae64931	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6501.26	9.02	31.65	2.95
8f20637b-d4d5-4d36-8ed0-3b675ef358aa	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	7718.93	8.93	34.17	2.95
5dc9a15e-ed9d-4308-b27b-fc9d9dc9e7c6	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C56H76O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	8612.08	8.91	40.18	2.94
319d4e69-ad07-4a45-b91e-b9362226f9f7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	7960.38	8.88	31.52	2.94
878eec44-8f56-441e-a353-571bb6961e9d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6131.85	9.06	31.67	2.94
167ab4e5-c416-444e-9e37-824ede080322	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	7715.06	8.91	34.16	2.93
146b22af-07a7-4c96-8b71-7687b8ec4aab	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C48H28O4S4]4[(C6H3NH2)(CO2)2]8	0	5563.96	8.9	35.32	2.93
9f3f22d4-cacb-469c-821a-cc3af221f668	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11453.48	9.14	60.95	2.93
d965caa3-d6a0-4f21-88b2-eb671bea2d3c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C56H76O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	7590.97	8.92	31.55	2.93
0061d404-88e4-4804-9df0-a1fa77575456	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3(CH3))(CO2)2]8	0	5186.77	9.06	31.68	2.92
27300769-ea25-4990-a8d6-614beebbec73	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3Br)(CO2)2]8	0	5705.73	9.06	31.69	2.92
750ca27a-2cc6-4857-93d3-3a9265d9306c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Fe4C40H44S4O4]4[(C6H3SO3)(CO2)2]8	0	5707.01	9.06	31.68	2.92
e3a32299-c834-44b0-9e85-8572e14348b6	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C56H76O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	7956.51	8.86	31.48	2.92
ea0419cc-ca8a-42c5-a5f2-61158544dcd0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C40H44O4S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7206.27	8.99	40.04	2.92

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
5b42b506-f2f9-4eb6-be13-8a44421120bc	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6019.64	9.08	31.68	2.92
1c97c0be-c889-4dd4-8101-dcaf5c1d49aa	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	5907.39	9.03	31.64	2.92
e2710f96-23b7-46eb-b6ef-7eeea4dd5924	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5539.19	9.08	31.68	2.92
089adb76-644e-4d54-a895-a56e3de101ba	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5426.98	9.07	31.68	2.92
00c7cf0f-67a3-46c6-8f61-6fe0c7b05cfb	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3OCOCHCH2(CO2)2]8	0	5634.93	9.04	31.65	2.92
50f0e0b8-7c68-423b-b0fc-be985d9ef0f2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5515	9.07	31.68	2.92
eed99a9f-8d70-4b3f-9a1e-917c59bfcbfc	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6309.25	9.01	33.99	2.92
88beab3d-c8f5-49b6-9f02-1b125d653cb6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6404.66	9.04	31.64	2.92
eebb9d0c-657e-4b23-b9c4-276549d5808d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3CO2CH3(CO2)2]8	0	5538.85	9.03	31.65	2.92
a69d5099-2589-4531-a815-fd12d86dc900	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3(NO2))(CO2)2]8	0	5434.54	9.06	31.68	2.92
8dab8036-aa83-419e-8254-888dcf5aa193	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5554.97	9.07	31.68	2.92
f4b096c6-a636-403c-a007-9b8ae529953f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3NH2)(CO2)2]8	0	5194.68	9.06	31.68	2.92
229142a1-c3cc-4794-b846-a6229b49f7a9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5506.94	9.07	31.68	2.92
ce5da740-f330-4e7b-ac81-78614e2b0653	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5523.4	9.08	31.68	2.92
81132245-512d-4b04-9d09-89bf5609c210	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	7587.1	8.91	31.51	2.92
917eed12-299b-45f4-ae69-fa1c24b3d218	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6507.94	9.06	32.52	2.92
99532833-b859-48e6-96d5-09c21a65bb5b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6179.55	9.07	31.67	2.92
5ab62dbc-e06f-4089-9271-f08713778d47	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7526.11	8.91	40.06	2.91
2dbe9440-aed2-4706-a072-54b204f542a7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6549.09	9.09	40.23	2.91
78ca70aa-7a9a-4ce2-9020-cd4fc23f9c9f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6517.44	9.08	31.66	2.91
e9008593-65ff-4e8e-866b-f4182abb62ea	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6550.7	8.97	31.52	2.91
f5e30e7f-ffe8-4cb1-9d8f-9e038f9c4367	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3(CH3))(CO2)2]8	0	5556.05	8.91	35.32	2.91
34498fe3-628a-428f-ba84-42987a047168	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	6820.2	9.07	34.45	2.91
4d5c2d02-9d88-42ec-980d-8036b1d56130	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12912.6	9.07	61	2.91
301e1f8d-8746-4b25-bcba-3d91ef48c622	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	5651.4	9.04	31.64	2.91
88b2c5a4-5083-4132-9eef-22aa8748deaa	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7967.05	8.93	32.66	2.91
13079996-f754-419b-b6f4-3aa509bac24e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3SO3)(CO2)2]8	0	7166.12	8.9	31.59	2.9
91a51220-baf4-4ad3-a724-1db5852d7daf	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3(CH3))(CO2)2]8	0	6645.89	8.9	31.59	2.9
aecd9670-427f-4a37-a9e6-29e3fd5c3290	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3Br)(CO2)2]8	0	7164.85	8.89	31.6	2.9
e136e5a9-b92e-40aa-946c-c6de9cc1a0a9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	8008.21	8.97	40.34	2.9
8e4ba84f-31fd-46ec-b1a2-e87f57eb316b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	7366.51	8.89	31.52	2.9
0f8d103f-fedf-47b2-a8a8-641d484eaf4f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6372.02	9.05	35.85	2.9
199513f1-27aa-49ad-9495-4a73c5b816ed	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6629.09	8.92	35.29	2.9
9a981bae-2eed-4126-9914-129999fc967e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	6886.1	8.91	31.58	2.9
aaec3198-880a-4661-9ac5-56f75dc8b462	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6998.31	8.92	31.57	2.9
938dbb0b-b857-4788-9b98-64a14d33c9f6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	7478.76	8.94	31.56	2.9
4613788e-af9d-46f8-8803-792aa15c608f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[C6H3CO2CH3(CO2)2]8	0	6997.97	8.87	31.56	2.9
60f5f2ab-b4d6-45ea-84db-fed59716fcae	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6974.12	8.92	31.58	2.9
ba434b14-a0dd-46dd-b0bc-a39dae54c621	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	7094.05	8.88	31.55	2.9
f11df548-b326-4e95-9c99-09dbaebf1bb9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	7863.78	8.9	31.52	2.9
97eeef21-a4b2-4ec9-9d79-6f2e16e57ecf	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3(NO2))(CO2)2]8	0	6893.66	8.89	31.6	2.9
2d6e7e24-5d9d-4c81-970c-0134dce1d117	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	5995.6	9.03	31.64	2.9
0e577cfb-9e7b-4cba-867c-94abdd76c3d9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3NH2)(CO2)2]8	0	6653.8	8.89	31.6	2.9
952ec918-f5db-4da0-9cf3-6f229000e8d7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6966.06	8.91	31.58	2.9
8f9161d1-fdf0-4e86-97c1-3a55066057fe	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	6773.51	9.06	48.37	2.9
a84cf959-e4d7-4a33-98b4-690255d7bb49	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	8279.32	8.94	34.59	2.9
ebf0d659-a867-4122-9998-40de6f98e02b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	7014.09	8.92	31.58	2.9
10d8c909-8dd3-41cc-bb93-0f601ab0a754	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12908.73	9.06	60.99	2.9
ada7dd4f-157e-429c-a3fe-1d886c2bee54	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6228.5	9.05	31.66	2.9
cec5db39-91fd-4c08-b80f-16317bc33ea4	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(((C6H3)C(CH3)3)(CO2)2]8	0	6982.52	8.93	31.57	2.9
02ae818c-43e6-4682-acca-d4497d7dffef	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	5867.6	9.03	31.64	2.9
b3d92fba-e331-4ee1-9e5a-080bed94c767	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	7638.67	8.93	31.55	2.9

