

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

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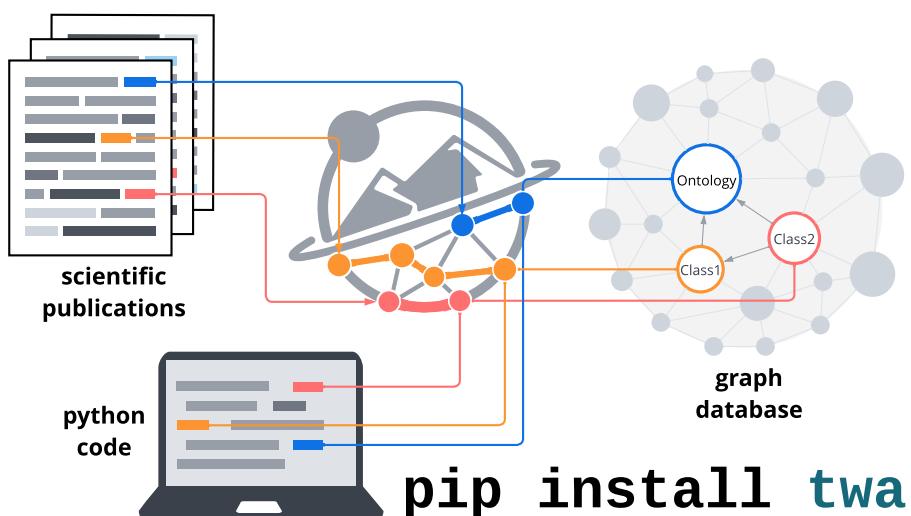
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Abstract

Data-driven discovery is crucial in scientific domains, yet the lack of standardised data management hinders reproducibility. In chemical science, this is exacerbated by fragmented data formats. The World Avatar (TWA) addresses these challenges *via* a dynamic knowledge graph historically provided in Java-based toolkits. We present `twa`, an open-source Python package that lowers the barrier to semantic data management. Its object-graph mapper (OGM) synchronises Python class hierarchies with RDF knowledge graphs, streamlining ontology-driven data integration and automated workflows. We demonstrate `twa`'s capacity to unify fragmented chemical data and accelerate research through use cases in molecular design and AI-assisted synthesis protocol extraction for metal-organic polyhedra (MOPs). Our approach expands the existing OntoMOPs knowledge graph by adding 799 new MOPs derived from combinatorial assembly models. By abstracting complex SPARQL queries behind a user-friendly interface, `twa` fosters transparent, reproducible knowledge-driven discovery. The package is freely available *via* pip install `twa` or <https://pypi.org/project/twa/>.



Highlights

- Introduced `twa` Python package for democratising dynamic knowledge graphs.
- Developed OGM to automatically synchronise Python objects with RDF graphs.
- Automated design and geometry assembly of metal-organic polyhedra.
- Integrated LLMs for streamlined MOP synthesis protocol extraction.
- Enabled reusable, ontology-driven workflows for AI-assisted cheminformatics.

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1 Introduction

Modern scientific and industrial domains generate digital data at an unprecedented scale, yet interoperability remains hampered by fragmented formats and siloed architectures [39]. These barriers limit data integration and reuse, undermining the potential of cross-domain collaboration. To address this, semantic web technologies systematise data into machine-readable formats that encode conceptual relationships, thus enabling cross-disciplinary interoperability [7]. A core manifestation of the semantic web is the knowledge graph, which has become indispensable for scientific and industrial innovation, due to its ability to harmonise and automate data workflows [21, 42].

A field that stands to benefit significantly from such innovation is chemistry, where researchers handle complex information on molecular structures, reaction pathways, and experimental protocols. Ontologies offer a powerful framework for encoding these data in a formal and computationally interpretable manner [29, 54]. Through adherence to semantic web standards, chemists can unify and automate disparate workflows, ultimately accelerating discovery [6, 30]. Despite the evident value of this approach, chemistry ontologies remain underutilised [29]. Many researchers find them challenging to maintain and extend, given the delicate balance between stability and adaptability that is essential for effective knowledge representation [13, 45].

Managing the evolution of ontologies requires robust version control, comprehensive documentation, and consistent input from domain experts. While some software solutions and collaborative workflows support these needs [38, 46], they are typically designed for expert programmers and require substantial knowledge of ontologies. This is particularly acute in AI-driven chemistry, where ontologies have immense potential to unify complex data but have seen limited adoption [4, 23]. As a result, user-friendly tools in widely adopted languages such as Python are sorely needed to lower entry barriers for non-experts, ensuring transparency, reproducibility, and broader adoption.

Over the past decade, object graph mappers (OGMs) have evolved from object-relational mappers (ORMs), which simplify database interactions by mapping object-oriented programming constructs to relational schemas [34]. OGMs extend this approach to graph databases, allowing developers to work with structured knowledge while abstracting away query complexity. However, most existing Python-based OGMs are designed for property-graph databases, such as `GQLAlchemy` [40] and `neomodel` [41], while RDF-backed OGMs are predominantly developed in Java [9, 19, 57] or TypeScript [24]. In Python, RDF-focused OGMs remain scarce, with `Owlready2` [33] being one of the few available options. Despite its utility, `Owlready2`, along with its extension for material science [11], is primarily designed for local ontology files rather than remote triple stores and lacks robust built-in type validation. Although `Owlready2` offers an experimental quadstore approach that converts ontologies into SQL databases, this functionality does not fully support distributed or scalable SPARQL-based knowledge graphs. Consequently, its application remains limited in the context of scalable, distributed knowledge graph systems [6].

The World Avatar (TWA) is a distributed, dynamic knowledge graph designed to create a digital replica of the physical world [2, 56]. It employs software agents to synchronise digital environments with geographically distributed physical systems [6]. For

seamless integration, modifying its states entirely through Python programmes is essential, necessitating an OGM solution tailored for distributed applications. To address this need, we introduce a Python-based OGM specifically designed for remote RDF-backed graph databases, featuring built-in type validation. This solution bridges modern scientific applications with the semantic web ecosystem and integrates directly with `twa`, the Python wrapper for The World Avatar project. By providing a vendor-neutral and standardised approach to managing RDF data structures, our OGM enhances accessibility and interoperability in chemical research.

Furthermore, as large language models (LLMs) gain traction in automating tasks within chemistry [8, 12, 37, 49], integrating OGMs with AI-driven methods unlocks new opportunities for structured hypothesis generation and data analysis. This work aims to accelerate the adoption of graph-based data management in chemistry, fostering a globally connected research network through an accessible and open-source Python toolkit.

The remainder of this paper is structured as follows. Section 2 situates our work within the broader context of the World Avatar project. Section 3 details the technical underpinnings of the proposed OGM, while Section 4 demonstrates its utility through use cases in metal-organic polyhedra. Finally, Section 5 presents conclusions and perspectives for future development.

2 The World Avatar

The World Avatar (TWA) is an open, interoperable digital ecosystem that integrates dynamic knowledge graphs and autonomous software agents to create a scalable digital twin of the physical world. It bridges domain silos using ontologies and linked data principles to enable cross-disciplinary interoperability. Emphasising collaborative and agent-based intelligence [5], TWA supports applications from molecular and material discovery [30] to urban resilience planning [56]. Specifically, in the chemistry domain, TWA supports chemical species ontology [45], rational design of novel reticular and porous materials [28, 32], natural language question-answering system [66], and distributed self-driving laboratories [6, 50].

A key challenge across projects was the steep learning curve of Java and the inherent complexity of ontologies, making it difficult to onboard new team members. To improve accessibility, we developed a Python wrapper as a more accessible alternative. However, team members often had to write repetitive SPARQL boilerplate code to access graph data, particularly when working with the same ontology across different projects. This not only increased development time but also introduced inconsistencies when modifications to the same ontology were needed for cross-domain applications. Moreover, developers had to manually update their SPARQL scripts to ensure meaningful results as ontologies evolved. To address these issues, we set out to develop a reusable software package that simplifies access to knowledge graphs by replacing repetitive SPARQL queries and complex Java-based workflows with a more efficient, consistent, and Python-native approach. This integration also enhances ontology version control for better change tracking and streamlined updates.

3 Object graph mapper

Building on years of experience in knowledge graph development, we present the `twa` Python package as a comprehensive solution for more intuitive and efficient knowledge graph management. By abstracting interactions with the underlying graph database, `twa` simplifies ontology development and population. A central feature of this package is its object-graph mapper (OGM), which provides a unified and scalable way to interact with knowledge graphs using object-oriented principles. This section introduces the core component of `twa`, the OGM, highlighting its role in streamlining ontology management and enhancing interoperability in modern scientific applications.

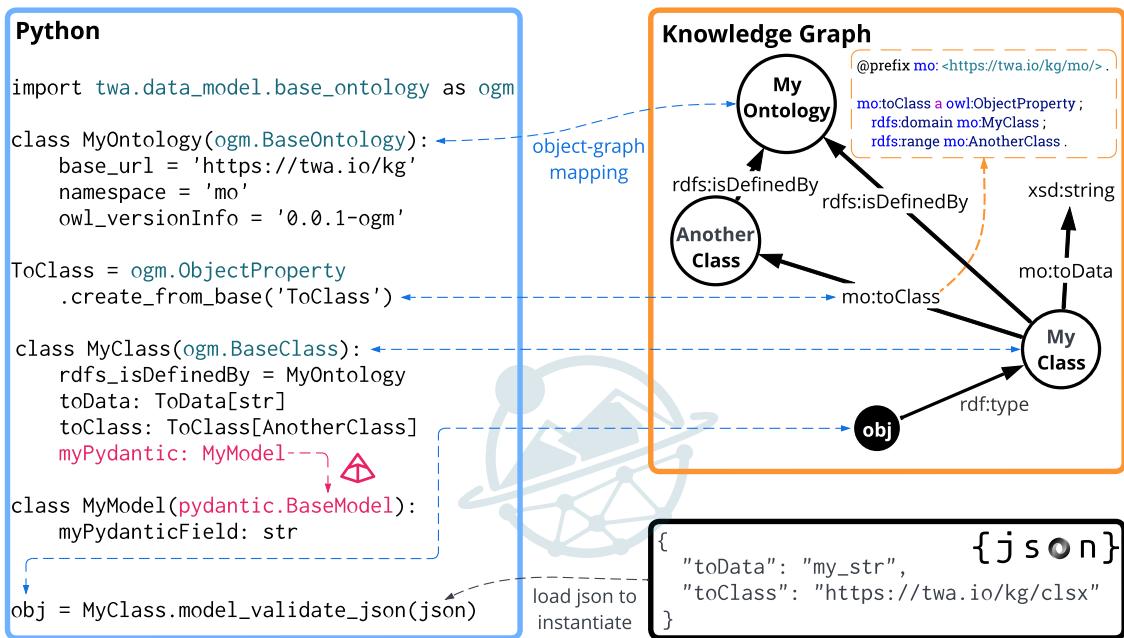


Figure 1: Overview of the object graph mapper (OGM) as an inter-exchange bridge between Python objects, RDF triples in knowledge graphs, as well as JSON data used in modern applications.

Figure 1 presents an overview of the OGM, which enables semantic translation between Python objects, knowledge graphs, and JSON data. By leveraging Pydantic [47] for structured data modelling and RDFLib [48] for representing RDF triples, OGM bridges object-oriented programming with semantic web technologies.

Figure 2 exemplifies how OGM in the `twa` Python package simplifies ontology management by abstracting complexities of querying and updating knowledge graphs. Developers only need to specify the endpoint, without worrying about manually writing SPARQL queries. Ontologies emerge naturally as a byproduct of defining relationships in Python, with a single function called exporting them as structured graph data. Similarly, pulling and pushing objects to and from the knowledge graph is streamlined through intuitive Python functions. This approach facilitates rapid prototyping and reduces the cognitive burden on developers, making semantic web technologies more accessible and efficient.

Python

```
from twa.kg_operations import PySparqlClient

# initialise SPARQL client
endpoint = 'http://my-sparql-endpoint/'
client = PySparqlClient(endpoint, endpoint)

# export TBox as triples
MyOntology.export_to_triple_store(client)

# export TBox as triples locally
MyOntology.export_to_owl('my_ontology.owl')

# pull/push objects from/to knowledge graph
my_obj = MyClass.pull_from_kg('my-iri',
client, -1)
my_other_obj = AnotherClass(...)
my_obj.toClass.add(my_other_obj)
my_obj.push_to_kg(client, -1)
```



Abstracted communication with knowledge graph

Built-in alignment of ontologies with Python codes

Git-like operation between Python objects and knowledge graph triples

Figure 2: Example usage of the `twa` Python package for interacting with knowledge graphs at both the TBox and ABox levels.

The core components of OGM include `BaseOntology`, `BaseClass`, `ObjectProperty`, and `DatatypeProperty`, which provide a direct mapping between Python classes and ontological concepts in the terminology component (TBox) of a knowledge graph, while instances correspond to assertion component (ABox). Designed to follow the standard subclassing mechanism in Python, these base classes can be extended by users to define domain-specific ontologies. Since they inherit from `pydantic.BaseModel`, they seamlessly integrate semantic functions while remaining compatible with native Pydantic features, such as JSON parsing and validation. This enables structured JSON data, including outputs from large language models (LLMs), to be directly instantiated as Python objects while preserving alignment with formal ontologies. Additionally, OGM provides utility functions for exporting defined ontologies as description logic, ensuring interoperability with standard semantic reasoning tools.

Figure 3 illustrates the core functionalities of OGM for enabling object-level interaction between Python and the knowledge graph. These rely on two key algorithms that ensure consistent and efficient data synchronisation. The `pull_from_kg` function (Alg. 1) retrieves data from the graph and instantiates or updates corresponding Python objects. It dynamically resolves the appropriate Python class for a given node based on its `rdf:type` label and the class inheritance hierarchy in Python. The algorithm supports recursive loading of linked objects, with a recursion depth parameter that controls whether nested structures are fetched to a specified depth or infinitely. To optimise performance and prevent redundant operations, it maintains a cache of object states, mitigating race conditions during concurrent pulls. The `push_to_kg` function (Alg. 2) propagates local changes from in-memory objects back to the knowledge graph. It computes the differences between the cached graph state and the current Python values to determine which triples need to be added or removed. To prevent infinite loops when traversing cyclic structures, it tracks processed nodes during traversal.

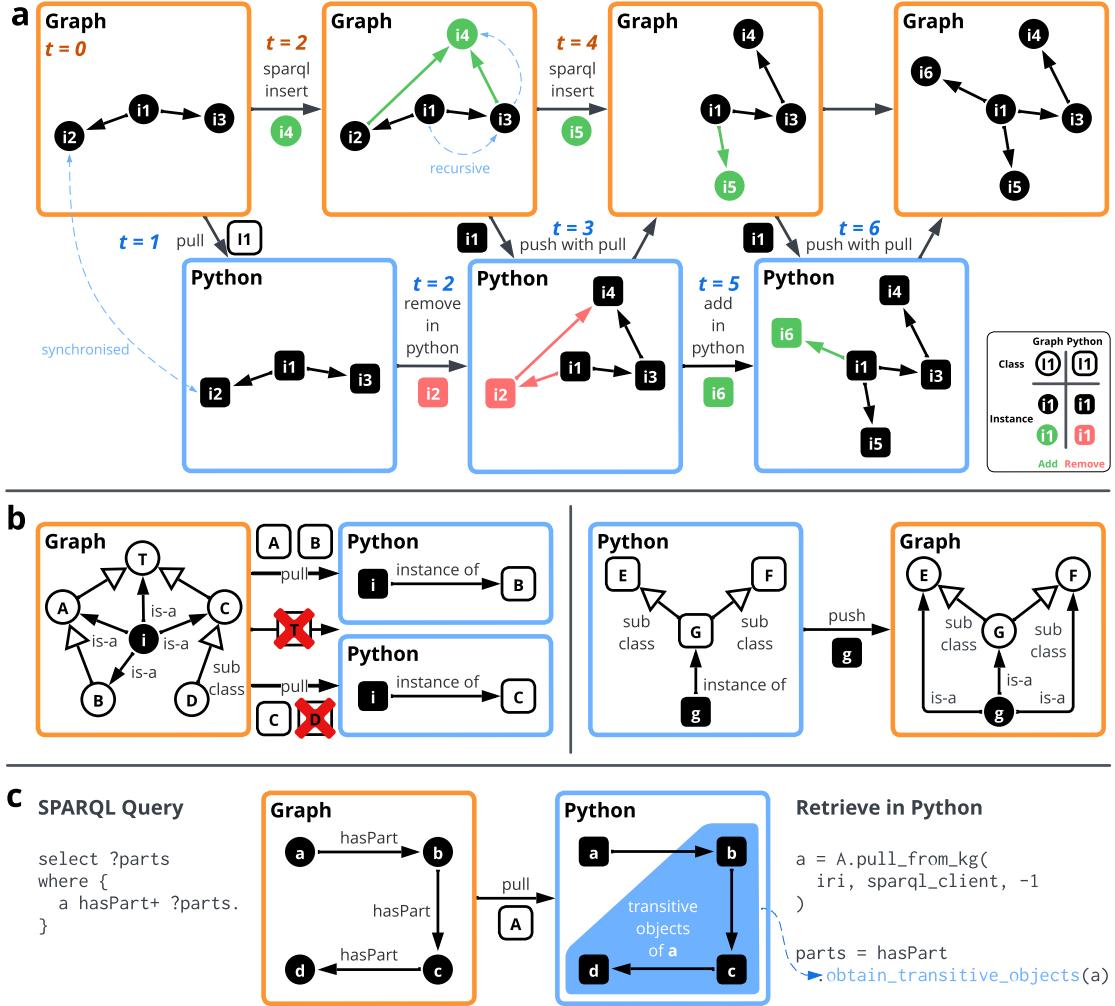


Figure 3: Illustration of three key features of the package: (a) recursive synchronisation between Python objects and the graph database, (b) multi-inheritance resolution in object and class hierarchies, and (c) transitive property handling for navigating relationships across multiple levels.

3.1 Recursive synchronisation

Figure 3(a) illustrates the Git-like recursive push and pull operations, where changes in the graph, such as SPARQL insertions of nodes **i4** and **i5**, and modifications in Python objects, such as the removal of **i2** or the addition of **i6**, are propagated in both directions. This mechanism ensures that Python objects remain aligned with the knowledge graph, even when updates are made externally.