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Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
fa9c9d65-63b9-40bc-85bc-d562712d1d86	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6181.29	9.01	31.54	2.9
29bcf314-d7d6-4167-80da-99d7a7276535	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3Br)(CO2)2]8	0	7160.98	8.87	31.56	2.89
6007bfc5-1fae-413d-abb5-4cfb3d181716	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3(CH3))(CO2)2]8	0	6642.02	8.88	31.55	2.89
a24515f1-911a-4ee2-93ce-e331e68ec4a4	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6870.54	8.87	35.26	2.89
ec4cc858-6563-44ce-8d0d-aea78875b29b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7976.56	8.95	31.52	2.89
b585af74-efad-4fb1-819d-2ec377d4d2c5	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	7362.64	8.87	31.48	2.89
099a09f7-75a6-4a77-be4f-f413d165c567	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6994.43	8.91	31.53	2.89
14c0e493-1563-413e-b42d-3fa007f3a42f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	7474.89	8.92	31.52	2.89
22f5cf6b-06c4-4685-b12a-365c6075c7be	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3CO2CH3(CO2)2]8	0	6994.09	8.86	31.51	2.89
9a067530-7175-49d1-acdd-04dcd54a1200	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	7831.14	8.91	35.98	2.89
a4b9192d-3b4e-4014-98f0-d3a83652fa9c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3(NO2))(CO2)2]8	0	6889.79	8.88	31.55	2.89
b90fcb8d-f937-46e1-847b-fcb2d4a5a92b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	6882.22	8.9	31.54	2.89
5e6769a5-97c0-4b91-b668-deb42238784e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6970.25	8.9	31.53	2.89
74ba5f89-7c7a-487b-94ee-2b823a05ef88	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	7859.91	8.88	31.48	2.89
ce21d653-30b2-4ff2-861e-d9626907295f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	7090.18	8.86	31.51	2.89
3466ced0-a718-42f6-ac7b-6a146e3f5bde	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3NH2)(CO2)2]8	0	6649.92	8.88	31.55	2.89
66aecc0e-1ab4-4ac9-968a-e3edaee4df44	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	7687.62	8.92	31.53	2.89
0485cf0d-055f-49f3-a093-73a71ab73203	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(CO2)3]8	-8	5979.97	7.79	31.41	2.89
ea4c1682-6240-4b39-9274-717ab2d15765	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	8232.63	8.95	48.48	2.89
aabfc508-6b51-438f-891a-c46a10117b55	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11502.92	9.09	60.92	2.89
3d1f25c2-3146-4779-82b0-5f386e1f751d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6962.18	8.89	31.54	2.89
64f55c08-3355-4741-8641-f12ee1865f77	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	6978.65	8.91	31.52	2.89
a73729f1-cda9-4fd9-b5e4-fc7fa877077b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	7010.22	8.9	31.53	2.89
9ff6b676-fa51-4e13-a915-ef7fdda2dedb	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3SO3)(CO2)2]8	0	7162.25	8.88	31.55	2.89
5835a6f5-ff78-4b1e-87f9-f5b333084e2a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7963.18	8.91	32.64	2.89
67b2890f-db02-4627-9ba2-44c0687ffe9b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6501.13	8.92	35.29	2.89
99ccd0ca-ebe9-4d17-99cd-2a2f3cdcc4c2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	7110.52	8.89	31.53	2.89
d87d4c0b-1ed9-4ae4-a6f4-cd8421a85ca2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	7634.79	8.91	31.51	2.89
fa7ab05f-6316-4675-8f22-538cb3ea3160	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	5763.61	9.03	31.65	2.89
036dbe57-c521-44b4-bd47-7584e74299df	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3SO3)(CO2)2]8	0	5756.44	9.01	31.55	2.88
3b2a53fb-5673-4f4f-a9a3-1dc8c7e7dd99	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7972.68	8.94	31.47	2.88
7e6421cf-4083-41d0-884c-fe5c3a0417c9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3(CH3))(CO2)2]8	0	5236.21	9.01	31.55	2.88
9167ba30-9f0b-49a6-b649-e976ff9b2764	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	8004.33	8.95	40.33	2.88
b0b3003d-8a67-4b18-9d28-24c93bc25654	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3Br)(CO2)2]8	0	5755.17	9.01	31.56	2.88
5998bd0b-e160-4175-9f04-282a1eb08139	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5588.63	9.02	31.55	2.88
7f9acaf4-e494-4622-a72d-81046b17236e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6069.08	9.03	31.55	2.88
00e6f15d-a9a7-498f-b4f0-e530a88a5637	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	5956.83	8.98	31.51	2.88
eb749534-fc4b-40b0-840a-18026ec3e559	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	7222.73	8.89	31.53	2.88
638e10bd-30af-4c18-88d4-d7192087b139	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5476.42	9.02	31.55	2.88
252d584c-325f-45b1-83b1-2d20f8ac0e06	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3CO2CH3(CO2)2]8	0	5588.29	8.98	31.52	2.88
2c58e94e-6d07-463c-98c5-8fefb70f4341	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3OCOCHCH2(CO2)2]8	0	5684.37	8.98	31.52	2.88
b5a25379-92fa-468c-8180-8e267b002a9a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5564.44	9.02	31.55	2.88
eea6cb1f-cf63-4738-b04c-4c2d296b079d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6454.1	8.99	31.51	2.88
ae9ba024-d5bb-451e-97dd-60fc67c648a8	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3(NO2))(CO2)2]8	0	5483.98	9.01	31.56	2.88
19f05b17-d782-482b-a23e-e533b1722ca2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	8275.44	8.92	34.57	2.88
4db4515d-5958-4b39-a047-4aa81b69f3c3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3NH2)(CO2)2]8	0	5244.12	9.01	31.56	2.88
389642dd-2e4b-48d9-9a26-115ddfbd0855	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5556.38	9.02	31.55	2.88
7d959bfc-dfa4-4ae3-8f5c-9bd22850dffd	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5604.41	9.02	31.55	2.88
81e5edca-99ee-4e71-ba54-dcf72c472e34	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	7454.72	8.89	31.52	2.88
b088eaec-ae48-49c3-97de-7649ecd5b977	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5572.84	9.03	31.55	2.88
1456b28b-fb47-4aaa-8b90-d4851215ba24	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	7106.65	8.87	31.49	2.88
5008a367-6c80-4bee-8c8d-80fd0c077bea	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Fe4C40H44S4O4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	6707.99	9.04	31.89	2.88