To achieve this, OGM maintains three sets of values for each node connection (*i.e.*, object or datatype properties). The *local state* represents the current state of Python objects, the *cached state* stores the last known version retrieved from the knowledge graph, and the *fetched state* reflects the latest values obtained from the graph if the pull is flagged before the push. When synchronising, OGM first compares the fetched and cached states

to identify external modifications that should be instantiated in Python. It then compares the cached and local states to detect changes made within Python that should be pushed to the graph. Users can provide a flag to enforce an overwrite of local modifications when pulling from the remote graph, ensuring that externally introduced changes take precedence in case of conflicts. This design enables multiple clients to operate concurrently on the same knowledge graph, similar to how developers collaborate on software projects using Git.

The recursive synchronisation mechanism operates at configurable depths, allowing users to control the extent of traversal during pull and push operations. A depth of 0 limits synchronisation to direct relationships, while a positive integer n restricts recursion to n levels. A depth of -1 enables full recursion, ensuring that updates propagate through all relationship links in the graph. This flexibility ensures that OGM can handle complex knowledge graphs efficiently while maintaining consistency between Python objects and the graph database.

Listing 1 presents an example demonstrating how recursive synchronisation is performed as shown in Fig. 3(a). The process begins by pulling an instance and its connected objects from the knowledge graph into Python. After external modifications are made directly in the graph, a local deletion is performed in Python. The push operation then ensures that all changes, including those made externally and locally, are properly reconciled. Finally, a new instance is created and linked to the existing object, and another push is executed to propagate the update recursively.

3.2 Multi-inheritance resolution

In ontologies with subclass hierarchies, a single entity can often be viewed through multiple facets, leading to multiple class labels (*i.e.*, `rdf:type`) for the same instance. This phenomenon, known as multiple inheritance [43], is common in knowledge representation systems. For example, the Climate Resilience Demonstrator (CReDo) project [3] develops a digital twin of infrastructure networks to assess their resilience to climate events such as flooding and extreme heat. In their implementation, each node in the infrastructure network is instantiated both as an `Asset`, which stores essential information, and as a `Site`, which is used for visualisation. When performing analyses, it is crucial to retrieve only the relevant aspects of the data to maintain computational efficiency, especially when the digital twin is operated at the national level.

Figure 3(b) illustrates how OGM resolves such multiple-inheritance scenarios. When pulling an instance from the knowledge graph, OGM determines its Python instantiation based on the method resolution order (MRO) of the class hierarchy. The system identifies the deepest subclass at the intersection of the class used for pulling and the instance's assigned types in the knowledge graph. For example, as node **i** is labelled with multiple classes, it will always be instantiated as the most specific subclass, such as leaf class **B** when pulled using either **A** or **B**. If multiple parallel leaf classes exist, such as when pulling **i** using **T** and encountering both **B** and **C**, OGM raises an error to prevent ambiguity. The user must explicitly use either **B** or **C** to prevent the conflict. An error is also raised if an instance is pulled using a class that is not assigned as its type in the knowledge graph,

even if it exists in the class hierarchies, such as attempting to pull `i` using `D`.

This approach ensures that Python objects correctly inherit the relevant properties while preserving the structure of the knowledge graph. Additionally, when pushing local changes back to the graph, OGM guarantees that unpulled portions remain untouched, preventing unintended data loss. Listing 2 provides a minimal example demonstrating this behaviour.

3.3 Transitive property

Transitive properties play a fundamental role in ontology modelling by enabling efficient reasoning over hierarchical and dependency-based relationships. They allow relationships to be inferred across multiple levels, ensuring a more comprehensive and structured representation of complex systems. Figure 3(c) illustrates the retrieval of transitive properties using native SPARQL queries and OGM in Python, highlighting the difference in approach.

In SPARQL, transitive properties are retrieved using property paths, which efficiently traverse hierarchical relationships directly within the query. OGM achieves this capability by implementing recursion, allowing Python objects to interact dynamically with connected entities. This recursive traversal is particularly useful in scientific domains where hierarchical relationships are prevalent, such as laboratory setups, reaction networks, or material dependency structures.

For instance (see Listing 3), in a lab setup, if Beaker A is part of Reaction Setup X, which itself is part of Experiment Y, transitive reasoning infers that Beaker A is part of Experiment Y. Similarly, if Clamp B is part of Stand C, and Stand C is part of Reaction Setup X, the entire component hierarchy can be traced. Such reasoning ensures precise representation and management of complex equipment arrangements, enhancing the efficiency and reliability of lab operations [51].

By leveraging transitive reasoning, OGM enhances the usability of knowledge graphs by providing structured access to indirect relationships while preserving the interpretability of object-oriented representations in Python. This integration of SPARQL’s declarative querying with OGM’s recursive traversal ensures that complex hierarchical structures can be navigated and manipulated seamlessly in a programmatic environment.

4 Use cases for reticular chemistry

Metal-organic polyhedra (MOPs) can be described as structures formed by metal- and organic-based chemical building units (CBUs) that resemble regular polyhedra [10, 18, 28, 59]. The rational design of MOPs, as well as other cage-like assemblies, requires domain experts to carefully consider both the chemical compatibility and geometric complementarity of the constituent CBUs [25, 28]. Didactical research involving children’s construction of polyhedral models from toys has shown that no formal geometric training is necessary to assemble such shapes [26, 27], indicating that some form of cognitive visualisation is involved in the reasoning process. Motivated by these insights, the concepts of assembly models (AMs) and generic building units (GBUs) were introduced as mental “blueprints” for systematically designing MOPs from available CBUs [28]. These ideas were first formalised in the OntoMOPs ontology [28], in which the CBUs were further classified as species using the OntoSpecies ontology [45].

The MOP discovery agent employs an algorithm based on set operations to identify which CBUs can be combined without generating undesirable strain [28]. In an analysis of 151 experimentally reported MOPs constructed from 137 unique CBUs, the dataset was effectively organised into 18 AMs and 7 GBUs. According to the discovery agent, as many as 1418 new MOPs could be rationally designed [28], and several of these predicted structures have been confirmed by experimental synthesis [61]. This targeted approach substantially narrows down the potential design space, originally estimated to be approximately 80,000 possibilities, thus allowing more focused and efficient computational and experimental investigations [28].

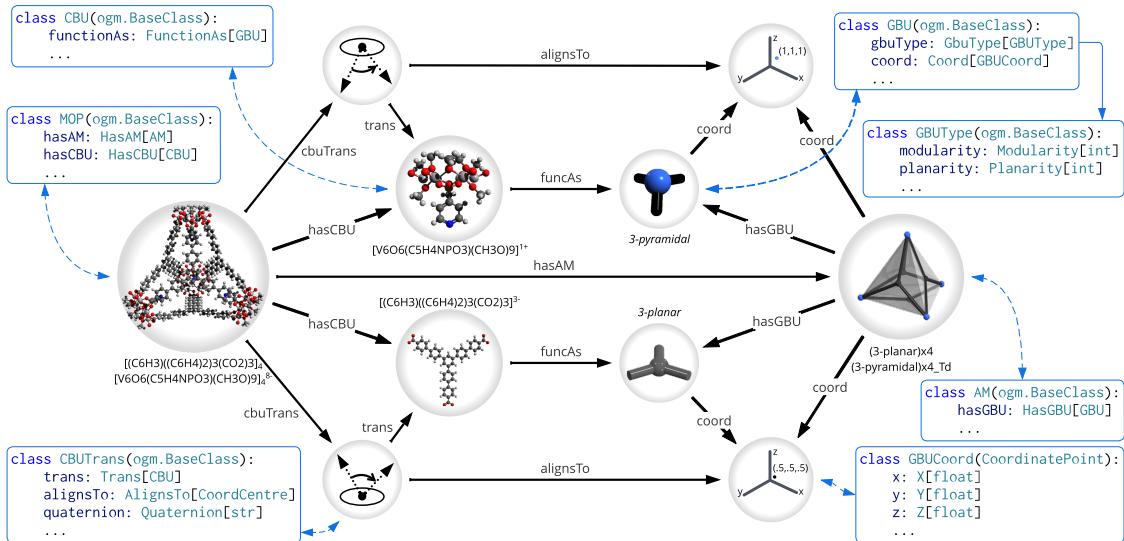


Figure 4: Representation of MOPs, CBUs, GBUs, AMs as part of OntoMOPs [28], key geometric concepts used in the assembly modelling of MOPs [31], and additional concepts added for semantic construction using the OGM. Class and relation names are abbreviated for clarity.

Figure 4 depicts a MOP $[(\text{C}_6\text{H}_3)((\text{C}_6\text{H}_4)_2)_3(\text{CO}_2)_3]_4[\text{V}_6\text{O}_6(\text{C}_5\text{H}_4\text{NPO}_3)(\text{CH}_3\text{O})_9]^{8-}$, which

follows the AM topology $(3\text{-planar})_4(3\text{-pyramidal})_4\text{-T}_d$. The assembly model (AM) prescribes two types of generic building units (GBUs), “3–planar” and “3–pyramidal”, each appearing four times and identified by their spatial coordinates. Instances of the “3–planar” GBU connect to three “3–pyramidal” GBUs, forming the polyhedral framework. This hierarchical representation was implemented *via* the OGM method to encode both chemical structure and geometric relationship [28]. Beyond rational design, the OGM method also includes automated assembly modelling of MOPs [31].

4.1 Semantic geometry construction

In our previous work, we introduced an automated rational design framework for MOPs, leveraging assembly models (AMs) and generic building units (GBUs) [28]. Building on that foundation, subsequent developments extended the process of assembly modelling to generate structural information about MOPs, thereby enabling computational analyses of cavity and pore sizing [31]. This work generalises these earlier methods and integrates them into the OGM infrastructure, providing a single, modular pipeline for constructing computation-ready 3D geometries of MOPs.

Figure 5 illustrates our semantic assembly workflow, which generalises and refines the vector-transformation approach from prior work [31]. The process begins with identifying binding sites for the chemical building units (CBUs), as shown in Fig. 5(a). Each binding site is defined as the centroid of a user-labeled binding fragment, corresponding to the atomic group(s) involved in bonding, inspired by “connection points” as implemented in geometry-based assembly for metal-organic framework [20]. A 2D circle is fitted through these binding sites, defining a plane whose normal vector serves as the “fingerprint vector” of the CBU. To ensure a unique orientational reference, we compute the cross-product of this fingerprint vector with a secondary vector extending from the circle’s centre to the nearest binding site. For CBUs functioning as 4–planar GBUs with an ideal D_{2h} symmetry, the secondary vector is instead defined from the centre to the shortest edges between two binding sites. The centroid of the CBU’s atoms, projected onto the normal vector of this plane, is designated as the assembly centre.

Next, Fig. 5(b) illustrates the quaternion-based alignment of the CBU fingerprint vector with that of its corresponding GBU in the AM. The fingerprint vectors of these GBUs are computed using the same procedure. Once rotational alignment is achieved, a translation vector is computed to place the rotated CBU at the appropriate distance for bonding (Fig. 5(c)). This step adjusts the distance between each CBU’s centre and binding site by half the bond length for calculation, preserving structural fidelity [31]. These adjustments prevent bonds from being too short, which would otherwise be difficult (though not impossible) to correct in future geometry optimisations [1]. Scaling factors are determined per GBU type to maintain the proportional relationships dictated by the symmetric AM topology, ensuring consistency across all CBU transformations. A 3D MOP geometry derived by the OGM implementation is shown in Fig. 5(d), whole details on the construction steps are provided as part of Appendix A.4.

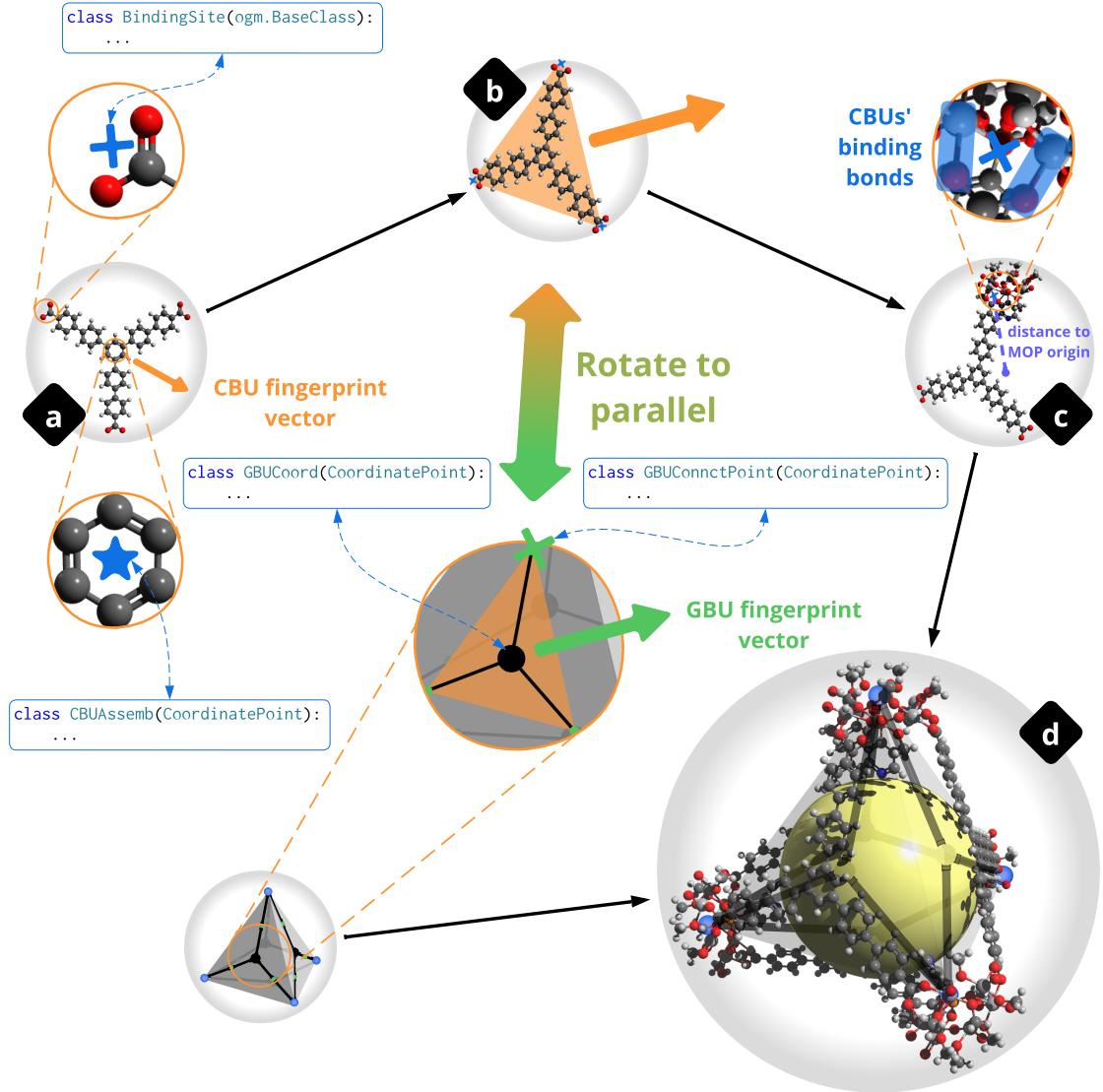


Figure 5: Automated semantic assembly of MOPs following the OGM implementation, inspired by previously developed geometry assembly protocol [31]: (a) assignment of binding sites and calculation of the fingerprint vector for CBUs, (b) quaternion-based alignment of CBUs and GBUs via their fingerprint vectors, (c) calculation of translation vectors to shift CBUs such that their binding bonds are equidistant from the origin of MOPs, and (d) transformation of CBUs into the final 3D MOP geometry, re-centred at the origin.

4.1.1 Expanding the chemical space of MOPs

We first tested our geometry construction algorithm on an expanded dataset that builds upon the original OntoMOPs set introduced by Kondinski and co-workers [28, 31]. Specifically, we incorporated two new assembly models (AM19 and AM20) and 15 additional MOPs from the literature that were not present in the original knowledge graph (see Ta-

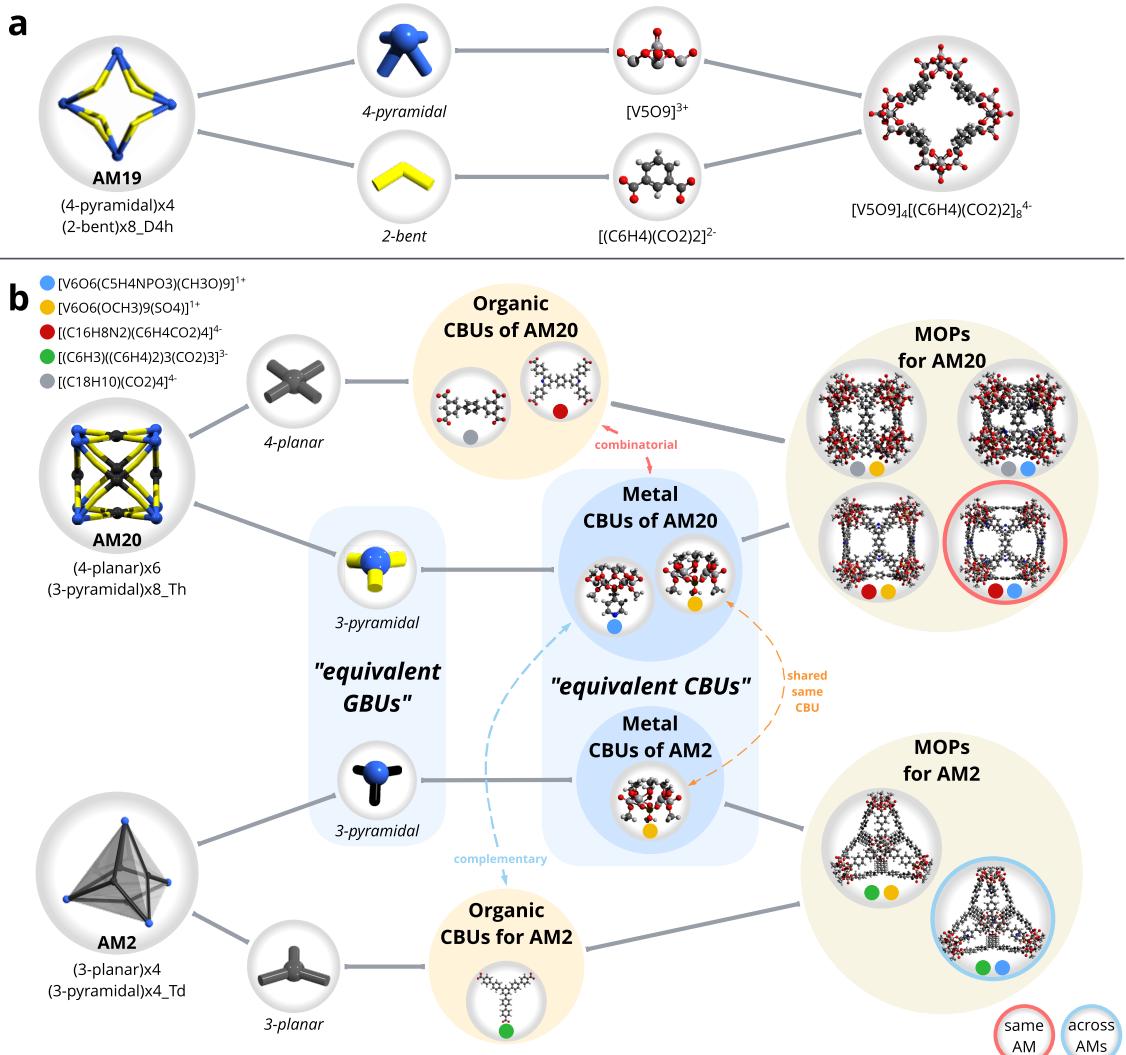


Figure 6: Examples of expanded chemical space resulting from the new AMs and MOPs introduced in this work. (a) A MOP $[V_5O_9]_4[(C_6H_4)(CO_2)_2]_8^{4-}$, added from the literature [65] and assembled with existing CBUs under an unseen AM topology $(4\text{-pyramidal})_4(2\text{-bent})_8\text{-}D_{4h}$ (AM19). (b) Rational design of new MOPs using Listings 4 and 5, showing internal combinatorial CBU assembly for $(4\text{-planar})_6(3\text{-pyramidal})_8\text{-}T_h$ (AM20) in Listing 4, and broader CBU swaps across compatible AMs (e.g., $(3\text{-planar})_4(3\text{-pyramidal})_4\text{-}T_d$, AM2) in Listing 5.

bles 1 and 2). Figure 6(a) highlights one such newly added MOP, $[V_5O_9]_4[(C_6H_4)(CO_2)_2]_8^{4-}$, which follows the newly defined AM ($4\text{-pyramidal})_4(2\text{-bent})_8-D_{4h}$ (AM19).