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
54acc0b9-c81a-46a0-bc5d-bed13731c569	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6557.37	9.01	32.48	2.88
d721791e-f007-49ab-844e-83fba0a7a2c6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6228.99	9.02	31.54	2.88
eee3abd8-bffe-4f74-98e1-a2cd86a9f51a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	7326.72	8.89	31.52	2.88
35f0ca26-7c7d-4e04-9e1f-5232508f7a88	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6598.53	9.03	40.19	2.87
39a6d371-fb3b-460e-9042-f66ca0fc2837	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3Br)(CO2)2]8	0	6075.01	8.9	35.32	2.87
626df82b-38bb-4447-ba7a-49056299ce57	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6566.88	9.03	31.53	2.87
9cf94ee1-72e2-4c62-abf5-7b3e3dcb1831	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5908.47	8.92	35.3	2.87
4410ccaa-7c58-4fa0-bffe-06c984f4c899	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6388.92	8.93	35.29	2.87
125a984c-db00-47b8-8ef0-72b9637a401d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3OCOCHCH2(CO2)2]8	0	6004.21	8.88	35.28	2.87
53685cc7-a3be-44ef-9b78-645267906ae3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5884.28	8.92	35.31	2.87
b45188e3-0cb5-492e-8619-bc66e49c64ba	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5796.26	8.92	35.31	2.87
b3451d07-1b95-46b4-9475-81f306caea06	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3(NO2))(CO2)2]8	0	5803.82	8.9	35.32	2.87
fcff3175-5b7e-48ce-bc3f-c92563093f08	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	7827.27	8.9	35.96	2.87
02b935b7-faf9-47fc-b7b6-1cbcda1ca168	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	7683.75	8.9	31.49	2.87
0e87a69c-bdfd-4d33-8154-092524452b20	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	6869.64	9.01	34.41	2.87
366fcd9d-b014-44b6-8838-af1dead7b18f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	7450.84	8.88	31.48	2.87
82df6371-deb0-4805-abd0-de52f1fceafa	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	8228.75	8.93	48.47	2.87
396931fb-730d-4159-aa72-ae1be958ac5a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11822.76	9.02	60.91	2.87
352e21bd-9c41-4b61-8014-66f27d9abf56	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5924.25	8.92	35.31	2.87
4f10bc36-4ef1-41d4-b474-6a4ae56a292b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5876.22	8.91	35.31	2.87
15644b52-b28b-4065-831f-c2d00d76c2e3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5892.68	8.93	35.3	2.87
e4f7ee0b-4a21-4cf0-aa0c-e79063598f48	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3SO3)(CO2)2]8	0	6076.28	8.91	35.32	2.87
5f27be49-acd9-4897-8004-1eb7226f3667	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	7322.85	8.87	31.48	2.87
6a66f02c-251f-4073-b8bc-56413e353473	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6877.21	8.92	35.28	2.87
d0f2a564-02d4-4b3a-9f56-e4e51e035065	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C56H76O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	8167.11	8.91	32.03	2.87
e8e26fa2-2985-42d7-96ff-c563b8e3701c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	5700.84	8.99	31.51	2.87
3f96ea9f-4385-41fe-a7cc-3f3f8a38d924	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6918.37	8.95	40.2	2.86
453e5ce1-a09d-4b85-8904-2998d10a3648	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	7218.86	8.87	31.48	2.86
ed733558-2364-4548-9cd0-b1b7212f90ee	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6276.67	8.88	35.26	2.86
1e12a592-7513-4712-b758-144d4b4ca032	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3CO2CH3(CO2)2]8	0	5908.13	8.88	35.29	2.86
c54e41fc-de88-4aa3-ba9b-f92e22cfb760	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6421.46	8.99	35.8	2.86
8b4c5e88-2835-4605-9a5a-1aedc77d2605	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6773.94	8.89	35.26	2.86
201eaf86-78b7-4dce-9d70-291f620c6d2b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6277.94	9	31.53	2.86
459e0664-dafd-48c7-b8e6-13bacd230f28	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6045.04	8.98	31.51	2.86
87d7c907-1f08-4953-aa6e-5c69e4596231	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	7189.48	8.92	35.28	2.86
a41be135-fde4-4027-9d15-8942fb79b8f2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	6822.95	9.01	48.34	2.86
81b897ad-f4a3-4aae-88b5-9029164cce89	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	5917.04	8.98	31.51	2.86
c39f7735-3752-4440-9e8d-020fbb189e0c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6548.83	8.92	35.29	2.86
95aa97bd-5a42-499c-994c-b5a497c29d6a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6886.72	8.94	35.26	2.85
6506a4c4-88f9-402f-800f-ff8e5dbe6a7f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6741.3	8.9	35.81	2.85
2a34c495-73c0-4aff-9e13-4d6612533cf4	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6597.78	8.91	35.27	2.85
833ca412-898e-4132-80a9-a110b633b1ac	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	5813.05	8.98	31.52	2.85
93f27699-c7ce-482e-a5fc-e028b4bba24a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	6020.68	8.89	35.27	2.85
bb1fd111-4c93-47f3-9af8-bea816dccf93	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C56H76O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	8163.23	8.89	32.01	2.85
c53966d8-fa20-4e44-9135-287d742a3de2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	6820.55	8.91	39.84	2.84
99b68d8c-e1f5-471e-80df-b9854b6dd163	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	6132.89	8.89	35.26	2.84
56205ec0-411e-4d9a-9c27-6cb9d6c3506a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	7142.79	8.93	48.35	2.84
8ca883c7-4fa2-4567-a602-b4d40bc43bb2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6364.88	8.89	35.26	2.84
6da19650-2ed3-45b9-8d42-372f47334f0b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O4S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	6757.43	8.99	31.85	2.84
fc6d8290-1e4b-4d37-8ca4-c69dc58eebff	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	6236.88	8.89	35.26	2.84
04e19c84-c5aa-4ca7-8ffe-3d8cc2518261	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	5923.53	8.93	33.74	2.83
a616ba19-1a75-4aa3-8fa6-bc565c139373	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C48H28O4S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	7077.27	8.9	35.29	2.83

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
12172464-83de-4234-8847-5e9eaccdc462	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	6816.7	8.89	39.83	2.82
9bee3372-1f84-414f-9064-c6e77ae43c32	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6164.98	8.89	30.09	2.82
b83be569-b610-414d-8eed-ce91fc50bce9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	5919.68	8.91	33.72	2.82
76ac77ea-31cd-45c0-8eb6-a3314837057d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	5795.57	8.94	27.3	2.82
bda8eed8-ad7f-46fa-83cb-3d93826aacb8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6161.13	8.87	30.07	2.81
21f3cbe2-3861-453b-95b0-792508fa0890	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7164.17	8.81	39.83	2.8
454a6954-b499-49e5-9822-9a92397f91f5	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	5683.36	8.95	27.07	2.8
df9f5487-7dfd-4aa9-8650-becf0c90ff10	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11117.2	8.97	60.78	2.8
3449c91e-33c7-4e1a-b386-843a443f5153	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6171.65	8.93	32.26	2.8
e8165d1b-d129-4753-9d1d-a355f32057c1	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	5791.73	8.91	27.28	2.8
5e023ca6-e819-46a3-af75-b0e9259f61fb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3(CH3))(CO2)2]8	0	4850.49	8.95	26.92	2.79
b8ea8b6b-4599-41b4-bde1-ce383b041941	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6212.81	8.95	39.98	2.79
cb1af04e-c636-4219-b5ee-3cf57802613f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3Br)(CO2)2]8	0	5369.45	8.95	26.92	2.79
f25af201-7502-4cc1-a794-eca7ce88b990	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3SO3)(CO2)2]8	0	5370.72	8.95	26.92	2.79
48e45f47-b393-4c15-a2c2-a2d6b3f60eb0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	5571.11	8.91	27.05	2.79
d7efdd3c-b721-4bc0-8048-70f83a68a54d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5202.91	8.96	26.92	2.79
edc6c882-85cb-48f0-be77-5ef96214f36a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6267.15	8.83	33.72	2.79
f79e9737-3d94-4b70-b7ab-81e9334edda6	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5090.7	8.95	26.92	2.79
a88c3749-be98-40cf-a8d4-159576a572cb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5178.72	8.95	26.92	2.79
aaa75d64-e2aa-448b-b444-6be580cb8fe6	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3CO2CH3(CO2)2]8	0	5202.57	8.92	26.9	2.79
b51e4a7d-e66a-40c9-828c-13bd18471db9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6068.38	8.92	26.88	2.79
dbb83da4-440c-4cfa-b4ae-f62c2ea40291	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	5298.65	8.92	26.89	2.79
c6423a36-00cf-4446-9805-e88f84104feb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3(NO2))(CO2)2]8	0	5098.26	8.95	26.92	2.79
00de1f4b-698a-478e-8b3d-279a2a36ce19	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5218.69	8.95	26.92	2.79
47545069-5119-4b21-8d39-ff54618c27d3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	6483.92	8.93	34.2	2.79
c6a8af33-eecf-445a-a7c3-903514267a4b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3NH2)(CO2)2]8	0	4858.4	8.95	26.92	2.79
20b5684f-5a89-49b5-928d-2e5534706577	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5187.12	8.96	26.92	2.79
a409d753-071b-45bc-a742-d27bf9008bba	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5170.66	8.95	26.92	2.79
1effed26-86f9-4986-87c0-77a9808882d5	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	5843.27	8.95	26.91	2.79
136c5bd7-094f-461b-b391-757dbeb46ce0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3SO3)(CO2)2]8	0	5366.88	8.93	26.88	2.78
232a9002-7e1c-4c14-9e11-571aa3a91aaa	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3(CH3))(CO2)2]8	0	4846.64	8.93	26.88	2.78
5b03b50b-cd55-4614-8795-8b2f4a03601b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	6508.6	8.78	32.21	2.78
e747a559-ce13-4819-8964-ce2ba7e435c0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6181.16	8.94	26.9	2.78
e4b550c0-8d7f-44ca-baff-8f085ca2ea90	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3Br)(CO2)2]8	0	5365.6	8.93	26.88	2.78
0978dd58-83fa-4368-94f3-265836660ed0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5086.85	8.93	26.88	2.78
ad2642a1-ff00-4c6d-a52b-b5c1ba049569	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	5567.26	8.88	27.03	2.78
04b4e3f2-944c-45b8-b2a5-e54e6b45054a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5199.06	8.93	26.88	2.78
6c57b5d4-1c1c-433d-b615-ffb0a294ab83	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6035.74	8.91	35.55	2.78
f09b15f8-703d-42e1-a576-64b6090e0dbd	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	5679.51	8.93	27.05	2.78
60d53b37-2907-42c9-aaa0-3b0a6d75336d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	5294.81	8.9	26.85	2.78
5c5a2d47-df4c-46a1-813c-9ea06c5c9850	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6064.53	8.89	26.84	2.78
a76c01fd-3a6b-4244-83f2-4abf140a814f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5174.87	8.93	26.88	2.78
911477ad-c167-44be-8607-c638fd8ab6c8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3(NO2))(CO2)2]8	0	5094.41	8.93	26.88	2.78
1f9da9c0-1b90-44e1-9f26-37f925e20299	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5214.85	8.93	26.88	2.78
4e4bdce5-d56e-49b8-b642-fa6520a7cabe	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3NH2)(CO2)2]8	0	4854.55	8.93	26.88	2.78
60ebf570-c0b5-4574-b787-629b5e87f367	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	5892.22	8.92	27.11	2.78
d394b939-1c08-41ce-9576-8b0a42463bd9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5183.28	8.93	26.88	2.78
ec39e82f-ef31-4ced-9175-a77bf2ae6564	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5166.81	8.93	26.88	2.78
fdc82daa-d61d-4e95-9e13-535ad7ca65e0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11113.35	8.94	60.77	2.78
7f80ff7e-389b-4c97-a71a-dbbf81a4e089	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	5315.12	8.92	26.88	2.78
d2b8f985-2c45-450a-8389-51fe9fc6e263	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6167.81	8.91	32.24	2.78
34e5751d-b0b2-4f83-83c2-61c08bc8c748	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6208.96	8.92	39.96	2.77