To systematically broaden the design space, we applied the algorithms in Listings 4 and 5 to interchange compatible metal and organic CBUs across the newly added AMs. In contrast to Listing 4, which strictly assembles CBUs already proven compatible with the same AM, Listing 5 allows for inter-AM CBU exchanges, provided both AMs share at least one common CBU. Figure 6(b) illustrates how this generates novel combinations, such as leveraging AM20 ($(4\text{-planar})_6(3\text{-pyramidal})_8-T_h$) and AM2 ($(3\text{-planar})_4(3\text{-pyramidal})_4-T_d$). Overall, these expansions yielded 799 newly designed MOPs derived from a base set of 1584. A summary of the new structures is listed in Table 3, with further details in Table 4.

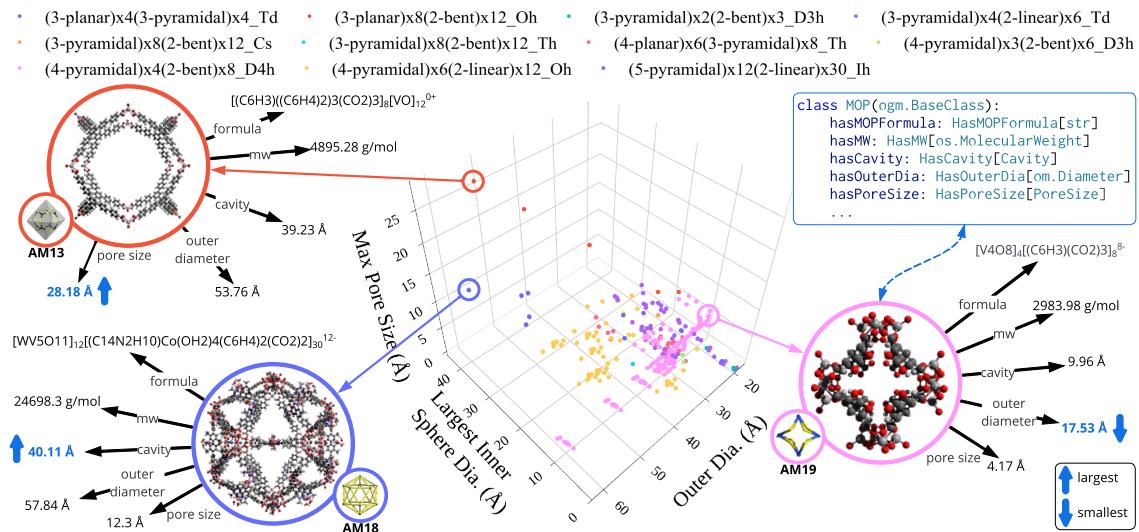


Figure 7: Visualisation of the expanded chemical space of 799 MOPs, highlighting structural properties such as maximum pore size, largest inner sphere diameter (a proxy for cavity size), and outer diameter. Points are colour-coded by their AM, and specific examples are circled to indicate extremes within the design space.

Figure 7 offers an overview of these 799 new MOPs, based on structural properties computed from the 3D geometries. Each MOP is re-centred on its geometric midpoint to streamline calculations. The *largest inner sphere diameter* measures the distance from the centre to the closest atom (adjusted by covalent radii), while *outer diameter* captures the farthest atom. The *maximum pore size* is obtained by projecting atomic positions onto vectors connecting the MOP centre to the centroid of ring-forming GBUs. The mathematical details behind these estimations are given in Appendix A.4.

Among the newly generated structures, certain AM19-based MOPs stand out for their compactness, exhibiting relatively small cavities. This is primarily due to the “ 4-pyramidal ” metallic CBUs and “ 2-bent ” organic CBUs with narrow dihedral angles. Conversely, other AMs that incorporate bulkier organic linkers display significantly larger pore sizes, emphasising how AM geometry and CBU composition drive structural properties.

These findings validate our OGM workflow implementation. By leveraging semantic data representation and automated assembly, developers can focus on high-level design logic

while leaving the recursive data retrieval and consistency checks to the OGM. This eliminates extensive scripting and facilitates the pre-screen of promising candidates before expensive density functional theory (DFT) optimisations. This continuing effort builds on the rational design concepts outlined in Kondinski et al. [28, 31] and highlights how a semantic-driven approach can streamline large-scale molecular design. Future work will explore the application of structural viability, based on computational chemistry protocols as proposed by Hoffmann et al. [22].

4.2 Extraction of synthesis protocols using LLMs

Following the automated rational design and geometry construction, the chemical relevance of newly designed MOPs ultimately depends on their experimental synthesis. However, such validation often faces bottlenecks due to the inefficiency of traditional trial-and-error synthesis methods. The self-assembly of these structures offers the potential to reliably predict synthesis procedures based on building units and assembly models. Connecting computational design with experimental realisation requires the systematic inference of synthesis protocols from literature procedures. Unfortunately, such protocols are often documented inconsistently across scientific publications and in non-machine-readable formats. Large language models (LLMs) show promise in addressing these challenges by extracting detailed synthesis information from the scientific literature to infer new synthesis routes [35, 55, 67].

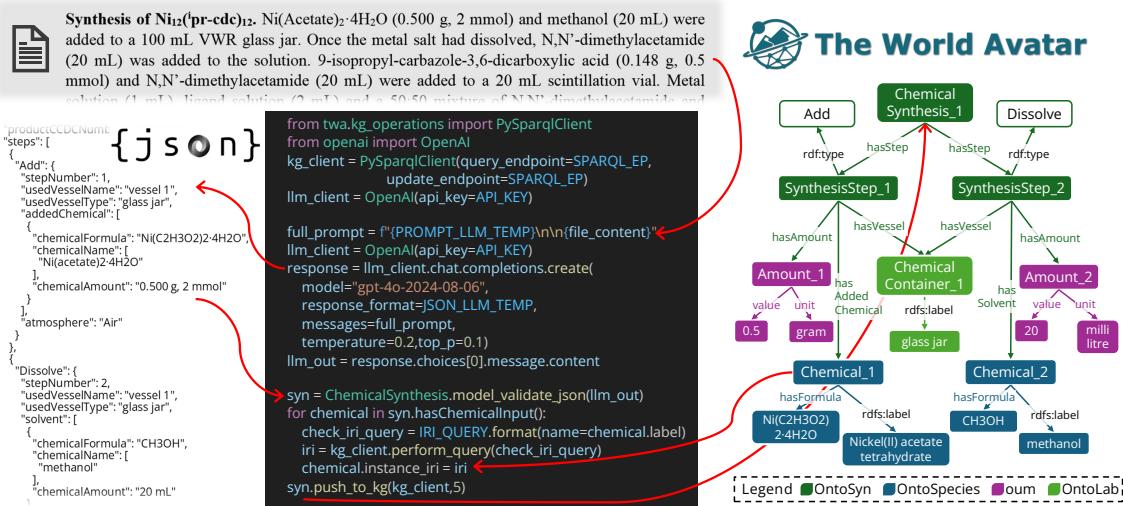


Figure 8: Automated extraction of MOPs synthesis protocols from literature using LLMs and integration into knowledge graphs using OGM. Supplementary information is processed through the OpenAI Python API to generate structured JSON outputs, which are then loaded by OGM to expand the knowledge graph.

Figure 8 illustrates the integration of LLMs with OGM to bridge unstructured literature with computable chemical knowledge. The pipeline automates the extraction of synthesis protocols from scientific literature, such as supplementary information in journal articles, using the OpenAI Python API [44] with domain-specific prompts. The LLM-generated

structured JSON outputs are then loaded into the knowledge graph through OGM. This integration establishes a bidirectional connection between unstructured text and semantic triples, enabling the instantiation of new knowledge derived from LLMs while leveraging existing structured knowledge to guide LLM prompts. By simplifying the transformation of data between JSON, Python objects, and graph nodes, this approach minimises coding overhead for researchers while ensuring compatibility with existing workflows. Full technical details of this implementation are provided in Saluz [52].

4.3 Natural language question answering

As OGM recursively pushes all generated triples to the knowledge graph, newly generated MOPs can be seamlessly queried by the chatbot Marie [32, 58], enabling interactive exploration of calculated properties and their interrelationships. This functionality allows researchers to connect computational results to practical applications, such as screening MOPs with specific properties. Figure 9 illustrates this through chained queries: the user first queries AMs with octahedral geometry and then identifies the largest pore size among MOPs associated with a selected AM. Next, observing the presence of a specific CBU within the identified MOP inspires a query for other MOPs formed from the same CBU. Marie retrieves detailed information, including structural visualisation and data from both literature and computational predictions. Future work includes integrating OGM into Marie’s codebase to enable dynamic data retrieval and modification during interactions.

5 Conclusions

In this work, we introduced `twa` (the World Avatar) Python package, a comprehensive framework that democratises the creation and management of dynamic knowledge graphs. By abstracting SPARQL queries and ontology manipulation, `twa` enables developers to build and maintain RDF-based knowledge structures in a familiar Python environment. Its modular design facilitates seamless integration with existing Python ecosystems, while its core object graph mapper (OGM) provides a versatile means of synchronising semantic data between Python classes and RDF-backed graph databases. Through demonstrating how the OGM facilitates the automation of geometry assembly and synthesis protocol extraction for metal-organic polyhedra, we have shown that domain-specific abstractions can significantly streamline the handling of hierarchical and relational data, thus lowering barriers to the broader adoption of knowledge-graph technologies in scientific research.

Looking ahead, future developments will integrate continuous integration/deployment (CI/CD) pipelines to maintain multi-namespace ontology consistency, enhance reasoning capabilities [33], and expand SPARQL querying through property-path functionality. Equally important is improving interoperability with standards such as SHACL [60] and the Object-Oriented Linked Data Schema [53]. To enhance OGM usability, further extensions will automate the generation of Python class hierarchies from existing ontologies. The synergy between ontologies and large language models (LLMs), demonstrated in the automated synthesis-extraction use case, presents a promising avenue for agentic workflows that harness structured knowledge in cutting-edge AI applications. Through deeper

What assembly models are representative of **octahedron** geometry



The assembly models that are representative of octahedron geometry include:

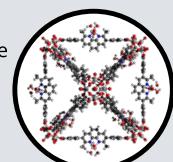
- (3-planar)x8(4-pyramidal)x6, Symmetry Point Group: Oh
- **(4-pyramidal)x6(2-linear)x12, Symmetry Point Group: Oh**
- (4-planar)x6(3-pyramidal)x8, Symmetry Point Group: Oh
- (4-pyramidal)x6(3-pyramidal)x8, Symmetry Point Group: Oh

Which MOP with AM **(4-pyramidal)x6(2-linear)x12_Oh** has the **largest pore size diameter** value



The Metal-Organic Polyhedron (MOP) with the specified assembly model (4-pyramidal)x6(2-linear)x12_Oh that has the largest pore size diameter value is represented by the following details:

- Formula: **[V5O9]6[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]12**
- Pore Size Diameter: **11.49 Ångströms**
- Provenance: **TWA OGM**

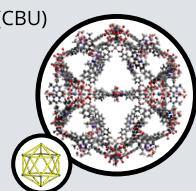


For the largest **outer diameter** value of MOPs with **CBU** **[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]**, what is its assembly model and its **pore size**



For the Metal-Organic Polyhedron (MOP) with the Chemical Building Unit (CBU) formula **[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]**, the following details are provided:

- Formula: **[WV5O11]12[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]30**
- Assembly Model: **(5-pyramidal)x12(2-linear)x30**
- Pore Size: **12.30 Ångströms**
- Outer Diameter: **57.84 Ångströms**



What MOP has AM **(5-pyramidal)x12(2-linear)x30** and what are their **inner sphere diameters**



For the Metal-Organic Polyhedron (MOP) with the Chemical Building Unit (CBU) formula **[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]**, the following details are provided:

1. MOP Formula:
[WV5O11]12[(C6H4N)2(CO2)2]30
Inner Sphere Diameter:
35.68 Ångströms
2. MOP Formula:
[V6O11]12[(C14N2H10)Co(OH2)4(C6H4)2(CO2)2]30
Inner Sphere Diameter:
40.07 Ångströms
3. ...

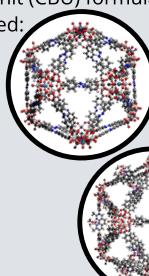


Figure 9: Illustration of Marie's natural language interface for exploratory queries on MOPs data via chained questions.

integration of LLMs with the OGM, twa may help advance the field towards autonomous research ecosystems, in which data-driven digital discovery is more efficient and transparent.

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Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT in order to enhance the readability and language of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

Data and code availability

All data covered in this research can be automatically queried through TWA-Marie interface (<https://theworldavatar.io/demos/marie>). The `twa` Python package is publicly available at the following links:

- PyPI: <https://pypi.org/project/twa/>
- GitHub: https://github.com/TheWorldAvatar/BaseLib/tree/main/python_wrapper
- Documentation: <https://cambridge-cares.github.io/TheWorldAvatar>

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 */  

1 Function pull_from_kg(iris, client, recursion, overwrite):  

2     instances, opf, dpf ← [], {}, {};  

    /* Iterate over copy to avoid modifying iris list during iteration */  

3     for iri in copy(iris) do  

4         if iri ∈ G.loading() then  

5             iri.remove(iri);  

6         else  

7             G.add_to_loading(iri);  

8         flag_pull ← |recursion| > 0;  

9         if recursion > -1 then  

10            recursion ← max(recursion - 1, 0);  

11        else  

12            recursion ← -1;  

13        nodes ← client.query(iris);  

14        for iri, props in nodes do  

            /* Resolve class from the intersection of rdf:type and Python MRO */  

15            if rdf_type ∉ props or props[rdf_type] ∉ cls.mro then  

16                G.remove_loading(iri);  

17                raise No suitable (sub)class identified for iri;  

18            node_cls ← G.get_cls(props[rdf_type]);  

            /* Process object properties recursively */  

19            for op in cls.object_properties() do  

20                if op ∈ props then  

21                    if flag_pull then  

22                        op_cls ← G.get_cls(op);  

                        opf[op] ← op_cls.pull_from_kg(props[op], client, recursion, overwrite);  

23  

            /* Process data properties (non-recursive) */  

24            for dp in cls.data_properties() do  

25                if dp ∈ props then  

26                    dp_cls ← G.get_cls(dp);  

                    dpf[dp] ← props[dp];  

27  

            /* Process rdfs properties (omitted here for brevity...) */  

            /* Update existing instance or create new */  

28            if iri ∈ G then  

29                instance ← G.get(iri);  

30                instance.update_cache(**opf, **dpf, overwrite);  

                /* update with fetched values */  

31            else  

32                instance ← cls(**opf, **dpf);  

                /* construct with resolved class */  

33            instances.add(instance);  

34            G.remove_loading(iri);  

                /* mark completion */  

35        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 */
1 Function push_to_kg(client, recursion, pull, overwrite) :
2   if pull then
3     /* Pull the latest state from remote to avoid conflicts */
4     cls.pull_from_kg([self.instance_iri], client, recursion, overwrite); */
5   g_remove, g_add  $\leftarrow \emptyset, \emptyset$ ; /* initialising diff graphs */
6   /* Recursively collect triples to add/remove across linked objects */
7   g_remove, g_add  $\leftarrow \text{collect\_diff}(g\_remove, g\_add, recursion, traversed \leftarrow \emptyset);
8   client.update(g_remove, g_add); /* apply changes to triplestore */
9   /* Retry upon failure (omitted here for brevity...) */
10  return g_remove, g_add;

11 Function collect_diff(g_remove, g_add, recursion, traversed) :
12   if self.instance_iri  $\in$  traversed then
13     return g_remove, g_add; /* avoid duplicate or cyclic traversals */
14   traversed.add(self.instance_iri); /* mark this IRI as processed */
15   /* Process all fields (object/data properties) of the instance */
16   for f, field_info in self.model_fields do
17     predicate_cls  $\leftarrow$  field_info.type_annotation; /* get property class */
18     if issubclass(predicate_cls, BaseProperty) then
19       flag_collect  $\leftarrow$  |recursion|  $> 0$ ; /* depth control */
20       if recursion  $> -1 then
21         recursion  $\leftarrow$  max(recursion - 1, 0); /* decrement finite recursion */
22       else
23         recursion  $\leftarrow -1$ ; /* remain infinite recursion */
24       /* Compute diff between cached and local values; fetched values have already been
25        dealt with in function pull_from_kg */
26       cache  $\leftarrow$  self.cache[f]; /* last known KG state */
27       local  $\leftarrow$  getattr(self, f); /* current local state */
28       remove  $\leftarrow$  cache - local; /* triples to delete */
29       add  $\leftarrow$  local - cache; /* triples to add */
30       for r in remove do
31         g_remove.add_triple(self.instance_iri, predicate_cls.iri, r);
32       for a in add do
33         g_add.add_triple(self.instance_iri, predicate_cls.iri, a);
34       /* Recurse into linked objects (if recursion allowed) */
35       if flag_collect and issubclass(predicate_cls, ObjectProperty) then
36         for o in cache  $\cup$  local do
37           /* Existing Python object, perform recursion */
38           if o  $\in G$  then
39             g_remove, g_add  $\leftarrow o.\text{collect\_diff}(g\_remove, g\_add, recursion, traversed);
40           /* If the object does not exist in Python then skip as they are never
41            modified locally */
42         /* Process rdfs properties (omitted here for brevity...) */
43       return g_remove, g_add;$$$ 
```

Listing 1: 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 2: 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 3: 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 \sqsubseteq OntoMOP:CoordinatePoint
OntoMOPs:CBUAssemblyCenter \sqsubseteq OntoMOP:CoordinatePoint
OntoMOPs:CoordinationCage \sqsubseteq OntoMOP:MolecularCage
OntoMOPs:DirectBinding \sqsubseteq OntoMOP:BindingDirection
OntoMOPs:GBUConnectingPoint \sqsubseteq OntoMOP:CoordinatePoint
OntoMOPs:GBUCoordinateCenter \sqsubseteq OntoMOP:CoordinatePoint
OntoMOPs:MetalOrganicPolyhedron \sqsubseteq OntoMOP:CoordinationCage
OntoMOPs:MetalOrganicPolyhedron \sqsubseteq OntoMOP:MolecularCage
OntoMOPs:MetalSite \sqsubseteq OntoMOP:BindingSite
OntoMOPs:OrganicSite \sqsubseteq OntoMOP:BindingSite
OntoMOPs:SidewayBinding \sqsubseteq OntoMOP:BindingDirection
 \exists OntoMOP:alignsTo. $\top \sqsubseteq$ OntoMOP:CBUAssemblyTransformation
 \exists OntoMOP:hasAssemblyModel. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasBindingDirection. $\top \sqsubseteq$ OntoMOP:ChemicalBuildingUnit
 \exists OntoMOP:hasBindingPoint. $\top \sqsubseteq$ (<https://www.theworldavatar.com/kg/ontomops/BindingSite> \sqcup OntoMOP:MetalSite \sqcup OntoMOP:OrganicSite)
 \exists OntoMOP:hasBindingSite. $\top \sqsubseteq$ OntoMOP:ChemicalBuildingUnit
 \exists OntoMOP:hasCBUAssemblyCenter. $\top \sqsubseteq$ OntoMOP:ChemicalBuildingUnit
 \exists OntoMOP:hasCBUAssemblyTransformation. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasCavity. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasChemicalBuildingUnit. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasGBUConnectingPoint. $\top \sqsubseteq$ (<https://www.theworldavatar.com/kg/ontomops/AssemblyModel> \sqcup OntoMOP:GBUCoordinateCenter)
 \exists OntoMOP:hasGBUCoordinateCenter. $\top \sqsubseteq$ (<https://www.theworldavatar.com/kg/ontomops/AssemblyModel> \sqcup OntoMOP:GenericBuildingUnit)
 \exists OntoMOP:hasGBTType. $\top \sqsubseteq$ OntoMOP:GenericBuildingUnit
 \exists OntoMOP:hasGenericBuildingUnit. $\top \sqsubseteq$ OntoMOP:AssemblyModel
 \exists OntoMOP:hasGenericBuildingUnitNumber. $\top \sqsubseteq$ OntoMOP:AssemblyModel
 \exists OntoMOP:hasLargestInnerSphereDiameter. $\top \sqsubseteq$ OntoMOP:Cavity
 \exists OntoMOP:hasOuterDiameter. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasPolyhedralShape. $\top \sqsubseteq$ OntoMOP:AssemblyModel
 \exists OntoMOP:hasPoreDiameter. $\top \sqsubseteq$ OntoMOP:PoreSize
 \exists OntoMOP:hasPoreRing. $\top \sqsubseteq$ OntoMOP:AssemblyModel
 \exists OntoMOP:hasPoreSize. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:hasProvenance. $\top \sqsubseteq$ OntoMOP:MetalOrganicPolyhedron
 \exists OntoMOP:isFormedBy. $\top \sqsubseteq$ OntoMOP:PoreRing
 \exists OntoMOP:isFunctioningAs. $\top \sqsubseteq$ OntoMOP:ChemicalBuildingUnit
 \exists OntoMOP:isNumberOf. $\top \sqsubseteq$ OntoMOP:GenericBuildingUnitNumber
 \exists OntoMOP:measuresRing. $\top \sqsubseteq$ OntoMOP:PoreSize
 \exists OntoMOP:transforms. $\top \sqsubseteq$ OntoMOP:CBUAssemblyTransformation
 $\top \sqsubseteq \forall$ OntoMOP:alignsTo.OntoMOPs:GBUCoordinateCenter

$\top \sqsubseteq \forall \text{OntoMOP:hasAssemblyModel}.\text{OntoMOPs:AssemblyModel}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasBindingDirection}.\text{OntoMOPs:BindingDirection}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasBindingPoint}.\text{OntoMOPs:BindingPoint}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasBindingSite}.\text{OntoMOPs:BindingSite}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasCBUAssemblyCenter}.\text{OntoMOPs:CBUAssemblyCenter}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasCBUAssemblyTransformation}.\text{OntoMOPs:CBUAssemblyTransformation}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasCavity}.\text{OntoMOPs:Cavity}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasChemicalBuildingUnit}.\text{OntoMOPs:ChemicalBuildingUnit}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasGBUConnectingPoint}.\text{OntoMOPs:GBUConnectingPoint}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasGBUCoordinateCenter}.\text{OntoMOPs:GBUCoordinateCenter}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasGBTType}.\text{OntoMOPs:GenericBuildingUnitType}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasGenericBuildingUnit}.\text{OntoMOPs:GenericBuildingUnit}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasGenericBuildingUnitNumber}.\text{OntoMOPs:GenericBuildingUnitNumber}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasLargestInnerSphereDiameter}.\text{om:Diameter}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasOuterDiameter}.\text{om:Diameter}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasPolyhedralShape}.\text{OntoMOPs:PolyhedralShape}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasPoreDiameter}.\text{om:Diameter}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasPoreRing}.\text{OntoMOPs:PoreRing}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasPoreSize}.\text{OntoMOPs:PoreSize}$
 $\top \sqsubseteq \forall \text{OntoMOP:hasProvenance}.\text{OntoMOPs:Provenance}$
 $\top \sqsubseteq \forall \text{OntoMOP:isFormedBy}.\text{OntoMOPs:GBUCoordinateCenter}$
 $\top \sqsubseteq \forall \text{OntoMOP:isFunctioningAs}.\text{OntoMOPs:GenericBuildingUnit}$
 $\top \sqsubseteq \forall \text{OntoMOP:isNumberOf}.\text{OntoMOPs:GenericBuildingUnit}$
 $\top \sqsubseteq \forall \text{OntoMOP:measuresRing}.\text{OntoMOPs:PoreRing}$
 $\top \sqsubseteq \forall \text{OntoMOP:transforms}.\text{OntoMOPs:ChemicalBuildingUnit}$
 $\exists \text{OntoMOP:hasBindingFragment}.\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/} \text{BindingSite} \sqcup \text{OntoMOP:MetalSite} \sqcup \text{OntoMOP:OrganicSite})$
 $\exists \text{OntoMOP:hasCBUFormula}.\top \sqsubseteq \text{OntoMOP:ChemicalBuildingUnit}$
 $\exists \text{OntoMOP:hasCCDCNumber}.\top \sqsubseteq \text{OntoMOP:MetalOrganicPolyhedron}$
 $\exists \text{OntoMOP:hasMOPFormula}.\top \sqsubseteq \text{OntoMOP:MetalOrganicPolyhedron}$
 $\exists \text{OntoMOP:hasModularity}.\top \sqsubseteq \text{OntoMOP:GenericBuildingUnitType}$
 $\exists \text{OntoMOP:hasOuterCoordinationNumber}.\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/} \text{BindingSite} \sqcup \text{OntoMOP:MetalSite} \sqcup \text{OntoMOP:OrganicSite})$
 $\exists \text{OntoMOP:hasPlanarity}.\top \sqsubseteq \text{OntoMOP:GenericBuildingUnitType}$
 $\exists \text{OntoMOP:hasProbingVector}.\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/} \text{PoreRing} \sqcup \text{OntoMOP:PoreSize})$
 $\exists \text{OntoMOP:hasReferenceDOI}.\top \sqsubseteq \text{OntoMOP:Provenance}$
 $\exists \text{OntoMOP:hasSymbol}.\top \sqsubseteq \text{OntoMOP:PolyhedralShape}$
 $\exists \text{OntoMOP:hasSymmetryPointGroup}.\top \sqsubseteq \text{OntoMOP:AssemblyModel}$
 $\exists \text{OntoMOP:hasUnitNumberValue}.\top \sqsubseteq \text{OntoMOP:GenericBuildingUnitNumber}$
 $\exists \text{OntoMOP:hasX}.\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/} \text{BindingPoint} \sqcup \text{OntoMOP:CBUAssemblyCenter} \sqcup \text{OntoMOP:CoordinatePoint} \sqcup \text{OntoMOP:GBUConnectingPoint} \sqcup \text{OntoMOP:GBUCoordinateCenter})$
 $\exists \text{OntoMOP:hasY}.\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/} \text{BindingPoint} \sqcup$

OntoMOP:CBUAssemblyCenter \sqcup OntoMOP:CoordinatePoint \sqcup OntoMOP:GBUConnectingPoint \sqcup OntoMOP:GBUCoordinateCenter)
 \exists OntoMOP:hasZ. $\top \sqsubseteq (\text{https://www.theworldavatar.com/kg/ontomops/BindingPoint} \sqcup$
 OntoMOP:CBUAssemblyCenter \sqcup OntoMOP:CoordinatePoint \sqcup OntoMOP:GBUConnectingPoint \sqcup OntoMOP:GBUCoordinateCenter)
 \exists OntoMOP:quaternionToRotate. $\top \sqsubseteq$ OntoMOP:CBUAssemblyTransformation
 \exists OntoMOP:scaleFactorToAlignCoordinateCenter. $\top \sqsubseteq$ OntoMOP:CBUAssemblyTransformation
 \exists OntoMOP:translationVectorToAlignOrigin. $\top \sqsubseteq$ OntoMOP:CBUAssemblyTransformation
 $\top \sqsubseteq \forall$ OntoMOP:hasBindingFragment.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasCBUFormula.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasCCDCNumber.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasMOPFormula.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasModularity.xsd:integer
 $\top \sqsubseteq \forall$ OntoMOP:hasOuterCoordinationNumber.xsd:integer
 $\top \sqsubseteq \forall$ OntoMOP:hasPlanarity.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasProbingVector.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasReferenceDOI.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasSymbol.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasSymmetryPointGroup.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:hasUnitNumberValue.xsd:integer
 $\top \sqsubseteq \forall$ OntoMOP:hasX.xsd:double
 $\top \sqsubseteq \forall$ OntoMOP:hasY.xsd:double
 $\top \sqsubseteq \forall$ OntoMOP:hasZ.xsd:double
 $\top \sqsubseteq \forall$ OntoMOP:quaternionToRotate.xsd:string
 $\top \sqsubseteq \forall$ OntoMOP:scaleFactorToAlignCoordinateCenter.xsd:double
 $\top \sqsubseteq \forall$ OntoMOP:translationVectorToAlignOrigin.xsd:string

A.3 Ontologised algorithms for the rational design of MOPs

The two algorithms developed in our previous work [28] to expand the chemical space of MOPs were ontologised herein as SPARQL queries. The first algorithm (Listing 4) constructs MOPs using chemically complementary CBUs restricted to a single AM without allowing CBU exchanges between different AMs, whereas the second algorithm (Listing 5) expands MOP construction by enabling CBU exchanges between different AMs, increasing versatility and the number of possible structures.

Listing 4: *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 5: 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.*, $(4\text{-planar})_6(3\text{-pyramidal})_8T_h$ and $(3\text{-planar})_4(3\text{-pyramidal})_4T_d$, 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.*, $(m_i-p_i)_{n_i}$. 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:

$$\mathcal{A} = \left(\prod_{i=1}^N (m_i-p_i)_{n_i} \right) \text{-sym}$$

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:

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

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):

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

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):

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

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

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

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

$$\mathbf{V}_i = [\mathbf{v}_{i,1} \ \mathbf{v}_{i,2} \ \mathbf{v}_{i,3}]$$

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 :

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

where $\text{Proj}_{\pi_i}(\mathbf{B}_{i,k})$ 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:

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

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

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

where \otimes denotes quaternion rotation.

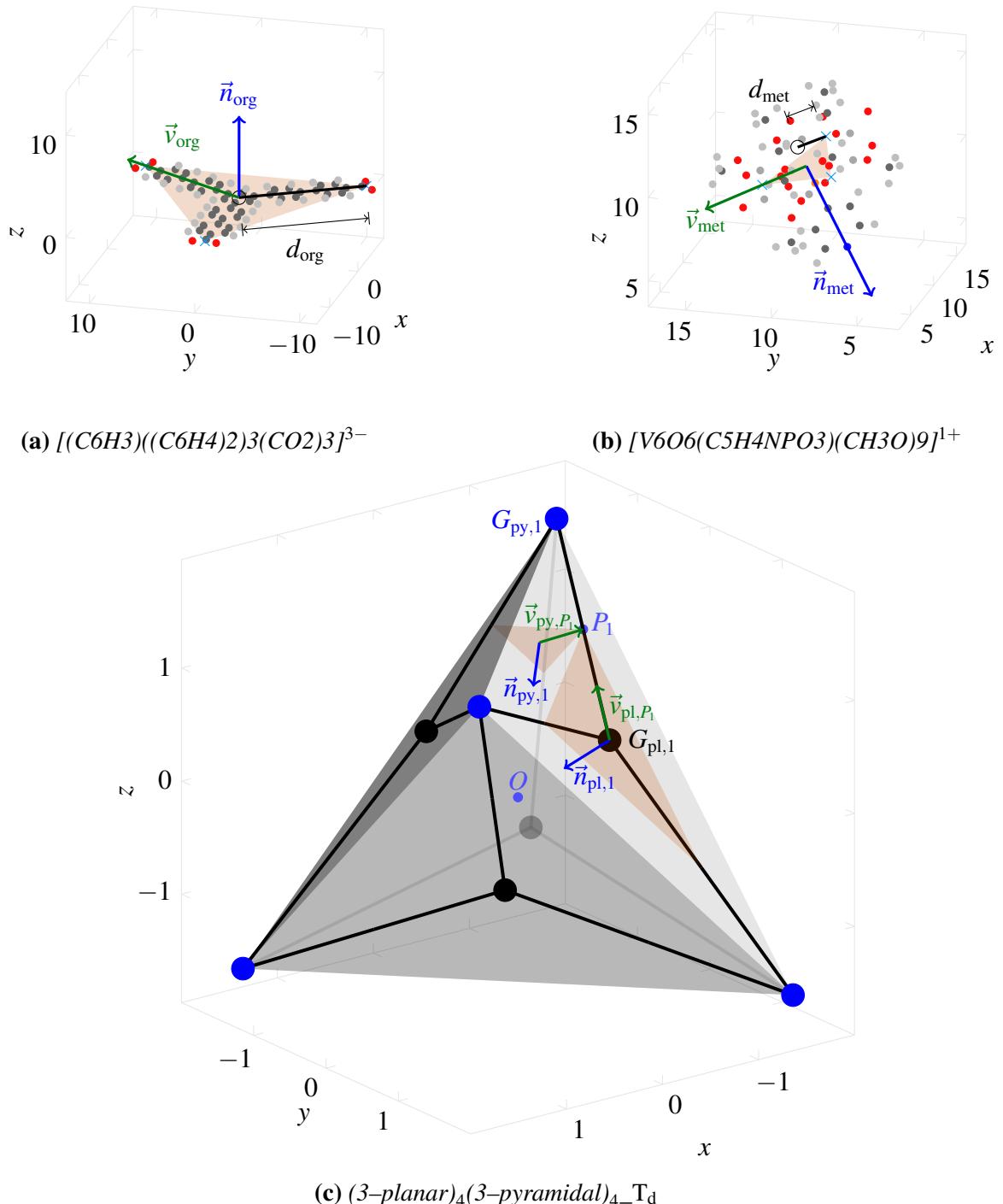


Figure 10: Visualisation for fingerprint vector rotation in the geometry stitching algorithm using OGM to align CBUs (organic/metal - (a)/(b)) and their corresponding GBUs (3-planar/3-pyramidal).

Figure 10 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

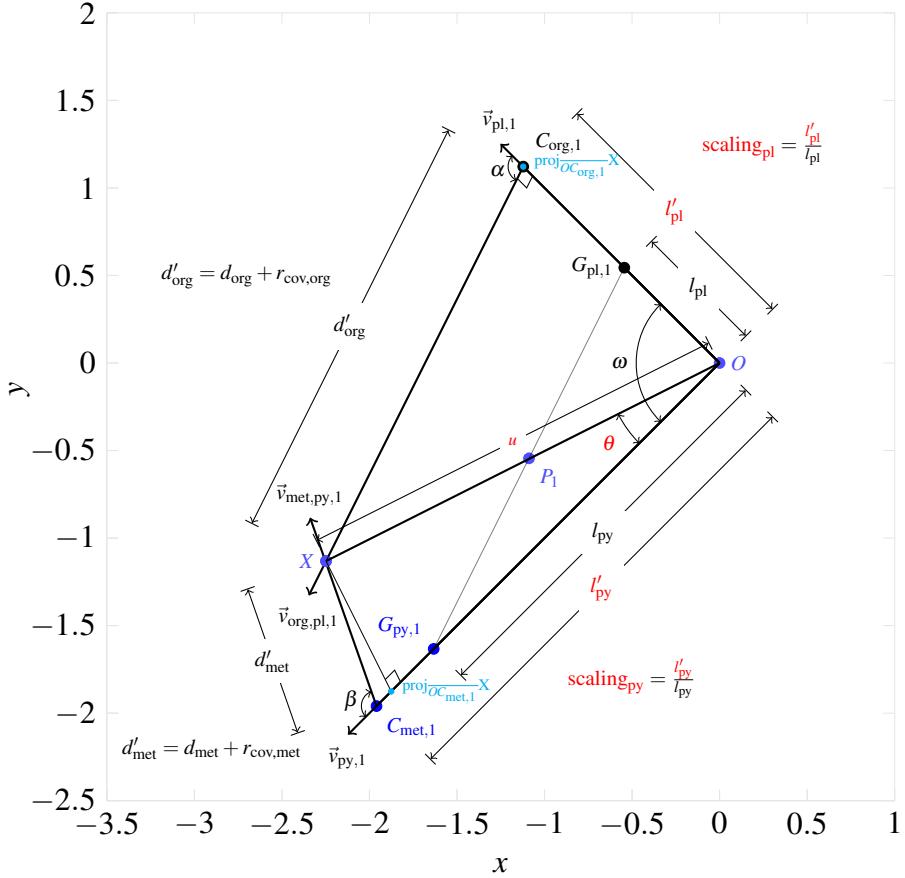


Figure 11: The scaling factor calculation per GBU Type for the MOP shown in Fig. 10 using the OGM-based MOP geometry stitching algorithm. The geometry to be solved is projected on the X-Y plane. Note that the scaling factors ($\text{scaling}_{\text{py}}$ and $\text{scaling}_{\text{pl}}$) are only for illustrative purposes and do not reflect the actual scale of this MOP.

Figure 11 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, $\vec{v}_{\text{py},1}$ and $\vec{v}_{\text{pl},1}$; 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 $(0,0,0)$:

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

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

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

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:

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

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:

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

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 1: New AMs (in boldface) and MOPs added to the original OntoMOPs knowledge graph as the foundation for the subsequent expansion with Listing 5. 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-pyramidal) ₄ (2-linear) ₆ -T _d	[Zr ₃ O(OH) ₃ (C ₅ H ₅) ₃] ₄ [(C ₈ H ₈)(C ₆ H ₄) ₂ (CO ₂) ₂] ₆	4	4210.29	1955211	[17]