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
21692f36-5e99-4cda-b652-16642205e02a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3CO2CH3(CO2)2]8	0	5198.72	8.9	26.85	2.77
02196cd6-ce4c-456e-99c4-e72114a24766	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	6437.23	8.92	48.16	2.77
8c00edda-d7db-4174-bf63-84ac93a5d318	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	5659.32	8.91	26.88	2.77
f9053291-df9a-47ed-aea7-7dd130b942bb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	6480.07	8.91	34.18	2.77
14e79c66-f935-421c-8803-b0c81323b7dd	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	5839.42	8.92	26.87	2.77
30579e80-c8e5-43fa-9132-05bb70b12554	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	5531.32	8.91	26.88	2.77
503f084a-0640-4530-add7-5c6339d1305e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	5311.27	8.89	26.84	2.77
b0d19b68-9134-4b94-abd9-b93f77823e04	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6139.2	8.83	32.24	2.77
d97be55e-9b3e-4b1a-90a9-f14e64785ea3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	5427.33	8.91	26.89	2.77
3aabe34a-8c9f-46ad-ab76-56b1d47cb154	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6177.31	8.92	26.86	2.76
6ed21ec4-58a3-438d-9bca-a354e9e8d512	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6031.89	8.89	35.53	2.76
0a049fd4-369c-4d0b-93a9-ebc2e3dbfb2f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	5888.37	8.9	27.09	2.76
0d922a38-0965-4bc5-bbff-8f54d1a7d063	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	6433.38	8.89	48.14	2.76
b50fe756-6661-4f6f-a325-92d91c91d5b0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	11460.83	8.88	60.76	2.76
0fe719ec-4961-42d7-a9cc-dc38e67e5b33	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H12O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	6371.71	8.91	31.63	2.76
06b15a50-7999-47bf-b97a-a8b96891d5ef	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3SO3)(CO2)2]8	0	5714.35	8.84	32.26	2.75
ccf470f1-a4d6-4acf-bda6-49b54f14c6d7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3(CH3))(CO2)2]8	0	5194.12	8.84	32.26	2.75
c1d381bb-80fe-4452-9c60-fcbd19764046	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3Br)(CO2)2]8	0	5713.07	8.84	32.26	2.75
5edf6bf1-e349-44ce-81f3-42dac08bfc69	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	5914.74	8.8	32.21	2.75
d6885041-7011-48d6-a8da-32a0677cea68	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	5423.48	8.89	26.84	2.75
0d418434-0603-4f47-bf54-9ccba73f0a67	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3CO2CH3(CO2)2]8	0	5546.19	8.81	32.23	2.75
56f99ede-a996-4e6b-a8d1-016127ac116b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	5546.53	8.85	32.25	2.75
81c8187e-fa60-41f8-80f9-ce133eda075e	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6026.99	8.85	32.25	2.75
8df9e68d-07f1-4159-bdf4-533c76daf6e0	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5434.32	8.84	32.26	2.75
bd969362-3d5f-49b6-b455-06dfdc4a5038	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	5522.35	8.84	32.25	2.75
d0f3b81c-da93-4c34-9cdc-62b4dca8ed2b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	5642.28	8.81	32.23	2.75
e6268857-1f2a-4af1-88e8-76ddc95e9b8d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6412.01	8.81	32.21	2.75
6a73ee24-012c-4095-a73f-afc4ccf6228c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3(NO2))(CO2)2]8	0	5441.89	8.84	32.26	2.75
da6eae44-88bb-46e5-a56b-c747dead08d4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3NH2)(CO2)2]8	0	5202.02	8.84	32.26	2.75
60a3e478-d72b-4ed6-9711-02de8cb00ae9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	5562.32	8.84	32.25	2.75
45c01b83-8cf7-4ea9-a481-798ee198dae9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	5655.47	8.89	26.84	2.75
587f9aba-4125-45e8-b86e-d45f62d1ba9d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	5530.75	8.85	32.25	2.75
8f28a216-a105-46a8-a50b-5881abe42b2f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	5514.28	8.84	32.26	2.75
7452f159-2673-4c08-a911-0f7ffb2b82ee	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6186.89	8.84	32.24	2.75
a569846b-bf27-4959-ab9c-dba1e680b3e7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	6515.28	8.83	32.25	2.75
bc70f06b-f460-4c6f-90b4-fe627a9e9924	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	5527.47	8.89	26.84	2.75
0afba2d4-7837-4260-910b-2161444e733d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	6524.78	8.84	32.23	2.74
2849d7b7-f81f-4c9f-80c1-e8ed22b54775	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	6556.43	8.85	39.96	2.74
441c66ea-7a18-43e0-b0c0-a295fef80fee	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	6827.54	8.83	34.19	2.74
a9bb3c00-4201-45fa-8466-8bc8ed6782a3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	5658.74	8.81	32.22	2.74
e29ed1f3-253e-4ea5-9153-68183b4e7000	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C24H12O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	6367.86	8.89	31.61	2.74
dbe91f12-fd5c-429b-86e8-514cf96381af	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	5770.95	8.8	32.22	2.73
f8a13d9a-0650-4770-b756-cf92ba858922	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6379.36	8.81	35.53	2.73
172c8451-97ef-41a7-a859-a157bc6d183c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6002.94	8.8	32.21	2.73
8cdedc12-d645-4cab-91ef-aa1ebc80acb8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6235.85	8.82	32.23	2.73
97e1f2e9-d157-4bf7-8d4f-3c4983bc9266	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	6780.85	8.82	48.15	2.73
6c0e5848-b1d7-417f-9753-930aae90c67f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	5874.95	8.8	32.21	2.73
178f9e36-6d37-4a70-9d88-76196555801f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Mg4C40H44O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	6715.33	8.81	32.24	2.71
bf47e1b0-c040-4f08-aa10-61077c2679da	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	-16	8085.43	8.72	39.72	2.7
2b2bc298-3f24-4648-90b3-bb4053ba3227	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	-16	7188.41	8.74	33.56	2.69
65270415-e483-4833-9330-8ef5f4d0611f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3CH2CS3C4H9(CO2)2]8	-16	7429.86	8.7	29.95	2.68
81141fb7-c512-4e30-a732-dbd2af4b0222	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3(CH3))(CO2)2]8	0	5744.33	8.54	31.49	2.68