	[V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₄ [(C ₆ H ₄ N) ₂ (CO ₂) ₂] ₆	-8	4717.49	2259643	[61]
	[V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₄ [(C ₁₀ H ₆)(C ₆ H ₄) ₂ (CO ₂) ₂] ₆	-8	5306.45	2359340	[62]
	[V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₄ [(C ₁₄ H ₈)(C ₆ H ₄) ₂ (CO ₂) ₂] ₆	-8	5606.45	2359341	[62]
(4-pyramidal) ₆ (2-linear) ₁₂ -O _h	[V ₅ O ₉] ₆ [(C ₁₄ H ₈)(CO ₂) ₂] ₁₂	-6	5563.22	2024518	[15]
	[Co ₄ C ₄₀ H ₄₄ O ₁₂ S ₄] ₆	0	13414.08	2176774	[36]
	[(C ₁₄ N ₂ H ₁₀)Co(OH ₂) ₄ (C ₆ H ₄) ₂ (CO ₂) ₂] ₁₂				
(3-planar) ₈ (2-bent) ₁₂ -O _h	[(C ₃ N ₃)(C ₆ H ₄) ₃ (CO ₂) ₃] ₈ [VO] ₁₂	0	4310.24	1864118	[14]
(4-pyramidal)₄(2-bent)₈-D_{4h}	[V ₅ O ₉] ₄ [(C ₆ H ₄)(CO ₂) ₂] ₈	-4	2907.73	1435110	[65]
(4-planar)₆(3-pyramidal)₈-T_h	[(C ₆ H ₃) ₂ (CO ₂) ₄] ₆ [V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₈	-16	8173.54	1583722	[16]
	[(C ₆ H ₃ N) ₂ (CO ₂) ₄] ₆ [V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₈	-16	8341.66	1985926	[16]
	[(C ₆ H ₃ C) ₂ (CO ₂) ₄] ₆ [V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₈	-16	8317.90	1985927	[16]
	[(C ₁₈ H ₁₀)(CO ₂) ₄] ₆ [V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₈	-16	8629.90	1985928	[16]
	[(C ₁₈ H ₁₀)(CO ₂) ₄] ₆ [V ₆ O ₆ (C ₅ H ₄ NPO ₃)(CH ₃ O) ₉] ₈	-16	9117.88	2211525	[63]
	[(C ₁₆ H ₈ N ₂)(C ₆ H ₄ CO ₂) ₄] ₆ [V ₆ O ₆ (OCH ₃) ₉ (SO ₄)] ₈	-16	10468.30	2278526	[64]
	[(C ₁₆ H ₈ N ₂)(C ₆ H ₄ CO ₂) ₄] ₆ [V ₇ O ₁₀ (OCH ₃) ₉] ₈	-24	10619.31	2278527	[64]

Table 2: 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 5. 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 ₈ H ₈)(C ₆ H ₄) ₂ (CO ₂) ₂]	Organic	-2	344.4	2-linear	102307057
[(C ₁₄ N ₂ H ₁₀)Co(OH ₂) ₄ (C ₆ H ₄) ₂ (CO ₂) ₂]	Organic	-2	577.46	2-linear	[36]
[(C ₆ H ₄ N) ₂ (CO ₂) ₂]	Organic	-2	268.24	2-linear	11471
[(C ₁₀ H ₆)(C ₆ H ₄) ₂ (CO ₂) ₂]	Organic	-2	366.4	2-linear	101160939
[(C ₁₄ H ₈)(C ₆ H ₄) ₂ (CO ₂) ₂]	Organic	-2	416.4	2-linear	12149442
[V ₆ O ₆ (C ₅ H ₄ NPO ₃)(CH ₃ O) ₉]	Metal	1	838.01	3-pyramidal	[63]
[(C ₆ H ₃) ₂ (CO ₂) ₄]	Organic	-4	326.24	4-planar	15840397
[(C ₆ H ₃ N) ₂ (CO ₂) ₄]	Organic	-4	354.26	4-planar	15526883
[(C ₆ H ₃ C) 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 ₈ N ₂)(C ₆ H ₄ CO ₂) ₄]	Organic	-4	708.7	4-planar	132570336

Table 3: Number of new MOPs generated using Listing 5 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 5
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-b6cce614935a8	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	6289a747-62f9-49a7-a6da-4e074b99a328	210	2	300
12	(3-pyramidal) ₈ (2-bent) ₁₂ _T _h	f738bfd8-8f73-4321-9888-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}	3a3bcc5-4834-4aa9-963e-0d89df7a5242	400	0	400
18	(5-pyramidal) ₁₂ (2-linear) ₃₀ _I _h	4d34c0b4-2a4b-4f16-98dd-97e5ce7349a5	28	0	40
19	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	35076129-4856-4f04-a535-58e41810b4d2	0	1	600
20	(4-planar) ₆ (3-pyramidal) ₈ _T _h	03f32815-d43d-4fc4-94da-4157573cc668	0	7	35

¹The serial numbers of the existing AMs (1–18) align with those used in Kondinski et al. [28].

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

A.6 Algorithmic output for new assemblies

Table 4: Summary of the new metal-organic polyhedron proposed in this work using Listing 5.

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)
9a0ec222-93b7-46cf-b83f-7906cce7ad5e	(3-planar) ₄ (3-pyramidal) ₄ _Td	[(C6H3)((C6H4)2)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5398.04	16.64	38.04	10.53
fc30d610-2fe7-4c83-8739-6f222918daa	(3-planar) ₄ (3-pyramidal) ₄ _Td	[(C6H3)(C2C6H4)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5381.91	14.79	34.13	10.08
d3afe1fd-7a63-4a39-a3f5-c4379732d67	(3-planar) ₄ (3-pyramidal) ₄ _Td	[(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 _Td	[(C6H3)(C6H4)3(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	5093.65	9.06	28.57	7.1
648e3939-fbf1-4f52-a782-616f15db675	(3-planar) ₄ (3-pyramidal) ₄ _Td	[(CSNH3)2(CO2)2]4[V6O6(C5H4NPO3)(CH3O)9]4	-4	4320.79	2.26	22.22	1.55
f2a4d626-8276-4732-a5a-e39444c7a74d	(3-planar) ₄ (3-pyramidal) ₄ _Td	[(C6H3)(CO2)3]4[V6O6(C5H4NPO3)(CH3O)9]4	-8	4180.51	0.13	20.23	0
ecd8412e-9490-4e89-b334-f3d39407310e	(3-planar) ₈ (2-bent) ₁₂ O ₆	[(C6H3)((C6H4)2)3(CO2)3]8[VO]12	0	4895.28	39.23	53.76	28.18
713c0a1f-95a3-414b-b158-f489c238ffcc0	(3-planar) ₈ (2-bent) ₁₂ O ₆	[(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 ₆	[(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 ₆	[(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 ₆	[(C6H3)(CO2)3]8[VO]12	0	2460.21	14.53	23.32	9.42
02672e2a-5068-4217-b5fc-a7c9750b4b0	(3-pyramidal) ₂ (2-bent) ₃ D _{3h}	[V6O6(C5H4NPO3)(CH3O)9]2[C2H4O2(C6H3S03)2(CO2)2]3	-10	3051.14	4.95	24.68	3.98
ac83c99d-11c0-487-9c82-25bffa430711	(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
c246c22b-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-b98a9f7dacf7b	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V6O6(OCH3)9(SO4)]4[(C14N2H10)Co(OH)2(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(OH)2(C6H4)2(CO2)2]6	-8	6816.8	17.68	39.02	13.63
cb4f6f02-4f2d-418d-2299-87d71733d9d	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V7O10(OCH3)9]4[(C14N2H10)Co(OH)2(C6H4)2(CO2)2]6	-12	6648.31	17.38	39.18	13.38
a8eab9dc-1b22-4e15-8fe7-d790503c036d	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V7O10(OCH3)9]4[(C6H4)2(CO2)2]6	-12	4792.99	17.47	32.11	13
1d4c9fc3-f175-4b71-b7b8-5fcabe95810	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V6O6(C5H4NPO3)(CH3O)9]4[(C6H4)2(CO2)2]6	-8	4937.43	12.89	32.31	12.07
bbc59d07-f9be-4c1a-be9a-3a0d02a2c7e8	(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
3eed9c7-8fd9-4996-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-69223929818b	(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(OH)2(C6H4)2(CO2)2]6	0	5614.82	14.05	38.27	10.67
eddf055-6bb6-be42-1d21-9a1a-b6c06d967b5	(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
f655b1f7-18f6-484b-b9e5-d448c85ch327	(3-pyramidal) ₄ (2-linear) ₆ T _d	[Zr3O(H3)3(C5H5)3]4[(C14N2H10)Co(OH)2(C6H4)2(CO2)2]6	4	5608.65	12.6	37.11	9.49
91fd9d00-96a6-48d8-ac5-463e7a3e9d2d	(3-pyramidal) ₄ (2-linear) ₆ T _d	[Zr3O(H3)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(OH)2(C6H4)2(CO2)2]6	0	4880.32	12.33	35.78	9.28
efb5342c-064c-4930-9e90-a0188e16986	(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
032clcf7-2172-414a-9514-28a43824ca0	(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-d781ac034a	(3-pyramidal) ₄ (2-linear) ₆ T _d	[Fe3O(SO4)3(CSH5N)3]4[(C14N2H10)Co(OH)2(C6H4)2(CO2)2]6	4	6300.85	12.16	36.63	9.14
d773a08-445e-469b-bd77-d4ba9b17ce2	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V6O6(C5H4NPO3)(CH3O)9]4[(C16H12)2(CO2)2]6	-8	5105.75	9.74	29.25	9.1
143afe2d-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-1a82-40a8-85ab-87c131defe1	(3-pyramidal) ₄ (2-linear) ₆ T _d	[Fe3O(SO4)3(CSH5N)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
328e7538-0551-40b2-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
79ab46fb-6211-4635-a381-ef76492ad40	(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-b4a3-8df7-3187bd753a	(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-ab15-1cefcc3be8611	(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-f2462222c91	(3-pyramidal) ₄ (2-linear) ₆ T _d	[Fe3O(SO4)3(CSH5N)3]4[(C8H8)(C6H4)2(CO2)2]6	4	4902.49	8.95	31.66	7.14
2195aca-e785c-479e-af26-c413ab852899	(3-pyramidal) ₄ (2-linear) ₆ T _d	[V6O6(C5H4NPO3)(CH3O)9]4[(C10H6)(C6H4)2(CO2)2]6	-8	4637.08	7.16	26.81	6.67
fe5709c5-d9d7-45f8-be72-c5df2fc9b90	(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 4: (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
ca97daec-7ba50-41a7-9b21-5839eb3cdcb7	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[V6O6(CSH4NPO3)(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-b852-0fae64593dc7	(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)(C6H4)2(CO2)2]6	-12	4769.05	6.67	24.53	4.57
956c5a38-e619-475c-8e57-891088a4e4c	(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
681ef464-aa0c-4ae3-9633-39e9c946a07	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[Fe3O(SO4)3(CSH5N)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(CSH4NPO3)(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(CNH4NPO3)(CH3O)9]4[(C6H3NH2)(CO2)2]6	-8	4426.82	4.44	24.3	4.13
48737363-25a9-42b9-a583-527245486d5	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[V6O6(CSH4NPO3)(CH3O)9]4[(C6H4)(CO2)2]6	-8	4336.73	4.44	24.25	4.11
86e06ab7-109f-4ba1-b55a-a761db54471	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[V6O6(CSH4NPO3)(CH3O)9]4[(C14H8)(CO2)2]6	-8	4937.54	4.31	24.84	3.97
96cd57a2-c06f-4cd3-a3fd-ce13fd0a517	(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-c73102b8c9e	(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(CSH5N)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-2e25-4126-99e9-28a490493947	(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-e9d1-907e-e9dc2644b958	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[Fe3O(SO4)3(CSH5N)3]4[(C14H8)(CO2)2]6	4	4421.59	2.05	21.65	0.72
2e7e0f25-3e49-4877-a28b-961a69c231	(3-pyramidal) ₄ (2-linear) ₆ -T _d	[V6O6(CSH4NPO3)(CH3O)9]4[C204]6	-8	3880.16	0	19.41	0
549f16f31-6f10-4a05-b165-087c433f509	(3-pyramidal) ₈ (2-bent) ₁₂ -C ₈	[V6O6(CSH4NPO3)(CH3O)9]8[(CSH5)(CH3)(CO2)2]12	-16	9082.65	12.54	32.29	10
792aef56-9301-42cb-8fc7-2e10fd2ccce	(3-pyramidal) ₈ (2-bent) ₁₂ -T _h	[PW9037Ni6NH2C4H3]8[(C6H3)(OCH3)(CO2)2]12	-24	23903.77	13.07	38.24	3.06
ac2a61be-ace3-4d8b-a2ba-c74716828f0	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C16H8N2)(C6H4CO2)4]6[V6O6(CSH4NPO3)(CH3O)9]8	-16	10956.28	21.46	40.73	8.9
793015c2-1cd2-498a-9ba4-1057c9fc290d	(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(HO)2(CO2)3]8	0	7083.33	19.49	37.54	5.74
8744df1bc-2b24-4563-ab00-2dc814eca94	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C16H8N2)(C6H4CO2)4]6[Fe3O(SO4)3(CSH5N)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)(CO2)4]6[Pd3PO(C3H7N)3]8	0	6257.55	13.14	26.47	4.16
dc95add3-e84d-4df5-8084-3d27c576331	(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-41ff-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
3e25529e-f5e7-44d0-980a-0de147001e1	(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
c82fbf8e-4b6-4410-4tf0-cc7389ad708	(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
cd843f3f-e064-c19-85ec-18e0ec1486	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C6H3N)2(CO2)4]6[V6O6(CSH4NPO3)(CH3O)9]8	-16	8829.64	10.12	29.64	2.32
b0e5526-0388-44b0-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-c8b1-4dc8-aae4-95489907a60	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C6H3C)2(CO2)4]6[V3O2(HO)2(CO2)3]8	8	6389.57	12.43	27.52	2.28
7748425b-2d7c-42f3-90df-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-891dccc8461a1	(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-43d0-860f-59306c36cb15	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C6H3C)2(CO2)4]6[V3O2(HO)2(HCO2)3]8	0	4932.93	12.15	26.22	2.05
343cd95b-2da2-4946-9ef4-2a9d38a98802	(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
8d77525c-021e-4ff9-ba2-10554c5264cf	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C6H3N)2(CO2)4]6[V3O2(HO)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
10933be1-e9e8-485e-91ee-81b5039ca273	(4-planar) ₆ (3-pyramidal) ₈ -T _h	[(C18H10)(CO2)4]6[V3O2(HO)2(HCO2)3]8	0	5244.93	12.11	27.5	1.18
9ad1115d-3235-4a78-b3d-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
3fff4b8e-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[V3O2(HO)2(HCO2)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-4261-9959-28d8758e608	(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
6be143c1-6429-4899-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-1b19-4f13-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-l75aa94e715f	(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 4: (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-pyramidal) ₃ (2-bent) ₆ _D _{3h}	[Zn4C40H44O12S4] ₃ [(C4H2S)(CO ₂) ₂]6	0	4340.62	6.52	30.01	2.94
c975a140-2f44-4da9-954b-bfaea7f098a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3) ₂ (CO ₂) ₂]8	-4	3500.33	13.33	24.8	9.31
846d20cc-3dbb-4548-a309-fa679105494e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	3232.57	12.87	21.97	8.91
6ba1f2c6-8147-4956-b587-0251b07a65da	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	6036.44	11.83	39.75	8.39
ba5f8318-5d17-46f0-92ab-89e208a0c992	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C56H76012S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	6572.19	11.96	36.52	8.39
05d6f468-69cb-4b43-a8a8-95aa73f61598	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	5667.16	11.99	36.17	8.37
6e7c17b-e6bf-457c-92ab-97408bcd767d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	5716.6	11.93	36.04	8.34
009fc610-69d0-4203-b5f4-3bdc0901e143	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	7126.28	11.83	36.18	8.31
7aa54b76-c139-4cf3-b1e3-2b2e20cb0a23	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76012S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	7122.41	11.81	36.13	8.3
057d132f-866b-4075-8a4e-730e01cb1138	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	5330.88	11.87	31.45	8.28
23f2d5ad-3c19-45d6-9ba5-bcf5962d4649	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	5327.03	11.84	31.4	8.27
fd5698be-7c17-419b-b853-a772fb3b504a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	5674.51	11.76	36.89	8.2
bbea90f3-d2e1-4d26-952f-f2ec9e003e0b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H18O24S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	-16	6595.76	11.68	34.52	8.16
03e6a62e-56f7-4038-a2d1-09fdff212ce5	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C10H6)(CO ₂) ₂]8	-4	3308.2	12.3	23.18	8.1
07d04db5-4415-477e-bf28-4169a3f663e1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	6224.72	11.46	35.93	8.1
4f1f007f-af1d-4f05-8b24-3a83c55ce88d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	6331.87	11.44	35.89	8.09
39420859-2035-49dc-8e8b-1a0dc6a3030c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C10H6)(CO ₂) ₂]8	0	3040.43	11.86	20.45	7.67
056b2b2-5287-4f23-8ee8-53b0b863c34	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ [(C6H3) ₂ (CO ₂) ₂]8	0	6228.56	10.71	35.86	7.62
c4ab94d7-ac74-4ec8-a072-e5eb9475a75	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C10H6)(CO ₂) ₂]8	0	5844.31	10.86	38.24	7.14
16131400-e991-4db0-8b20-6835c240bcbb1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C56H76012S4] ₄ [(C10H6)(CO ₂) ₂]8	0	6380.06	10.99	34.96	7.12
8b433046-80f9-9a3e-056f47545c636	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C10H6)(CO ₂) ₂]8	0	5475.03	11.01	34.64	7.11