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
f7161bf0-3baa-49c5-b367-ebfe2b79f2b3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3N2C6H3(CH3)2(CO2)2]8	-16	7060.45	8.75	29.92	2.68
918c1f11-4f09-4d91-a846-4ff0583e700c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[(C6H3(CH3))(CO2)2]8	0	5851.48	8.53	31.45	2.67
304a020a-7384-48dc-8fb1-6fe5eccee70a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3NH2)(CO2)2]8	-16	6123.28	8.76	29.92	2.66
55cbad87-3205-4754-8bfc-102101b4af71	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	-16	12382.08	8.78	60.67	2.66
4a9f6a87-0084-4cf7-93c0-2d59062a2693	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3Br)(CO2)2]8	-16	6634.33	8.76	29.92	2.65
b5ca84c5-9395-403a-98a1-67a5151861e8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3(CH3))(CO2)2]8	-16	6115.37	8.76	29.92	2.65
0a41b4d4-8a80-4ea5-aa02-ce1776d6ea76	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	-16	6835.99	8.72	29.88	2.65
1757676c-7e0f-4565-9e1d-2e86bd53e283	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	-16	6948.24	8.76	29.92	2.65
93345b1e-7997-4b22-a9f3-056aa43f7c2f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OCH2CH3)(CO2)2]8	-16	6355.58	8.76	29.92	2.65
d14e4641-b05f-4e26-aca7-ae5c37a42ffc	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	-16	6467.79	8.77	29.92	2.65
3306ef05-d2b4-4931-8246-ce94afbb2fad	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3CO2CH3(CO2)2]8	-16	6467.45	8.73	29.9	2.65
e1cd0d60-eaf4-4fab-afb2-4ff19b98af54	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3(NO2))(CO2)2]8	-16	6363.14	8.76	29.92	2.65
48085b7b-849b-45a1-b22e-5ece125c012c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H2O)(CH2CHCH2)(CO2)2]8	-16	6443.6	8.77	29.92	2.65
98c97a1f-5ad2-4038-946e-f15712981018	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	-16	7333.26	8.73	29.89	2.65
8c081c6d-1767-468a-9e15-85ba4075833a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3OCOCHCH2(CO2)2]8	-16	6563.53	8.73	29.89	2.65
404e6fa0-591b-40b6-8697-fa1edc6bc242	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OC2H4OH)(CO2)2]8	-16	6483.57	8.77	29.92	2.65
90230e86-3784-4ea4-936e-c439256594b4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OCH2C2H)(CO2)2]8	-16	6435.54	8.76	29.92	2.65
8b5e050d-3200-4cc0-9401-461c0992b15f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[((C6H3)C(CH3)3)(CO2)2]8	-16	6452	8.77	29.92	2.65
02527590-024f-4170-9cc1-e24ba3163fc9	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3SO3)(CO2)2]8	-16	6635.6	8.76	29.92	2.65
41964391-30ae-4797-9a71-f03b170f05a5	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	-16	7108.15	8.76	29.91	2.65
9ca0436c-14bd-4b3c-a1f1-1f857ab746f4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	-16	7436.53	8.74	32.12	2.65
4994cabe-a6e1-49c3-9053-c9f44f9ea683	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)O(CH2)11CH3(CO2)2]8	-16	7477.69	8.76	39.83	2.64
608373c7-dd21-40b8-8f9a-319e6297c4db	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3C2Si(C3H7)3(CO2)2]8	-16	7446.04	8.75	29.9	2.64
f21dc008-821b-42bc-81cc-b6b2cffebd62	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	-16	7300.62	8.72	35.37	2.64
3e8a01be-2e19-41f4-b9b7-d68f6b8f1f5f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3NH2)(CO2)2]8	0	5752.24	8.54	31.49	2.64
9be03fff-07ca-4a6f-9ca6-8877e08bf9b8	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	-16	7748.8	8.74	34.07	2.64
19570eb7-f6df-4832-bf62-f4373e9f3769	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)O(CH2)3CH3(CO2)2]8	-16	6580	8.73	29.89	2.64
cb445570-24f2-4785-92fd-0d866d8244d1	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)O(CH2)4CH3(CO2)2]8	-16	6692.21	8.72	29.89	2.63
3e0660b2-0c20-49fa-a58d-2eb2537fd69f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[(C6H3NH2)(CO2)2]8	0	5859.38	8.53	31.45	2.63
62546655-cdf3-4dff-b9d5-247e7e562783	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	-16	7157.1	8.73	29.9	2.63
6f853735-3222-47cf-86d1-5a605df29434	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)O(CH2)13CH3(CO2)2]8	-16	7702.11	8.73	48.04	2.63
dc07d72e-572d-45df-98af-2084221b681b	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[C6H3NHCO2C(CH3)3(CO2)2]8	-16	6924.2	8.72	29.88	2.63
7def8f3e-9007-45e2-8664-03a2fa02195a	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)NHCOC(CH3)3(CO2)2]8	-16	6796.2	8.72	29.88	2.63
1d4e3707-9be4-461b-9388-a81c38ba6d74	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Co4C24H8O24S8]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	-16	7636.59	8.72	31.49	2.62
8e4e459b-9d2e-4e92-a283-5bad4546d9b3	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[((C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7714.39	8.49	39.54	2.53
91e15d85-89ff-432d-8e4a-5c5928aa8b4f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6817.37	8.52	33.31	2.53
23baa8d0-f4bb-4fd8-b923-afb2492b0d64	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[C6H3CH2CS3C4H9(CO2)2]8	0	7058.82	8.47	31.46	2.52
9b0e1a38-ac40-4287-aeb1-753a13b2449d	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[((C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7821.53	8.47	39.53	2.52
db5a0c9f-8d5c-431b-9de4-28ad0aee5c8f	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	7165.96	8.46	31.42	2.51
3c6f7c0c-a71c-4e68-bfaa-d410386138e7	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6924.51	8.5	33.3	2.51
c263e2eb-f30e-4d63-aadf-c75447ea2641	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6689.41	8.52	31.49	2.51
610fd487-aaaf-4808-a8cc-9be968aea621	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Zn4C40H44O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6796.56	8.51	31.45	2.5
18c2134f-0a26-4602-9bdc-1447097d5beb	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3Br)(CO2)2]8	0	6263.29	8.54	31.49	2.49
ab0614e8-2220-490e-a03a-2b36b248862c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3SO3)(CO2)2]8	0	6264.56	8.54	31.49	2.49
e4112085-c303-4456-a1dd-93be41eb4294	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6464.95	8.49	31.46	2.49
2998f839-6d2f-43cf-9b57-3d7e45853f86	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6096.75	8.54	31.49	2.49
2f6b6a4f-6aab-4435-9cc0-b89cc58f4128	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[((C6H3)(N2(C6H4CH3))(CO2)2]8	0	6577.2	8.54	31.49	2.49
a8d308dc-2246-4007-a53d-87e8809dd4c4	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5984.54	8.54	31.49	2.49
72918148-cbfb-49fd-b567-6d802b7db15c	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6072.56	8.54	31.49	2.49
75e2f13d-219a-4a4d-90f4-059ff7d15946	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[((C6H3)CH2CS2(C6H5)(CO2)2]8	0	6962.22	8.5	31.46	2.49
91e14889-66d5-41f0-9b12-be456b1ade83	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[C6H3OCOCHCH2(CO2)2]8	0	6192.49	8.51	31.47	2.49
979dc45e-c73f-4df4-a040-7f79a4b3a999	(4–pyramidal)$_4$(2–bent)$_8$_D$_{4h}$	[Ni4C40H44S4O12]4[((C6H3(NO2))(CO2)2]8	0	5992.1	8.54	31.49	2.49

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
5f3a2a48-7c3e-4ce3-a2eb-d916d50bf0c1	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[((C6H3)C(CH3)3)(CO2)2]8	0	6080.96	8.54	31.49	2.49
aec0cf90-f368-4823-93c5-702c0d135d82	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OC2H4OH)(CO2)2]8	0	6112.53	8.54	31.49	2.49
dfc71108-3445-4892-aae8-ed34c6b7d04b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6064.5	8.54	31.49	2.49
9c18057a-ea3f-4184-9e39-dc198c18fec3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12011.04	8.54	60.52	2.49
7d16ead4-1971-43b6-827a-fbeb80b32aeb	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7065.49	8.51	31.91	2.49
71fabde5-8032-46e5-9bc0-97992f3f5bae	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3Br)(CO2)2]8	0	6370.43	8.53	31.45	2.48
6b0c0e59-7790-4ba3-9e03-86db27af799d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	7106.65	8.53	39.63	2.48
72d2428f-2a1d-44f3-8c6c-f9b0393bca3f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3SO3)(CO2)2]8	0	6371.71	8.53	31.45	2.48
6f2e029c-c533-4f89-a63b-96e4cbd5ac9b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	6091.68	8.53	31.45	2.48
983633dd-6318-48f0-8893-706b6cbf4c76	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6572.1	8.48	31.41	2.48
d3d4250d-29ab-47a0-9f16-d73776a03716	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6203.89	8.53	31.45	2.48
4376ae09-4683-43d0-99d3-4e90a081c21b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)N2(C6H4CH3))(CO2)2]8	0	6684.35	8.53	31.45	2.48
16c909ac-1eef-4c13-bf47-ce38ea49be8c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6179.71	8.53	31.45	2.48
2690d5a9-aad7-4a46-aac5-9c0859e5faaf	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	6299.64	8.49	31.42	2.48
e2988e6c-cb66-4e38-b863-846eba9e6ba1	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	7069.37	8.49	31.42	2.48
fcacc268-6efa-49e5-882a-bb9b66077112	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[C6H3CO2CH3(CO2)2]8	0	6096.41	8.51	31.47	2.48
9234f073-e3ea-4a22-94c9-888c6b9a7c06	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3(NO2))(CO2)2]8	0	6099.25	8.53	31.45	2.48
4c5012f2-e2a0-4f6c-96ac-ba8d65f2e836	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	7377.76	8.51	33.87	2.48
9e75eac7-163e-47d4-972e-559130ea77c7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	6219.68	8.53	31.45	2.48
998af7a3-5df5-47e8-9aef-54c2dd7ae0bc	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6171.64	8.53	31.45	2.48
af5a6b7d-8617-4c46-92d5-52a96bed96e7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	6188.11	8.53	31.45	2.48
a4f71d09-9864-4334-bf14-c6c2b596c808	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12118.19	8.52	60.51	2.48
2b35c4b2-42fc-4e6b-ba26-711dfaf462e9	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	6208.96	8.5	31.46	2.48
4439f5f9-9144-4f7f-b5ad-2d2b8ce2b574	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6737.11	8.53	31.49	2.48
c7a97273-20e1-4466-912a-561a4a8ca921	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7172.64	8.5	31.9	2.48
c766725f-df06-40ac-8b92-da4dc305749c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7075	8.52	31.48	2.47
d6972f23-bfcb-448a-bc01-da5818e0db6c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	7213.79	8.51	39.62	2.47
5b924e46-e54e-4475-949e-3e8165784de5	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6929.58	8.5	35.12	2.47
71be927b-ac8a-49c3-93db-7a7e6194f909	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[C6H3CO2CH3(CO2)2]8	0	6203.55	8.49	31.43	2.47
b78a7afb-c647-4850-b18e-6df963014c47	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	7331.07	8.5	47.87	2.47
bb77420c-f427-4340-9ae7-c1608011e4f2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	7484.9	8.5	33.86	2.47
f65105f1-7108-4f4e-a4d1-af0451b1f302	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6786.06	8.51	31.47	2.47
20583e67-3304-4c5e-9ede-8733e43d9b30	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6844.25	8.52	31.45	2.47
92af9cef-692c-4a24-b74e-0866e7b4678a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7182.14	8.51	31.44	2.46
4500393b-5a67-4698-b9b7-ebd2b83c5873	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	6321.17	8.49	31.46	2.46
71482eea-a5f3-4316-be1e-f18c18da778c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	7036.72	8.48	35.11	2.46
8ba39c2b-04ab-483f-baf0-c361385e46fe	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6893.21	8.49	31.43	2.46
a8e0b2fc-c50c-4b04-95cc-6a152768b2fa	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6553.16	8.49	31.46	2.46
6794f4c1-b7ad-465f-8243-931f03618aa3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	6316.1	8.49	31.42	2.46
f2defd5b-7235-4bb8-907a-d858d8d49154	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	6425.16	8.49	31.46	2.46
faab29dc-ec54-4d69-98a5-ab819c2c7185	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	6428.31	8.48	31.42	2.45
a4d57914-d751-4c99-8907-4cea076aa8c4	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	7438.21	8.48	47.86	2.45
556e791f-a21a-4d94-86c1-ed87d9b29d3d	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6660.3	8.48	31.41	2.45
0ad2849c-a372-4856-ba4a-09d033d47b8c	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	6532.31	8.48	31.42	2.45
12b94e3a-5823-43e5-85c6-3f62523fa95e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Ni4C40H44S4O12]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	7265.55	8.5	31.49	2.45
d8edc269-e631-44cd-865b-fff42f46539b	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Zn4C40H44O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	7372.69	8.48	31.45	2.44
84847434-1aa2-4e91-94bc-d2d0ce5752da	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3(CH3))(CO2)2]8	0	5748.17	7.8	31.42	2.21
e3cf0b44-f259-4b0f-85e3-3ab91de7533e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3NH2)(CO2)2]8	0	5756.08	7.8	31.42	2.14
569096b4-a500-473d-8164-23bd36291194	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7718.23	7.74	39.04	2.05
31f2494b-7f14-43b5-9b0a-340d9af0457a	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OC2H4)3(OH)(CO2)2]8	0	6821.21	7.77	32.62	2.05
6794980b-3c65-4ca2-8e8e-1f8a666ad098	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3CH2CS3C4H9(CO2)2]8	0	7062.66	7.73	31.39	2.04
60a7406a-9a00-427a-a441-fab60f5af304	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H2O)(CH2CHCH2)(CO2)2]8	0	6076.4	7.8	31.42	2.03