3d42506a-0ca0-4da4-b1d1-d13aa6d80b9c9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C10H6)(CO ₂) ₂]8	0	5524.47	10.96	34.51	7.07
9ebfb082-9916-4251-ad06-af4d13feac3e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C10H6)(CO ₂) ₂]8	0	6934.15	10.87	34.62	7.03
2da94335-7e07-47be-a238-d38966cd7fd	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C10H6)(CO ₂) ₂]8	0	5138.75	10.89	29.91	7.02
7c14ab97-432e-41b8-9a98-d7f4edadbe18	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76012S4] ₄ [(C10H6)(CO ₂) ₂]8	0	6930.27	10.85	34.57	7.02
a491a6d9-22f3-4800-91fb-b02a0771100a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [(C10H6)(CO ₂) ₂]8	0	5134.9	10.87	29.86	7.01
808c5596-104b-4895-bc11-72d8bae5cba3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ [(C10H6)(CO ₂) ₂]8	0	5482.37	10.79	35.32	6.93
5f018c78-110d-4020-bae6-l1d5f83d8e80	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H18O24S4] ₄ [(C10H6)(CO ₂) ₂]8	-16	6403.63	10.7	32.95	6.9
5531ba7a-90aa-43c6-a046-b99c0d89b56	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ [(C10H6)(CO ₂) ₂]8	0	6032.59	10.49	34.42	6.85
64116819-068d-446f-9185-f8c27468d5ac	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ [(C10H6)(CO ₂) ₂]8	0	6139.73	10.48	34.38	6.84
21301c3f-9e47-44d0-9f1f-b77faf97091	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ [(C10H6)(CO ₂) ₂]8	0	6036.43	9.78	34.34	6.35
7e33daa6-efb3-49df-a39a-11da157f670	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H4)(CO ₂) ₂]8	0	2639.97	9.96	17.54	5.47
69d240d4-72f4-4cac-9966-67f8c19ef76	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3OH)(CO ₂) ₂]8	-4	3035.73	10.42	20.02	5.02
9e96f6cb-d73c-4c08-b184-af683401050	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5443.84	8.9	35.32	4.95
ead2cc02-11cd-41c3-899b-1fc8955894d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OCH3)(CO ₂) ₂]8	-4	3147.94	10.42	20.02	4.85
e97fb070-106a-4832-89c5-5c528e2ad283	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H4)(CO ₂) ₂]8	0	5074.56	9.06	31.69	4.83
6bad4023-6513-4ba8-8dd8-10f8267fb3e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5124	9.01	31.56	4.79
dd635530-90b4-44d7-8e6a-6725bc467571	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H4)(CO ₂) ₂]8	0	4738.28	8.95	26.92	4.79
041ca318-264c-400a-95ea-04d576b273b0	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [(C6H4)(CO ₂) ₂]8	0	4734.43	8.93	26.88	4.78
f9718b5c-6471-430c-8f36-12838aa9bae	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C56H76012S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5979.59	9.02	31.94	4.78
683a0591-9610-49a5-bc57-bf43d781a315	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H4)(CO ₂) ₂]8	0	6533.68	8.89	31.6	4.69
442db98e-6a8a-47bb-ae6d-c482db1c9495	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(CO ₂) ₃]8	-12	3251.75	10.41	20.01	4.69
e60b7d67-7a41-4225-4976-87efcf75c6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76012S4] ₄ [(C6H4)(CO ₂) ₂]8	0	6529.81	8.87	31.56	4.68
aa6e1b64-39a4-4baa-bad2-452a0e8b4157	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ [(C6H4)(CO ₂) ₂]8	0	5632.12	8.54	31.49	4.66
f7dcda4f-2604-4072-9057-8028f856f8c3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H8O24S8] ₄ [(C6H4)(CO ₂) ₂]8	-16	6003.16	8.76	29.92	4.66
758c317a-350b-45a1-b567-bccccb55c2c00	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5081.9	8.84	32.26	4.65
c147bdc8-facd4f9e-9846-915e03268126	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5739.26	8.53	31.45	4.65
57004130-10bc-4053-9d90-565b9de6809	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3OH)(CO ₂) ₂]8	0	2767.96	9.96	17.54	4.5
e28033ce-5684-4853-96e6-04f6e6a1370	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)(OCH3)(CO ₂) ₂]8	0	2880.17	9.96	17.8	4.46
5b78e7f9-4dff-434a-a28f-c098cb6e6890	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)(CO ₂) ₃]8	-8	2983.98	9.96	17.53	4.17
59b035b7-071f-4926-a619-18995159137a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ [(C6H4)(CO ₂) ₂]8	0	5635.96	7.8	31.42	4.15
582e979c-8d8e-4cccd-b203-576f97ff118f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3OH)(CO ₂) ₂]8	0	5571.84	8.9	35.32	4.01

Continued

Table 4: (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 [(C6H ₃)(OCH ₃)(CO ₂) 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 [(C6H ₃ (CH ₃))(CO ₂) 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 [(C6H ₃ NH ₂)(CO ₂) ₂] ₈	-4	3027.85	10.42	20.02	3.91
82625b08-8b1a-4921-b3aa-f5edac65fa52	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	5314.77	9.07	31.68	3.86
6f165bb2-3af3-45a9-9ec3-74462b0aa169	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O4] ₄ [(C6H ₃ OH)(CO ₂) 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 [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	4978.49	8.95	26.92	3.83
1111b7a-b178-4582-969a-eba90073c2c7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	4866.28	8.95	26.92	3.83
97f41eca-f4c7-4f07-a4e3-6c489b97a5cce	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	5364.21	9.01	31.55	3.82
c60ce960-d9ce-4060-b364-8d89df76e878	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H76O12S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) 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 [(C6H ₃ OH)(CO ₂) ₂] ₈	0	5252	9.01	31.56	3.82
11e33ac3-cdb8-4d1d-9fc0-9c8ba4987c9c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	4862.43	8.93	26.88	3.81
9eda58a9-7bb7-4ec1-b490-9e9b4ed11817	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H76O12S4] ₄ [(C6H ₃ OH)(CO ₂) 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 [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	4974.64	8.93	26.88	3.81
13e02df-0b7a-4598-a04b-53b0b4d009fa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H ₂ O)(CH ₂ CH ₂ CH ₂)(CO ₂) ₂] ₈	-4	3348.17	10.42	22.15	3.74
02a2ee4-0c84-4324-8f8d-b821ca428f1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	5760.12	8.54	31.49	3.73
2faea5d7-1a20-494c-b1b1-b842505acd267	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	6773.89	8.9	31.59	3.72
1b5b790-7860-43d6-f949-0a859d8942b4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	6661.68	8.89	31.6	3.71
5dd1564f-ea9e-d41d-8af4-d47c2b41d9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn ₄ C40H44O12S4] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	5867.26	8.53	31.45	3.71
5792c164-d7e0-46dc-af4-224ec1b96f159	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	6770.01	8.89	31.55	3.71
663ed0ad-9134-46ae-be4c-19d04935f17a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H ₃ OH)(CO ₂) 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 [(C6H ₃ OH)(CO ₂) 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 [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	-16	6243.37	8.76	29.92	3.69
f6fc6ab9-38d1-439f-9b53-b48423553a9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C40H44O12S4] ₄ [(C6H ₃ OH)(CO ₂) ₂] ₈	0	5209.9	8.84	32.26	3.68
584e9f6c-60a2-4b94-8660-1d5e53138a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C40H44O12S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	5322.11	8.84	32.26	3.68
5e531cf-c6205-496f-a57c-906e01c1d84	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H28O4S4] ₄ [(C6H ₃)(CO ₂) 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 [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	5872.33	8.54	31.49	3.68
247e049b-ee08-46f4-ba1e-e19b47a97187	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn ₄ C40H44O12S4] ₄ [(C6H ₃)(OCH ₃)(CO ₂) ₂] ₈	0	5979.47	8.53	31.45	3.67
14d6012c-6598-4843-8322-f3ffe93596f7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O4] ₄ [(C6H ₃)(CO ₂) ₃] ₈	-8	5418.58	9.06	31.67	3.53
826478e9-d9de-4257-aa23-6e1503d9822	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ O ₃)(CO ₂) ₂] ₈	0	3272.41	9.96	18.67	3.52
224c83fc-24cc-4af8-93e0-029df96ee93d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ Br)(CO ₂) ₂] ₈	0	3271.14	9.96	17.54	3.52
4fb2b1d3-9339-4014-b5db-f5f6426c4eb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(CH ₃))(CO ₂) ₂] ₈	0	2752.18	9.96	17.54	3.52
39c45ef-fe18-44b2-9640-49de372a21d5	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ O)(CH ₂) ₁₁ CH ₃ (CO ₂) ₂] ₈	0	4114.49	9.95	40.72	3.52
f680391-fb9c7-45b8-ef4e-eee288b3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(C6H ₁₂ O ₂)(C9H ₅ O ₂)(CO ₂) ₂] ₈	0	4722.24	9.91	40.49	3.52
1c5e04fd-a911-4c7b-8e24-ec63ea9a04e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(OCH ₂ CH ₂ CH ₃)(CO ₂) ₂] ₈	0	3104.6	9.96	21.9	3.52
0fa6b0f8-2c2b-46ef-93d9-a9a57b311fb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₂ O)(CH ₂ CH ₂ CH ₂)(CO ₂) ₂] ₈	0	3080.41	9.96	21.78	3.52
e1248bce-8791-443c-aef0-4d81906e478	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(OCH ₂ CH ₃)(CO ₂) ₂] ₈	0	2992.38	9.96	20.17	3.52
7cf33184-6895-4d00-815c-3e611b2d67e9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(OC2H4) ₃ (OH)(CO ₂) ₂] ₈	0	3825.22	9.94	34.64	3.52
ef7cb2d4-b5d5-4d88-8614-8e8248bc61e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(N2(C6H ₄ CH ₃))(CO ₂) 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 [(C6H ₃ (NO ₂))(CO ₂) ₂] ₈	0	2999.95	9.96	17.94	3.52
dd313c87-542e-4fab-b9e5-f1480721059	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ NH ₂)(CO ₂) ₂] ₈	0	2760.08	9.96	17.54	3.52
03970ae-e3af-4dc8-8831-51d8083d1256	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ C6H ₂ (OC16H ₃₃)) ₃ (CO ₂) ₂] ₈	0	9018.89	9.96	61.36	3.52
0b2e88eb-4c2d-4b9b-a2fa-ec2d1b57746	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(OC2H4OH)(CO ₂) ₂] ₈	0	3120.38	9.96	22.34	3.52
f9fabfb-349a-4e8-9838-3312f279df1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(C3H6O ₂)(C9H5O ₂))(CO ₂) ₂] ₈	0	4385.6	9.94	34.89	3.52
6216bda7-1df4c7-8775-c27bc24454c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(C1CH ₃)(CO ₂) ₂] ₈	0	3088.81	9.96	19.91	3.52
f6312165-e2a1-4c96-e21-dcc20632f493	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(OCH ₂ C2H)(CO ₂) ₂] ₈	0	3072.34	9.96	22.4	3.52
01ba9ad7-32e5-441e-ad43-e42ab563cb9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(CH ₂)(C4N2H202CH ₃)(CO ₂) 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 [(C6H ₃ N2C6H ₃ (CH ₃)) ₂ (CO ₂) ₂] ₈	0	3697.26	9.94	28.07	3.52
bf677a7-92ee-402c-8404-93278861e57	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃)(C2H4O ₂)(CONH ₆ H ₅))(CO ₂) 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 [(C6H ₃ C2S5i(C3H7)3)(CO ₂) ₂] ₈	0	4082.85	9.94	26.99	3.51
b351c04-8447-4f6a-a612-6f76b692d15b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H ₃ CO2C2H4S4(CH ₃) ₃ (CO ₂) 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 [(C6H ₃ Br)(CO ₂) 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 [(C6H ₃ CH ₂ CS3C4H9(CO ₂) ₂] ₈	0	4066.67	9.9	30.79	3.5

Continued

Table 4: (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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)CH2CS2(C6H5)(CO2)] ₈	0	3970.07	9.92	25.29	3.5
37929ad8-25b2-42ba-a3db-55c4d3447852	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)CO2CH3(CO2)] ₈	0	3104.26	9.93	20.85	3.5
dff7668-1e56-44c5-a683-64a73129aebd	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)OCOCHCH2(CO2)] ₈	0	3200.34	9.93	22.47	3.5
8801c583-2167-4526-92dc-d6f655837e26	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H3)(CO2)] ₈	-8	5082.29	8.94	26.91	3.5
892bc8a2-bd65-4bc2-a5f2-ccdf5d28eadf6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)O(CH2)4CH3(CO2)] ₈	0	3329.02	9.92	27.07	3.5
b9aaea0a-a3bb-44e8-b3a7-806498d27a37	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)O(CH2)3CH3(CO2)] ₈	0	3216.81	9.92	24.49	3.5
1027d8ea-ca54-4555-a0ea-9d3c1b49f66	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)(OC2H4)] ₂ (OH)(CO2)] ₈	0	3472.8	9.91	27.9	3.49
8c72225a-ec3f-4aa6-bcc2-1923767a7ff	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)(OC2H4)] ₃ (OCH3)(CO2)] ₈	0	3937.43	9.92	36.45	3.49
1e0556fc-d700-4519-bf6c-3478bb582b9d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)NHCO2C(CH3)] ₃ (CO2)] ₈	0	3561	9.91	24.39	3.49
4d9a0a09-84ce-4851-bf53-a769c60f897	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)O(CH2)13CH3(CO2)] ₈	0	4338.92	9.92	48.76	3.49
e067a04a-7472-49b1-92dd-2e357922750d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H44O4S4] ₄ [(C6H3)(CO2)] ₈	-8	5468.01	9	31.54	3.49
a14bf1b-cabb-4f3a-9f74-5f385eb575f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)(C2H4O2)(C9H5O2)](CO2)] ₈	0	4273.39	9.92	32.33	3.49
cb4d1d4e4-9fa5-46c4-96b3-d6e84a863c58	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V4O8] ₄ [(C6H3)NHCOC(CH3)] ₃ (CO2)] ₈	0	3433.01	9.92	23.52	3.49
1b980ad2-e5f5-4357-9079-2591181065a8	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [(C6H3)(CO2)] ₈	-8	5078.45	8.92	26.87	3.48
62cc803b-2e3f-4154-9635-e5ef1f4fd3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C56H76O12S4] ₄ [(C6H3)(CO2)] ₈	-8	6323.61	9.02	31.92	3.48
2ece2eb8-5dac-4388-8e14-c3021a866354	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ [(C6H3)(CO2)] ₈	-8	5976.13	8.54	31.48	3.4
c67e05e4-21f8-4149-911f-a166edf36b69	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ [(C6H3)(CO2)] ₈	-8	6083.28	8.52	31.44	3.39
fd3cc09a-af10-4e0b-023-d46e623c3b37	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [(C6H3)(CO2)] ₈	-8	6877.69	8.89	31.58	3.38
5fefef1d-fab1-e445-8786-b4d37abb15e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H3)(CO2)] ₈	-8	6873.82	8.87	31.54	3.37
dd12d1c-8edf-4c8b-81a5-33a0eb0259b7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H8O24S8] ₄ [(C6H3)(CO2)] ₈	-24	6347.17	8.76	29.91	3.37
b46e96bd-acb-4fc3-88a0-6c9371299627	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ [(C6H3)(CO2)] ₈	-8	5425.92	8.83	32.25	3.35
f1a455d-d70b-44be-95bf-4446958d105	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OCH2C2H)](CO2)] ₈	-4	3340.11	10.42	22.78	3.23
ccb45327-e3c3-4ed0-abd6-a1e77591f66	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ [(C6H3OH)(CO2)] ₈	0	5763.96	7.8	31.42	3.21
03e1440c-702b-4705-ab5e-4667ba06201	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ [(C6H3)(OCH3)(CO2)] ₈	0	5876.17	7.8	31.42	3.21
f5047b2c-4226-4480-a455-b16dc57e137c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OCH2)11CH3](CO2)] ₈	-4	4382.26	10.4	41.08	3.11
66010140-f0a9-4e98-a793-d78eb9ca438	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OCH2CH2CH3)](CO2)] ₈	-4	3372.36	10.42	22.29	3.11
1968008c-6b08-49bc-b094-76f954fe5d5	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(N2(C6H4CH3))](CO2)] ₈	-4	3852.81	10.42	28.21	3.11
005f0468-975d-4d73-8ac5-3a035ca60f60d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(NO2)](CO2)] ₈	-4	3267.71	10.42	20.02	3.11
72288b20-2a8d-4da0-b204-5335ca38a092	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OCH2CH3)](CO2)] ₈	-4	3260.15	10.42	20.59	3.11
40a0887f-a1a1-46a0-968a-10f5aabdd0f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OC2H4)](OH)(CO2)] ₈	-4	4092.98	10.4	35.06	3.11
5b02d725-df8a-4cb4-9865-7732ccb121c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OC2H4OH)](CO2)] ₈	-4	3388.14	10.42	22.75	3.11
9d048b6c-1cf3-435f-9955-5156c3a3d68b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(C3H6O2)(C9H5O2)](CO2)] ₈	-4	4653.37	10.39	35.22	3.11
9a413da2-d88e-4c31-77dbf3b6c43	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)C6H2(O1C16H33)3](CO2)] ₈	-4	9286.65	10.42	61.63	3.11
c1f0e64-8b5f-42cd-92d8-178c8d21633	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(CH3)](CO2)] ₈	-4	3356.57	10.42	20.34	3.11
18fb3827-c7c5-42f0-a2a2-28c8519cc2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3SO3)](CO2)] ₈	-4	3540.18	10.42	20.02	3.11
26c89477-1ec3-4f31-9586-7bf6fa5f1185	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(C2H4O2)(C9H5O2)](CO2)] ₈	-4	4541.16	10.37	32.66	3.11
b473b78c-1086-4fe8-b7ea-44062e010f6d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)N2C6H3(CH3)](CO2)] ₈	-4	3965.02	10.4	28.43	3.11
61966025-af83-4e59-af0d-a5a1d60d78	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(C6H12O2)(C9H5O2)](CO2)] ₈	-4	4990	10.37	40.8	3.1
5ce0c201-f222-4aa0-6a1c17949fc68	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)C2Si(C3H7)](CO2)] ₈	-4	4350.61	10.4	27.39	3.1
8de55fe9-0843-4592-a803-fc078267e7c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(CH2)(C4N2H202CH3)](CO2)] ₈	-4	4012.72	10.41	26.18	3.1
a4f3ecbc-c241-486e-bca8-340582c02743	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(C2H4O2)(CONH6H5)](CO2)] ₈	-4	4341.11	10.39	33.33	3.1
79217c42-a9a5-4792-8c4c-d5c21ec9623f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)CO2CH3](CO2)] ₈	-4	3732.02	10.39	21.27	3.09
cbbffcc7-75c2-466a-90fd-dc0e2ab5e0eb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)CO2CH2CH2]2(C6H3)](CO2)] ₈	-4	3468.1	10.39	22.85	3.09
85e28bf4-93bb-48f0-aa2d-a8427925f3b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)CO2C2H4Si(CH3)3](CO2)] ₈	-4	4061.67	10.39	28.32	3.09
9fd5582a-9041-43bb-bd68-0f112f402e38	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)CH2CS3C4H9](CO2)] ₈	-4	4334.43	10.35	31.13	3.08
9ec3e022-e900-4a89-a045-9d727d93bc24	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OC2H4)](OH)(CO2)] ₈	-4	3740.56	10.37	28.3	3.08
f311fc8c-8a3-4b43-b66a-98cce2bd1e6a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)O(CH2)4CH3](CO2)] ₈	-4	3596.78	10.37	27.42	3.08
34e1cb4-649c-4bd7-acb1-e4a5e14db1f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)CH2CS2(C6H5)](CO2)] ₈	-4	4237.83	10.38	25.7	3.08
e40971d6-9fc5-475f-80cf-3396c3fc032e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)(OC2H4)](OCH3)](CO2)] ₈	-4	4205.19	10.37	36.88	3.08
0b24ea4a-fed4-4fa1-bbfbf-ddd1a0f957c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)NHCO2C(CH3)](CO2)] ₈	-4	3828.77	10.37	24.78	3.08
44e368cb-89b9-4eef-b8f3-aed4fbcb6870	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)O(CH2)13CH3](CO2)] ₈	-4	4606.68	10.37	49.04	3.08
0db45e56-63ad-4bed-b890-5d4601ee6fe6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₄ [(C6H3)NHCO2C(CH3)](CO2)] ₈	-4	3700.77	10.37	23.93	3.08

Continued

Table 4: (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[(C6H ₃ O(CH ₂) ₃ CH ₃ (CO ₂) ₂] ₈	-4	3484.57	10.38	24.85	3.08
deb93359-9efc-4a3a-9d94-ccf6e3a26f6d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C6H1202)(C9H5O ₂)](CO ₂) ₂] ₈	0	8061.86	9.06	40.28	3.05
d30532ae-4e52-4c61-80ca-8ddac192d1bc	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ CH ₂ CS ₃ C4H ₉ (CO ₂) ₂] ₈	0	7406.29	9.01	31.86	3.04
b6120179-3a69-4a18-92a5-d3d5e00e35f4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(OH)(CO ₂) ₂] ₈	0	7164.84	9.06	34.29	3.04
88fa4c45-659f-f4d5-8e2a-b723999fc292	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ N2C6H ₃ (CH ₃)(CO ₂) ₂] ₈	0	7036.88	9.05	31.89	3.03
9f4a8c38-aca0-45cd-96f6-leb6ab1540a4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C6H ₂ O(C16H ₃₃)(CO ₂) ₂] ₈	0	12358.51	9.2	61.07	3.01
66cdab96-7833-4ee5-9ed9-e5b910935261	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ O(CH ₂) ₁ CH ₃ (CO ₂) ₂] ₈	0	7454.12	9.1	40.44	3
715faa83-82db-4fd0-9869-287973b69c4a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ SO ₃)(CO ₂) ₂] ₈	0	6612.04	9.03	31.93	3
e1fdbecc0-3305-426e-926e-9ed343a6a63b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ (CH ₃))(CO ₂) ₂] ₈	0	6091.8	9.03	31.93	3
ea8512c1-4501-4911-8325-9f8917ad486b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H3Br)(CO ₂) ₂] ₈	0	6610.76	9.02	31.94	3
1a687303-13e5-476b-8896-8cf3325024b7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂ CH ₂ H ₃)(CO ₂) ₂] ₈	0	6444.22	9.05	31.91	3
7efd4a05-7196-4fb8-95f5-d2a68dd053a1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(N ₂ (C6H4CH ₃))(CO ₂) ₂] ₈	0	6924.67	9.06	31.9	3
d40984a9-d8fd-4233-8256-57c0060e186	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(2OH)(CO ₂) ₂] ₈	0	6812.42	9.02	31.86	3
91afeb21-6789-4a41-a530-c917bf6dc241	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂ CH ₃)(CO ₂) ₂] ₈	0	6332.01	9.04	31.92	3
405b15a9-75bc-4908-b808-96570ece91c7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ O)COCH ₂ CH ₂ (CO ₂) ₂] ₈	0	6539.97	9.01	31.89	3
8c80550f-902a-4a7d-86dd-727999b605cac	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ CO ₂ CH ₃)(CO ₂) ₂] ₈	0	6443.88	9	31.89	3
cac45fc0-dd9f-4ab7-99e6-b1b9c5381a7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ CH ₂ S ₂ (C6H ₅)(CO ₂) ₂] ₈	0	7309.69	9.03	31.86	3
bf7e93c6-7dbd-4732-8d4b-8d6172b57fb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₂ O)(CH ₂ CH ₂ CH ₂)(CO ₂) ₂] ₈	0	6420.03	9.05	31.91	3
bbfb23a-27e7-40b5-abc2-4e2c18a06373	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ (NO)) ₂ (CO ₂) ₂] ₈	0	6339.57	9.02	31.93	3
c00938f4-6c57-47ef-8225-6a3fa211568c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(OH)(CO ₂) ₂] ₈	0	6460.01	9.05	31.91	3
bbf2c88e-6a23-4014-b878-93cdf2073dd4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂ CH ₂)(CO ₂) ₂] ₈	0	6411.97	9.04	31.92	3
f796c39d-d109-4b7f-9922-d954a3035a1a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ NH ₂)(CO ₂) ₂] ₈	0	6099.71	9.02	31.93	3
b6ef5fbf-6c1b-4419-967a-f39a5c07dd1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(CH ₃)(CO ₂) ₂] ₈	0	6428.44	9.06	31.91	3
a95b1f13-8afc-49b5-9b6c-b0587ed0aab	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C2H ₄ O ₂)(CONHC6H ₅)(CO ₂) ₂] ₈	0	7412.97	9.06	32.75	3
f2e22acd-e402-426e-a509-51d41e7fb5e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(CH ₂)(C4N ₂ H ₂ OCH ₂)(CO ₂) ₂] ₈	0	7084.58	9.06	31.89	3
eb6f5064-8a54-44da-9067-4710861f31513	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C6H ₃ Si)(C3H ₇)(CO ₂) ₂] ₈	0	7422.47	9.08	31.85	2.99
deea5166-8a38-4c23-943a-017451368524	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(3OCH ₃)(CO ₂) ₂] ₈	0	7277.05	9.04	36.1	2.99
5c90419e-0b72-4fc9-a0c0-25bc969752c2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C3H ₆ O ₂)(CH ₉ H ₅ O ₂)(CO ₂) ₂] ₈	0	7725.23	9.06	34.68	2.99
89c73608-2385-4d49-8f08-22990528858e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂ CH ₃)(CO ₂) ₂] ₈	0	6556.43	9.02	31.87	2.99
430139d2-a93f-45c4-bd07-527f25a01602	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂)(C13CH ₃)(CO ₂) ₂] ₈	0	7678.54	9.08	48.56	2.98
c749515-d4af-4b6a-b779-2bc38d8424d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ CO ₂ CH ₄ Si)(CH ₃)(CO ₂) ₂] ₈	0	7133.53	9.05	31.87	2.98
fa7daab-4371-4ff1-96ed-18d95c606403	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃ HNCO ₂)(CH ₃)(CO ₂) ₂] ₈	0	6900.63	9.02	31.86	2.98
8f32a8f7-5e33-4b3d-8a8d-ea93f1e4fc7b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(NHCO ₂)(CH ₃)(CO ₂) ₂] ₈	0	6772.63	9.02	31.86	2.98
a133740a-5676-42d3-b4e3-74c0a96b0da	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(OCH ₂)(CH ₃)(CO ₂) ₂] ₈	0	6668.64	9.02	31.86	2.98
8fd6782d-4e04-4e2d-abfc-f0026ef1f8e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃)(C6H1202)(C9H5O ₂)](CO ₂) ₂	0	7156.83	9.05	40.08	2.96
1f59169-8474-481e-9c32-007478765a2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃)(OC ₂ H ₄)(3OH)(CO ₂) ₂] ₈	0	6259.81	9.06	34.04	2.96
93e1f1d4-ebcb3-4ac6-8005-74ccc9e2a86	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg ₄ C56H ₇ 601254]4[(C6H ₃)(C2H4O ₂)(CH ₉ H ₅ O ₂)](CO ₂) ₂	0	7613.02	9.04	32.12	2.96
05991b74-5980-44d4-b7b8-88794ad48f48	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C56H ₇ 601254]4[(C6H ₃)(C6H1202)(C9H5O ₂)](CO ₂) ₂	0	8615.95	8.93	40.2	2.95
899840c6-f7b3-4b6f-9460-108f8ae64931	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃ CH ₂ CS ₃ C4H ₉)(CO ₂) ₂] ₈	0	6501.26	9.02	31.65	2.95
8f20637b-d4d5-4d36-8d60-c3b675e9358aa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(3OH)(CO ₂) ₂] ₈	0	7718.93	8.93	34.17	2.95
5dc9a15e-ed9d-4308-b27b-ec9d9dc9e7c6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni ₄ C56H ₇ 601254]4[(C6H ₃)(C6H1202)(C9H5O ₂)](CO ₂) ₂	0	8612.08	8.91	40.18	2.94
319d4e9-ad07-4a45-b91e-b93d2226f97	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C56H ₇ 601254]4[(C6H ₃ CH ₂ CS ₃ C4H ₉)(CO ₂) ₂] ₈	0	7960.38	8.88	31.52	2.94
878eecc44-8f56-441e-a353-571bb6961e9d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃)(N ₂ (C6H4CH ₃))(CO ₂) ₂] ₈	0	6131.85	9.06	31.67	2.94
167ab4e5-c416-444e-9e37-824ede080322	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni ₄ C56H ₇ 601254]4[(C6H ₃)(OC ₂ H ₄)(3(OH)(CO ₂) ₂] ₈	0	7715.06	8.91	34.16	2.93
146b22af-07a7-4c96-8b71-7687b8ec4aab	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C48H28O4S4]4[(C6H ₃)(NH ₂)(CO ₂) ₂] ₈	0	5563.96	8.9	35.32	2.93
931f22d4-cach-469c-821a-cc3af221f668	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃)(C6H2)(OC16H33)(CO ₂) ₂] ₈	0	11453.48	9.14	60.95	2.93
d965caa3-d6a0-4f21-88b2-eb671bea2d3c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C56H ₇ 601254]4[(C6H ₃)(C6H3N2C6H3)(CH ₃)(CO ₂) ₂] ₈	0	7590.97	8.92	31.55	2.93
0061d404-88e4-4804-9d0-a1fa77575456	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H ₃)(CH ₃)(CO ₂) ₂] ₈	0	5186.77	9.06	31.68	2.92
27300769-ea25-4990-a8d6-614beebec73	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H3Br)(CO ₂) ₂] ₈	0	5705.73	9.06	31.69	2.92
750ca27a-2cc6-4857-93d3-3a9265d9306c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe ₄ C40H44S4O ₄]4[(C6H3SO ₃)(CO ₂) ₂] ₈	0	5707.01	9.06	31.68	2.92
e3a32299-c834-44b0-9e85-8572e14348b6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni ₄ C56H ₇ 601254]4[(C6H ₃ CH ₂ CS ₃ C4H ₉ (CO ₂) ₂] ₈	0	7956.51	8.86	31.48	2.92
ea041cc-c8a8-42c5-a5f2-611585440cd0	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co ₄ C40H44S4]4[(C6H ₃)(C6H1202)(C9H5O ₂)](CO ₂) ₂	0	7206.27	8.99	40.04	2.92

Continued

Table 4: (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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(N2(C6H4CH ₃))(CO ₂) ₂] ₈	0	6019.64	9.08	31.68	2.92
1c97c0be-c889-4dd4-8-101-dca5e1d49aa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OC2H ₄)(OH)(CO ₂) ₂] ₈	0	5907.39	9.03	31.64	2.92
e2710f96-23b7-46eb-b6ef-7eee4dd5924	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OCH2CH2CH ₃)(CO ₂) ₂] ₈	0	5539.19	9.08	31.68	2.92
089adbf76-644e-4d54-a895-a56e3de101ba	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OCH2CH ₃)(CO ₂) ₂] ₈	0	5426.98	9.07	31.68	2.92
00c7cf0f-67a3-46c6-8f61-6fe0c7b05cfb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃ O)COCHCH ₂ (CO ₂) ₂] ₈	0	5634.93	9.04	31.65	2.92
50f0e0b8-7c68-423b-b0fc-be985d9ef02	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₂ O)(CH2CHCH ₂)(CO ₂) ₂] ₈	0	5515	9.07	31.68	2.92
eed99af-8d70-4b3f-9a1e-917c59bfcbfc	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4] ₄ [(C6H ₃)(OC2H4)(3OH)(CO ₂) ₂] ₈	0	6309.25	9.01	33.99	2.92
88beab3d-c8f5-49b6-9f02-1b125d653cb6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(CH2CS2(C6H ₅))(CO ₂) ₂] ₈	0	6404.66	9.04	31.64	2.92
eebb9d0c-657e-4b23-b9c4-276549d5808d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃ CO2CH ₃)(CO ₂) ₂] ₈	0	5538.85	9.03	31.65	2.92
a69d5099-2589-4531-a815-f1d2b86cd900	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(NO ₂)](CO ₂) ₂] ₈	0	5434.54	9.06	31.68	2.92
8dab8036-aa83-419e-8254-888dcf5aa193	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OC2H4OH)(CO ₂) ₂] ₈	0	5554.97	9.07	31.68	2.92
f4b096c6-a636-403c-a007-9b8ae529953f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3NH2)(CO ₂) ₂] ₈	0	5194.68	9.06	31.68	2.92
229142a1-c3cc-4794-b846-a6229b49f7a9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OCH2C2H)(CO ₂) ₂] ₈	0	5506.94	9.07	31.68	2.92
ce5d740-f330-4e7b-ac81-78614e2b0653	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(C(CH ₃))](CO ₂) ₂] ₈	0	5523.4	9.08	31.68	2.92
81132245-512d-4b04-9d09-89bf5609c210	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76012S4] ₄ [(C6H3N2C6H3)(CH ₃)(CO ₂) ₂] ₈	0	7587.1	8.91	31.51	2.92
917eed12-299b-45f4-a6e9-fa1c24b3d218	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(C2H4O2)(CONHC6H5)(CO ₂) ₂] ₈	0	6507.94	9.06	32.52	2.92
99532833-b859-48e6-96d5-09c21a65bb5b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(CH2(C4N2H2O2CH ₃))(CO ₂) ₂] ₈	0	6179.55	9.07	31.67	2.92
5ab624ba-e06f-4089-9271-108713778d47	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(C6H12O2)(C9H5O2)](CO ₂) ₂] ₈	0	7526.11	8.91	40.06	2.91
2dbe9440-acd2-4706-a072-54b204542a7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(O(CH ₂))1CH3](CO ₂) ₂] ₈	0	6549.09	9.09	40.23	2.91
78ca70aa-7a9a-4ec2-9020-cd4fc239q9f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3C2Si(C3H ₇))(CO ₂) ₂] ₈	0	6517.44	9.08	31.66	2.91
e9008593-65ff-4e8e-8660-f4182abb62ea	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3CH2CS3C4H9)(CO ₂) ₂] ₈	0	6550.7	8.97	31.52	2.91
f5e30e7f-f8e8-4c1b-9d8f-9e0389e4367	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)(CH3)](CO ₂) ₂] ₈	0	5556.05	8.91	35.32	2.91
34498fe3-628a-428f-ba84-42987a047168	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(C3H6O2)(C9H5O2)](CO ₂) ₂] ₈	0	6820.2	9.07	34.45	2.91
4d5c2d02-9d88-42ec-980d-8036b1d56130	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H ₃)(C6H2)(C6H33)](CO ₂) ₂] ₈	0	12912.6	9.07	61	2.91
301e1f8d-8746-4b25-bcba-3d91ef48c622	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(O(CH ₂))3CH3](CO ₂) ₂] ₈	0	5651.4	9.04	31.64	2.91
88b2c54-5083-4132-9eef-22aa8748dea	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H ₃)(C2H4O2)(CONHC6H5)](CO ₂) ₂] ₈	0	7967.05	8.93	32.66	2.91
13079996-1754-419b-b6f4-3aa509ba24e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3S03)](CO ₂) ₂] ₈	0	7166.12	8.9	31.59	2.9
91a151220-ba4f-4ad3-a724-1db5852d7df	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(CH3)](CO ₂) ₂] ₈	0	6645.89	8.9	31.59	2.9
aeed9670-427f-4a37-a9e6-56f75dc8b42	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3Br)](CO ₂) ₂] ₈	0	7164.85	8.89	31.6	2.9