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
611aa697-85ed-46b0-952d-713e75a9d558	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3N2C6H3(CH3)2(CO2)2]8	0	6693.25	7.77	31.42	2.03
0980b395-b45e-48de-bc5d-0a214af420e7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3Br)(CO2)2]8	0	6267.13	7.8	31.42	2.01
34293b37-2cce-49bd-a305-40a69d077f95	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6581.04	7.79	31.42	2.01
3ca9a2f8-d86e-40de-a5c8-f1062bbe4969	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6100.59	7.8	31.42	2.01
a176f3ad-146b-4c78-830d-4174107d60df	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6468.79	7.74	31.38	2.01
ebcc31d4-6f34-4fac-96a0-48ff35798a5e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5988.38	7.8	31.42	2.01
9b8ea20b-9b05-48ce-9d7c-eef13a08ce7f	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3(NO2))(CO2)2]8	0	5995.94	7.8	31.42	2.01
d76ee113-a16d-4e02-988d-71eac2dbf6cf	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6966.06	7.75	31.39	2.01
d83df500-d27f-473b-b924-c4bf114b9c64	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3OCOCHCH2(CO2)2]8	0	6196.33	7.76	31.39	2.01
3c88ab7d-d630-4256-b179-14d5cdf471aa	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)C6H2(OC16H33)3(CO2)2]8	0	12014.88	7.79	60.09	2.01
afd013ec-2d1d-43a7-aacc-ddacffc4cbe6	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OC2H4OH)(CO2)2]8	0	6116.37	7.8	31.42	2.01
60123ba4-1ab3-4d24-9612-f584b5505ac3	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[((C6H3)C(CH3)3)(CO2)2]8	0	6084.8	7.8	31.42	2.01
4f22f8dc-60d1-4875-b52c-3dbc020133e7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OCH2C2H)(CO2)2]8	0	6068.34	7.8	31.42	2.01
22387da0-05fe-40ba-9e3c-cc12fa7bc792	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3SO3)(CO2)2]8	0	6268.4	7.8	31.42	2.01
fa01491c-36a4-4c0a-b78b-88cbdcd08fd4	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	0	7069.33	7.77	31.41	2.01
8e62fa5a-dec7-46ef-a195-9d97f6f4cfe2	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)O(CH2)11CH3(CO2)2]8	0	7110.49	7.78	39.07	2
cc2e2e30-4dec-402b-b403-2e9ad264ec10	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3CO2CH3(CO2)2]8	0	6100.25	7.76	31.4	2
3210f2cc-b48b-4b6d-ace0-f014659a697e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)((C3H6O2)(C9H5O2))(CO2)2]8	0	7381.6	7.77	33.34	2
a920d17e-0ecb-4fa3-9ef0-e816b7352438	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(CH2)(C4N2H2O2CH3)(CO2)2]8	0	6740.95	7.78	31.41	2
dea37fb3-4575-4006-b886-129b1ac4dae1	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3C2Si(C3H7)3(CO2)2]8	0	7078.84	7.77	31.41	1.99
17206358-0bbf-455e-8b7e-6101af658ea7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)(OC2H4)3(OCH3)(CO2)2]8	0	6933.42	7.75	34.42	1.99
ffdab926-bf9f-422a-9a5b-0ff724842967	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3CO2C2H4Si(CH3)3(CO2)2]8	0	6789.9	7.76	31.4	1.99
ef9f9801-808a-4e09-8010-50a6f44034d7	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)O(CH2)3CH3(CO2)2]8	0	6212.8	7.76	31.39	1.99
bb2bf47e-0bfc-40ec-8c79-824787bf779e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)O(CH2)4CH3(CO2)2]8	0	6325.01	7.75	31.39	1.98
482b24e3-4b93-4221-b902-d782322af9ed	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)O(CH2)13CH3(CO2)2]8	0	7334.91	7.75	47.41	1.98
6dbecf6f-cb5e-442f-ae82-4e0e4556cd3e	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[C6H3NHCO2C(CH3)3(CO2)2]8	0	6557	7.74	31.38	1.98
0283cd73-a838-4f79-9829-5ee727d2d649	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)NHCOC(CH3)3(CO2)2]8	0	6429	7.75	31.39	1.98
d7466a81-bd09-4314-ab30-000284fc4727	$(4\text{–pyramidal})_4(2\text{–bent})_8\_D_{4h}$	[Co4C40H44O12S4]4[(C6H3)((C2H4O2)(C9H5O2))(CO2)2]8	0	7269.39	7.75	31.42	1.97
4f26e7a2-24bf-4f28-9fb3-672e9eafcd9f	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V5O9]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	-6	9321.74	21.97	42.65	11.49
69394669-dca9-4a24-b5d3-99fac5ed2a1e	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	8920.09	21.38	39.06	11.15
4a74f863-9b8f-4ad2-bfd9-82c2f4eef614	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	13929.53	20.43	53.19	10.66
d8732ac5-26a1-4928-b83d-b37a72164ee0	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Fe4C40H44S4O4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	12571.98	20.32	52.63	10.58
f8069cab-7057-4468-8efe-dd3217e6b963	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C56H76O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	14760.66	20.26	52.8	10.57
7f2547f0-b4ea-442f-8609-de170e6c4fbf	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C56H76O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	14754.85	20.24	52.75	10.56
90dc4ca8-b819-4a10-9d7f-6cb9bf70f52d	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O4S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	12646.14	20.26	52.47	10.54
4d4b9f44-db3e-4321-8f71-034c71ea6ed1	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C48H28O4S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	13125.9	20.21	55.89	10.5
abaeec66-9bff-4da3-b105-4381643d19a0	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H12O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	12067.56	20.11	47.99	10.44
82ea5975-4501-4f57-ac7d-881c2bc55bc3	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C24H12O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	12061.79	20.09	47.94	10.42
cb35d857-3c7e-4c18-8d0e-052b8561fff0	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C40H44O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	12583	19.97	53.49	10.38
a7f8615d-e880-405a-be61-22241231dddd	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H8O24S8]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	-24	13964.88	19.87	51.06	10.29
e127cbb9-2b7e-4ffa-bdc0-c51257b04c8e	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C40H44S4O12]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	13408.32	19.57	51.96	10.12
e56026fd-115f-4cde-a9f3-302065542340	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Zn4C40H44O12S4]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12	0	13569.04	19.55	51.91	10.11
97c771e2-f3ca-47ea-85c3-9384a2fc8b2f	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V5O9]6[(C8H8)(C6H4)2(CO2)2]12	-6	6525.02	17.6	36.82	9.78
1a2e9246-6408-4ada-81d0-23f2b9bab4fa	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C8H8)(C6H4)2(CO2)2]12	0	6123.37	17.02	33.36	9.44
89700465-04e5-403f-9ece-4f10da9801a5	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V5O9]6[(C6H4N)2(CO2)2]12	-6	5611.1	21.41	34.25	9.26
9a078635-33be-4179-b687-0ccb67012b2f	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C6H4N)2(CO2)2]12	0	5209.45	20.83	30.85	8.96
c777c9ad-aab2-4492-bbb8-b5c874bd465b	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	11132.81	16.07	47.43	8.92
7518fb1f-3c02-4821-ba5b-68ce31a179be	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Fe4C40H44S4O4]6[(C8H8)(C6H4)2(CO2)2]12	0	9775.26	15.98	46.97	8.85
afd65214-3481-4bf0-9a85-e1d614431c47	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C56H76O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	11963.94	15.91	47.04	8.83
41455d2b-ccfb-4ab8-a22b-04234c5b7ec8	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C56H76O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	11958.13	15.88	46.99	8.81
d1cd50e4-edbe-496e-8914-8be824c4422f	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O4S4]6[(C8H8)(C6H4)2(CO2)2]12	0	9849.42	15.91	46.81	8.81
12bc8f29-50d1-4fd3-acc5-3fe60181b16d	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C48H28O4S4]6[(C8H8)(C6H4)2(CO2)2]12	0	10329.18	15.88	50.24	8.78

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Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
59932b68-4c41-47e7-b314-04b7a5b4477a	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H12O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	9270.84	15.76	42.29	8.71
d6e0e506-e957-44f7-b54a-6f6c3ba965c8	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C24H12O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	9265.07	15.73	42.24	8.69
88501790-da11-41e4-a441-2124bdd42153	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C40H44O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	9786.28	15.63	47.71	8.66
4214199c-7336-4ce9-84d7-1d94d084926e	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H8O24S8]6[(C8H8)(C6H4)2(CO2)2]12	-24	11168.16	15.52	45.32	8.57
eec819b5-e8ff-4e4d-88ab-c0a56c64d4cf	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C6H4N)2(CO2)2]12	0	10218.89	19.83	44.92	8.53
eb7b0325-af96-4d0d-8930-2fd84afe9491	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Fe4C40H44S4O4]6[(C6H4N)2(CO2)2]12	0	8861.34	19.74	44.5	8.46
a4439fd5-7adc-422c-be47-0c92bb442847	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C56H76O12S4]6[(C6H4N)2(CO2)2]12	0	11050.02	19.66	44.53	8.45
02d9c8ea-460d-4b88-be04-a7396ea0f1b9	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C56H76O12S4]6[(C6H4N)2(CO2)2]12	0	11044.21	19.64	44.48	8.43
32f68f31-491e-48af-be8a-019705df4e4c	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O4S4]6[(C6H4N)2(CO2)2]12	0	8935.5	19.67	44.35	8.42
b779cc44-7412-4fe7-90d8-47b6a9306cb8	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C40H44S4O12]6[(C8H8)(C6H4)2(CO2)2]12	0	10611.6	15.21	46.31	8.39
8a53ba23-165c-41ec-bbab-aeea729e7973	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C48H28O4S4]6[(C6H4N)2(CO2)2]12	0	9415.26	19.64	47.8	8.38
ed0a09e3-67e7-45b4-b097-dc9fbe4f16d8	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Zn4C40H44O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	10772.32	15.19	46.26	8.38
fe15e3e1-815b-4afc-899a-00f8166e0d66	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H12O12S4]6[(C6H4N)2(CO2)2]12	0	8356.92	19.54	39.8	8.33
b413a8b9-709e-4693-ab36-a5ddc92a1f05	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C24H12O12S4]6[(C6H4N)2(CO2)2]12	0	8351.15	19.52	39.74	8.31
c0986d30-17dc-4a8a-8065-0340e3fd3b11	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C40H44O12S4]6[(C6H4N)2(CO2)2]12	0	8872.36	19.38	45.23	8.27
80f13a6a-fb15-45cd-ae69-58104ac02007	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H8O24S8]6[(C6H4N)2(CO2)2]12	-24	10254.24	19.3	42.81	8.2
0dad802c-5b4a-4baf-a39a-96e130e533f0	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C40H44S4O12]6[(C6H4N)2(CO2)2]12	0	9697.68	19	43.85	8.05
80ce05a8-1b18-4fbe-9440-e823e1f81da2	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Zn4C40H44O12S4]6[(C6H4N)2(CO2)2]12	0	9858.4	18.98	43.8	8.04
e1eb9f40-c12f-4dbd-b138-78f178131661	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	10617.36	14.24	45.92	7.84
4982f707-19bf-4fa8-ba7d-527019681baa	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O12S4]6[(C6H4N)2(CO2)2]12	0	9703.44	18.03	43.46	7.58
50784e79-2315-4ab9-9e57-ddd8a19d6789	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V5O9]6[(C14H8)(C6H4)2(CO2)2]12	-6	7389.02	15.73	37	6.79
2285aa8d-85da-41b8-a76f-230cbb6db655	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C14H8)(C6H4)2(CO2)2]12	0	6987.37	15.15	33.54	6.46
a9de1c09-7cef-4445-8177-fed2bca00944	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11996.81	14.29	47.58	6
4f2982c9-9d46-4842-a15d-238d42b344d7	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Fe4C40H44S4O4]6[(C14H8)(C6H4)2(CO2)2]12	0	10639.26	14.18	47.12	5.92
a8efdb74-4a9c-45b0-ad97-76c059377c03	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C56H76O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	12827.94	14.13	47.19	5.91
12edcdbf-e0d6-4587-8fe0-4e194e8d70c9	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C56H76O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	12822.13	14.1	47.14	5.9
b7012e51-1b7d-4178-a55b-3314e5335e4a	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O4S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10713.42	14.11	46.97	5.89
c9a5e1ea-b848-4ebf-9a6f-7f8e28d7dc71	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C48H28O4S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11193.18	14.07	50.4	5.84
66494e67-a3b8-479f-b35b-5119bae7d755	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H12O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10134.84	13.93	42.45	5.78
89791dd5-c463-4542-875b-29d6c1d899bc	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C24H12O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10129.07	13.91	42.4	5.77
b715238e-1bd9-4ff7-9582-a115471cd2a2	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10650.28	13.87	47.85	5.73
adc3138f-775f-4fe6-b182-fc1602948eba	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H8O24S8]6[(C14H8)(C6H4)2(CO2)2]12	-24	12032.16	13.71	45.48	5.65
09b3a394-c3b0-49ac-a001-c61c41caaa93	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C40H44S4O12]6[(C14H8)(C6H4)2(CO2)2]12	0	11475.6	13.42	46.47	5.48
a5b4c153-750f-4ff6-8d2c-ca8f80627e49	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Zn4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11636.32	13.4	46.42	5.47
3931be65-9841-4194-b0e0-0569f0edfd55	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11481.36	12.47	46.08	4.97
144f304f-39b0-4f59-a927-3b85fa426520	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V5O9]6[(C10H6)(C6H4)2(CO2)2]12	-6	6789.02	17.81	37.13	4.6
97f6a41c-d98d-4514-8575-5028875f84f3	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C10H6)(C6H4)2(CO2)2]12	0	6387.37	17.25	33.68	4.29
d72f5cf4-627c-481e-b4f1-5df19b7e5642	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	11396.81	16.47	47.68	3.84
38622766-7769-4924-9d24-7f7e0b88f0f8	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Fe4C40H44S4O4]6[(C10H6)(C6H4)2(CO2)2]12	0	10039.26	16.36	47.23	3.77
199031bb-b99a-4a61-b41d-6913a7dd2c84	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C56H76O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	12227.94	16.32	47.29	3.75
0c804e03-ec30-4bc8-8f81-a7309e4ec9e5	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C56H76O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	12222.13	16.29	47.24	3.74
19915f07-9519-44f4-8aac-d8abcadfb25c	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O4S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10113.42	16.3	47.07	3.74
9220284b-25fc-475f-af59-31f0c08c0cca	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C48H28O4S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10593.18	16.25	50.5	3.7
dab29577-118c-41c3-a473-71a5770b542e	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H12O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	9534.84	16.1	42.55	3.64
d7a27b5b-6234-4ff9-bcc8-adf7b5ccba13	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C24H12O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	9529.07	16.07	42.5	3.63
f1f11162-3f7d-47fe-a776-32ac4111bd65	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C40H44O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10050.28	16.09	47.94	3.61
89729dea-cba1-4650-826b-634656dfd206	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C24H8O24S8]6[(C10H6)(C6H4)2(CO2)2]12	-24	11432.16	15.89	45.58	3.52
0b4ee1be-a498-4476-a088-76c79540e3a4	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Ni4C40H44S4O12]6[(C10H6)(C6H4)2(CO2)2]12	0	10875.6	15.62	46.57	3.37
7f18e406-1993-4935-a410-800b53a94582	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Zn4C40H44O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	11036.32	15.6	46.52	3.36
bbee264b-40d7-44f4-be23-af9956c6d6db	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Co4C40H44O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10881.36	14.7	46.18	2.91
2e1a7758-473b-47e6-9925-ec6024e4d702	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[V4O8]6[(C14H8)(CO2)2]12	0	5161.57	6.97	24.9	2.74
be5f6046-c68f-4048-bd5f-eeb0eaf9a2bb	$(4\text{–pyramidal})_6(2\text{–linear})_{12}\_O_h$	[Mg4C56H76O12S4]6[(C14H8)(CO2)2]12	0	10171.01	6.06	35.72	2.24

Continued

Table S4: *(Continued)*

MOP Partial IRI[1]	Assembly Model	MOP Formula[2]	Charge (e^-)	Molar Mass (g/mol)	Cavity Dia. (Å)	Outer Dia. (Å)	Max Pore Dia. (Å)
1b582eab-d686-4846-a54d-34bc523b7320	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Fe4C40H44S4O4]6[(C14H8)(CO2)2]12	0	8813.46	5.98	35.49	2.17
a4455a87-cf34-427c-a8ee-f7716e8652a5	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C56H76O12S4]6[(C14H8)(CO2)2]12	0	11002.14	5.91	35.33	2.15
aee563f6-3cfa-46cf-92bf-05037ec047b5	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Ni4C56H76O12S4]6[(C14H8)(CO2)2]12	0	10996.33	5.89	35.28	2.14
a8451939-13bd-4e7a-be72-5f69c4738623	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C40H44O4S4]6[(C14H8)(CO2)2]12	0	8887.62	5.92	35.34	2.14
5b6092cf-3a43-45ea-9f6d-91980f91d438	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C48H28O4S4]6[(C14H8)(CO2)2]12	0	9367.38	5.89	38.9	2.1
5f97331b-dea6-48f6-9116-f7648ca6988e	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C24H12O12S4]6[(C14H8)(CO2)2]12	0	8309.04	5.8	30.74	2.04
f85fa25d-aa4d-4355-8dc0-0ba322e2ca59	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Ni4C24H12O12S4]6[(C14H8)(CO2)2]12	0	8303.27	5.78	30.69	2.03
4bc8abe4-bf6b-42fd-b089-9974f51eb443	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Mg4C40H44O12S4]6[(C14H8)(CO2)2]12	0	8824.48	5.65	36.04	2
4c14ecfc-dbae-466a-b086-92a0c0545ba0	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C24H8O24S8]6[(C14H8)(CO2)2]12	-24	10206.36	5.58	33.69	1.91
ac77719e-9529-4938-93a2-5502b8dc7c88	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Ni4C40H44S4O12]6[(C14H8)(CO2)2]12	0	9649.8	5.31	34.96	1.74
b595104a-c0f8-4975-842e-71b57436c05f	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Zn4C40H44O12S4]6[(C14H8)(CO2)2]12	0	9810.52	5.29	34.91	1.73
e0a5de71-b159-4854-9222-ad1ec8adf9be	(4–pyramidal)$_6$(2–linear)$_{12}$_O$_h$	[Co4C40H44O12S4]6[(C14H8)(CO2)2]12	0	9655.56	4.46	34.58	1.24
5ea714af-9c55-403f-86e2-6cbfb6416c0d	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]30	-12	24698.3	40.11	57.84	12.3
dc398d5a-964f-4a68-8079-3bbc8d21beec	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]30	0	23103.52	40.07	57.83	12.27
f0b01b35-63aa-4d61-9af4-64d18b28ee3d	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C8H8)(C6H4)2(CO2)2]30	-12	17706.5	33.4	49.98	11.13
a0a50a47-3468-403b-a103-aeaf7f975031	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C8H8)(C6H4)2(CO2)2]30	0	16111.72	33.37	49.97	11.11
743da282-c399-4ac2-8857-9373c3a7a2b2	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C6H4N)2(CO2)2]30	0	13826.92	35.64	46.54	9.05
2dda2130-6733-46f9-a974-6c6b90eb4c69	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C6H4N)2(CO2)2]30	-12	15421.7	35.68	46.55	9.05
6aac6d83-befa-4d0a-b42c-eb761da3d864	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C14H8)(C6H4)2(CO2)2]30	-12	19866.5	31.11	50.18	8.43
bd66d7b5-2f3e-4dab-9267-f68ed5855f86	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C14H8)(C6H4)2(CO2)2]30	0	18271.72	31.07	50.18	8.41
d0df0b36-15a5-4a1f-9b5e-5e693737d581	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C10H6)(C6H4)2(CO2)2]30	-12	18366.5	32.25	50.29	6.34
82bbf0b7-4e81-4c80-9548-ec898ec78d58	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C10H6)(C6H4)2(CO2)2]30	0	16771.72	32.22	50.29	6.31
bd932909-9a2b-4fc2-93ab-0178d701703b	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[WV5O11]12[(C14H8)(CO2)2]30	-12	15302	17.67	35.99	4.57
175d1159-6abc-48d9-a9e3-9e7821a4a410	(5–pyramidal)$_{12}$(2–linear)$_{30}$_I$_h$	[V6O11]12[(C14H8)(CO2)2]30	0	13707.22	17.63	35.95	4.56

[1] *The complete IRI for all of the MOPs starts with* `https://www.theworldavatar.com/kg/ontomops/MetalOrganicPolyhedron_`

[2] *The MOP formulae are written in plain text format*

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