e136e5a9-b92e-40a4-946c-cde9cc1a0a9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(O(CH ₂))1CH3](CO ₂) ₂] ₈	0	8008.21	8.97	40.34	2.9
8e4ba84f-31fd-46ec-b1a2-e87f57eb316b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(OC2H4)(OH)](CO ₂) ₂] ₈	0	7366.51	8.89	31.52	2.9
0f8d103f-fedf-47b2-a8a8-641d484ef4f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H ₃)(OC2H4)(3OCH ₃)](CO ₂) ₂] ₈	0	6372.02	9.05	35.85	2.9
199513f1-27aa-49ad-9495-4a73c5b816ed	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)(OC2H4)(3OCH ₃)](CO ₂) ₂] ₈	0	6629.09	8.92	35.29	2.9
9a981bae-2eed-4126-9914-12999nf967e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(OCH2CH3)](CO ₂) ₂] ₈	0	6886.1	8.91	31.58	2.9
aaec3198-880a-4661-9a5-56f75dc8b462	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(OCH2CH2CH3)](CO ₂) ₂] ₈	0	6998.31	8.92	31.57	2.9
938dbb0b-b857-4788-9b98-6414d33c9f6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(N2(C6H4CH ₃))] (CO ₂) ₂] ₈	0	7478.76	8.94	31.56	2.9
4613788e-af9d-46f8-8803-792aa15c60f8	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(CO2CH3)](CO ₂) ₂] ₈	0	6997.97	8.87	31.56	2.9
60f52ab-b4d6-45ea-84db-fed59716fcae	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H2O)(CH2CHCH2)](CO ₂) ₂] ₈	0	6974.12	8.92	31.58	2.9
ba434b14-a0dd-46dd-b0bc-a39dac54c621	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3O)COCHCH ₂](CO ₂) ₂] ₈	0	7094.05	8.88	31.55	2.9
f11df548-b326-4e95-9c-99dhabf1bb9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(CH2CS2(C6H5))] (CO ₂) ₂] ₈	0	7863.78	8.9	31.52	2.9
97eeef21-a4b2-4ec9-9d79-6f2e16e57cef	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(NO ₂)](CO ₂) ₂] ₈	0	6893.66	8.89	31.6	2.9
2d6e7e24-5d9d-4e81-970c-0134cce1d117	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3NHCO2C(CH3 ₃))] (CO ₂) ₂] ₈	0	5995.6	9.03	31.64	2.9
0e577cfb-9e7b-4cba-867-94abdd7c3d9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3NH2)](CO ₂) ₂] ₈	0	6653.8	8.89	31.6	2.9
952e918-f5db-4da0-9cf3-6f229000e8d7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(OCH2C2H)](CO ₂) ₂] ₈	0	6966.06	8.91	31.58	2.9
8f9161d1-fd04-e86-97c1-3a5506657fe	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3)(O(CH ₂))3CH3)] (CO ₂) ₂] ₈	0	6773.51	9.06	48.37	2.9
a84cf959-e4d7-4a33-98b4-690255d7b49	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(C3H6O2)(C9H5O2)] (CO ₂) ₂] ₈	0	8279.32	8.94	34.59	2.9
ebf0d659-a867-4122-9998-40de6f98e02b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(OC2H4OH)](CO ₂) ₂] ₈	0	7014.09	8.92	31.58	2.9
10d8c909-8dd3-41cc-bb93-0f601ab0a754	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76012S4] ₄ [(C6H3)(C6H2)(C16H33)] (CO ₂) ₂] ₈	0	12908.73	9.06	60.99	2.9
ada7dd4f-157e-429f-a3fe-1d886c2bee54	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3CO2C2H45i(CH3 ₃))] (CO ₂) ₂] ₈	0	6228.5	9.05	31.66	2.9
ce5db39-91fd4-c08-b80f-16317bc33ea4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(C(CH3 ₃))] (CO ₂) ₂] ₈	0	6982.52	8.93	31.57	2.9
02ae818c-43e6-4682-acca-d4497d7dfief	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4O4] ₄ [(C6H3)NHCOC(CH3 ₃)] (CO ₂) ₂] ₈	0	5867.6	9.03	31.64	2.9
b3d92fba-e331-4ee1-9e5a-08bed94c767	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76012S4] ₄ [(C6H3)(CH2)(C4N2H2O2CH3)] (CO ₂) ₂] ₈	0	7638.67	8.93	31.55	2.9

Continued

Table 4: (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-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3Br)(CO2)2] ₈	0	7160.98	8.87	31.56	2.89
6007bfc5-1fae-413d-abbb-5cfb3d181716	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3(CH3))(CO2)2] ₈	0	6642.02	8.88	31.55	2.89
a24515f1-911a-4ec2-93ce-e331e68ec4a4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [C6H3CH2CS3C4H9(CO2)2] ₈	0	6870.54	8.87	35.26	2.89
ec4cc858-6563-44ce-8d0d-aea78875b29b	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3)(OC2H4) ₂ (OH)(CO2)2] ₈	0	7362.64	8.87	31.48	2.89
099a097-75a6-4a77-be4f-f413d165c567	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [C6H3CO2CH3(CO2)2] ₈	0	6994.09	8.86	31.51	2.89
9a067530-7175-49d1-acdd-04ddcd54a1200	(4-pyramidal) ₄ (2-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-d3a365269c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3(NO2))(CO2)2] ₈	0	6889.79	8.88	31.55	2.89
b90fc8d-937-461-847b-fcb2d4a5a92b	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H2O)(CH2CHCH2)(CO2)2] ₈	0	6970.25	8.9	31.53	2.89
74ba5f89-7c7a-487b-94ee-2b82a305e188	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3)CH2CS2(C6H5)(CO2)2] ₈	0	7859.91	8.88	31.48	2.89
ce21d653-30b2-4f2-861e-d9626907295f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [C6H3OCOCHCH2(CO2)2] ₈	0	7090.18	8.86	31.51	2.89
3466ced0-a718-42f6-acb7-6a146e3f5bde	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3NH2)(CO2)2] ₈	0	6649.92	8.88	31.55	2.89
66aacc0e-1ab4-4ac9-968a-3edaae4d44	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [C6H3CO2C2H4Si(CH3)3(CO2)2] ₈	0	7687.62	8.92	31.53	2.89
0485fc0d-055f-49f3-a93-73a1b73203	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(CO2)3] ₈	-8	5979.97	7.79	31.41	2.89
ea4c1682-6240-4b39-9274-717ab2d15765	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ (C6H3O)(CH2)13CH3(CO2)2] ₈	0	8232.63	8.95	48.48	2.89
aabb508-6b51-438f-891a-4c6a10117b55	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)C6H2(OCl16H3)3(CO2)2] ₈	0	11502.92	9.09	60.92	2.89
3d1f25c2-3146-4779-82b0-5f38e61f751d	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-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-b5e4-7cf8a877077b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3)(OC2H4OH)(CO2)2] ₈	0	7010.22	8.9	31.53	2.89
9ff6b676-fa51-4e13-9a15-e7ffd42dedb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3SO3)(CO2)2] ₈	0	7162.25	8.88	31.55	2.89
5835a6f5-f78-4b1e-879-f5b333084e2a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3)(C2H4O2)(CONHC6H5)(CO2)2] ₈	0	7963.18	8.91	32.64	2.89
67b2890f-db02-4627-9ba2-44c0687ff9b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [C6H3N2C6H3(CH3)2(CO2)2] ₈	0	6501.13	8.92	35.29	2.89
99cc0d0ca-eb9-4d17-99cd-2a2f3edcc4c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ (C6H3)(O(CH2)3CH3)(CO2)2] ₈	0	7110.52	8.89	31.53	2.89
d87d4c0b-1ed9-4ac4-a6f4-cd8421a5ca2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3)(CH2)(C4N2B2O2CH3)(CO2)2] ₈	0	7634.79	8.91	31.51	2.89
fa7ab05f-6316-4675-8822-538ch3ea3160	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4] ₄ [C6H3](O(CH2)4CH3)(CO2)2] ₈	0	5763.61	9.03	31.65	2.89
036dbe57-c521-44b4-bd47-7584e74299df	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3SO3)(CO2)2] ₈	0	5756.44	9.01	31.55	2.88
3b2a53fb-5673-4f49-a9a3-1dc8c7e7dd99	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ (C6H3C25i(C3H7)3(CO2)2] ₈	0	7972.68	8.94	31.47	2.88
7e6421cf-4083-41d0-884c-4e5c3a0417c9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(CH3)(CO2)2] ₈	0	5236.21	9.01	31.55	2.88
9167ba30-9f0b-49a6-9649-976ff9b2764	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3Br)(CO2)2] ₈	0	5755.17	9.01	31.56	2.88
5998hb0b-e160-4175-9f04-282a1eb08139	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(OCH2CH2CH3)(CO2)2] ₈	0	5588.63	9.02	31.55	2.88
79acaf4-c494-4622-a7d-8104b617236e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(N2(C6H4CH3))(CO2)2] ₈	0	6069.08	9.03	31.55	2.88
00e6f15d-a9a7-49ff-b4f0-e530a88a5637	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(OC2H4)(CO2)2] ₈	0	5956.83	8.98	31.51	2.88
eb749534-fc4b-4b0b-840a-18026ec3e559	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ (C6H3)(O(CH2)4CH3)(CO2)2] ₈	0	7222.73	8.89	31.53	2.88
638e10bd-30af-4c18-4c8-d192087b139	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(O(CH2)3CH3)(CO2)2] ₈	0	5476.42	9.02	31.55	2.88
252d584c-325f-45b1-83b1-2d208ac0e06	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3CO2CH3)(CO2)2] ₈	0	5588.29	8.98	31.52	2.88
2c58e94e-6d07-463c-98c5-8fe870f70f4341	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H20)(CH2CHCH2)(CO2)2] ₈	0	5564.44	9.02	31.55	2.88
eea6cb1f-cf63-4738-b04c-4c2d296b079d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(CH2CS2(C6H5)(CO2)2] ₈	0	6454.1	8.99	31.51	2.88
ae9ba024-d5bb-451e-974d-60fc67c648a8	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(O(C2H4)(CO2)2] ₈	0	5483.98	9.01	31.56	2.88
19f05b17-d782-482b-a23e-e533b1722ca2	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3NH2)(CO2)2] ₈	0	5244.12	9.01	31.56	2.88
389642dd-2e4b-48d9-9a26-115ddfb0855	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ (C6H3)(OCH2C2H)(CO2)2] ₈	0	5556.38	9.02	31.55	2.88
7d959bfc-dfa4-4ae3-8f5c-9b2d22850fdfd	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ (C6H3NHC02(C3H3)(CO2)2] ₈	0	7454.72	8.89	31.52	2.88
b088aec-ae48-49c3-97de-7649ecd5b977	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Fe4C40H44S4] ₄ (C6H3)((C2H4O2)(C9H5O2))(CO2)2] ₈	0	6707.99	9.04	31.89	2.88

Continued

Table 4: (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-be5d-bed13731c569	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(C2H4O ₂)(CONHC6H ₅)(CO ₂) ₂] ₈	0	6557.37	9.01	32.48	2.88
d721791e-f007-49ab-844e-83fa0a7a2c6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(CH ₂)(C4N2H ₂ O2CH ₃)(CO ₂) ₂] ₈	0	6228.99	9.02	31.54	2.88
eee3abd8-bffe-4f74-98e1-a2cd86a9f51a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [(C6H ₃)(NHCOC(CH ₃)) ₃ (CO ₂) ₂] ₈	0	7326.72	8.89	31.52	2.88
3500ca26-7c7d-4e04-9e1f-5232508f7a88	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(O(CH ₂)) ₁ CH ₃ (CO ₂) ₂] ₈	0	6598.53	9.03	40.19	2.87
39a6d371-fb3b-460e-9042-f66ca0fc2837	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3Br)(CO ₂) ₂] ₈	0	6075.01	8.9	35.32	2.87
626df82b-38bb-4447-ba7a-4905299ce57	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3C2Si(C3H ₇))(CO ₂) ₂] ₈	0	6566.88	9.03	31.53	2.87
9cf94ee1-72e2-4c62-abf5-7b3e3dc1831	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(OCH2CH2CH ₃)(CO ₂) ₂] ₈	0	5908.47	8.92	35.3	2.87
4410ccaa-7c58-4fa0-bff6-06c984f4899	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(N ₂ (C6H4C3))(CO ₂) ₂] ₈	0	6388.92	8.93	35.29	2.87
125a984c-db00-47b8-8ef0-72b9637a401d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3OCOCHCH ₂)(CO ₂) ₂] ₈	0	6004.21	8.88	35.28	2.87
53685c7-c3b4-44ef-9b78-645267906ae3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H2O)(CH2CHCH ₂)(CO ₂) ₂] ₈	0	5884.28	8.92	35.31	2.87
b45188e3-0cb5-492e-8619-bc66e49c64ba	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(OCH2CH3)(CO ₂) ₂] ₈	0	5796.26	8.92	35.31	2.87
b3451d07-1b95-46b4-9475-811306caeae06	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3(NO ₂))(CO ₂) ₂] ₈	0	5803.82	8.9	35.32	2.87
fcff3175-5b7e-48ce-bc3f-c92563093f08	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H ₃)(OC2H4) ₃ (OCH3)(CO ₂) ₂] ₈	0	7827.27	8.9	35.96	2.87
02b935b7-faf9-47fc-b7b6-1bcba1ca168	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H3CO2C2H4Si)(CH3) ₃ (CO ₂) ₂] ₈	0	7683.75	8.9	31.49	2.87
0e87a69c-bdfd-4d33-8154-09254452b20	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(C3H6O ₂)(C9H5O ₂))(CO ₂) ₂] ₈	0	6869.64	9.01	34.41	2.87
366fcfd-b014-446b-8838-af1d7b18f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H3NHC02C(CH3) ₃ (CO ₂) ₂] ₈	0	7450.84	8.88	31.48	2.87
82df6371-deb0-4805-abd0-0e52f1fceafa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H3O)(CH2) ₃ 13CH ₃ (CO ₂) ₂] ₈	0	8228.75	8.93	48.47	2.87
396931fb-730d-4159-aa72-ae1b958ac5a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)(C6H2(O)C16H3)(CO ₂) ₂] ₈	0	11822.76	9.02	60.91	2.87
352e21bd-9e41-4b61-8014-66f27d9abf56	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(O(C2H4OH))(CO ₂) ₂] ₈	0	5924.25	8.92	35.31	2.87
4f10b36-4ef1-4144-b474-6a4ae56a292b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)(OCH2C2H)(CO ₂) ₂] ₈	0	5876.22	8.91	35.31	2.87
15644b52-b28b-4065-831f-c2d00d76c2e3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)(C(CH3) ₂)(CO ₂) ₂] ₈	0	5892.68	8.93	35.3	2.87
e4f7e0b-4a21-4cf0-aao0-e79063598f48	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3SO ₃)(CO ₂) ₂] ₈	0	6076.28	8.91	35.32	2.87
5127b9e49-acd9-4897-8004-1eb7226f3667	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H3)NHCOC(CH3) ₃ (CO ₂) ₂] ₈	0	7322.85	8.87	31.48	2.87
6a66f02c-251f-4073-b8bc-56413c353473	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(C2H4O ₂)(CONHC6H ₅)(CO ₂) ₂] ₈	0	6877.21	8.92	35.28	2.87
d0f2a564-02d4-4b3a-9f56-e4e51e035065	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C56H76O12S4] ₄ [(C6H ₃)(C2H4O ₂)(C9H5O ₂))(CO ₂) ₂] ₈	0	8167.11	8.91	32.03	2.87
e8e26fa2-2985-42d7-96f1-563b8e3701c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(O(CH2CH3)(CO ₂) ₂) ₂] ₈	0	5700.84	8.99	31.51	2.87
3f96ea9f-4385-41fe-a7cc-3f3f8a3d924	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(O(CH2)11CH ₃)(CO ₂) ₂] ₈	0	6918.37	8.95	40.2	2.86
453e5c1-a09d-4b85-8904-2998d10a3648	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H ₃)(O(CH2)4CH3)(CO ₂) ₂] ₈	0	7218.86	8.87	31.48	2.86
ed733558-2364-4548-9cd0-b1b7212f90ee	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(OC2H4)(H2O)(CO ₂) ₂] ₈	0	6276.67	8.88	35.26	2.86
1e12a592-7513-4712-b758-144d4b4ca032	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3CO2CH3)(CO ₂) ₂] ₈	0	5908.13	8.88	35.29	2.86
c54e41fc-de88-4aa3-ba9b-9f2e22cf760	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(OC2H4)(3(OCH3)(CO ₂) ₂) ₂] ₈	0	6421.46	8.99	35.8	2.86
8b4c5e88-2835-4605-9a5a-1aedc77d605	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(CH2CS2)(C6H5)(CO ₂) ₂] ₈	0	6773.94	8.89	35.26	2.86
201ea9f-78b7-4dec-9d70-291620c6d2b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3CO2C2H4S)(C3H3)(CO ₂) ₂] ₈	0	6277.94	9	31.53	2.86
459e0664-daf4-48c7-b8e6-13bacd230f28	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3NHCO2C(CH3) ₃ (CO ₂) ₂] ₈	0	6045.04	8.98	31.51	2.86
87d7e07-907-1f08-4953-aafe-5c69e4596231	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(C(H6O2)(C9H5O2))(CO ₂) ₂] ₈	0	7189.48	8.92	35.28	2.86
a41be13-4cd4-4027-9d15-8942fb798b2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(O(CH2)13CH ₃)(CO ₂) ₂] ₈	0	6822.95	9.01	48.34	2.86
81b897ad-f4a3-4aae-88b5-9029164cce89	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(NHCOC(CH3) ₃ (CO ₂) ₂) ₂] ₈	0	5917.04	8.98	31.51	2.86
c397f735-3732-4440-9e8d-020bb189e0c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(CH2)(C4N2H ₂ O2CH3)(CO ₂) ₂] ₈	0	6548.83	8.92	35.29	2.86
95aa97bd-5a42-499c-b5a497c29d6a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3C2Si(C3H ₇))(CO ₂) ₂] ₈	0	6886.72	8.94	35.26	2.85
6506a4c4-889b-402f-800f-f8e5db6ea7f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H3NHCO2C(CH3) ₃ (CO ₂) ₂] ₈	0	6741.3	8.9	35.81	2.85
2a34c495-73c0-4aff-9e13-4d6612533cf4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3CO2C2H4Si(CH3) ₃ (CO ₂) ₂] ₈	0	6597.78	8.91	35.27	2.85
833ca412-898e-4132-80a9-11b63b1ac	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(O(CH2)4CH3)(CO ₂) ₂] ₈	0	5813.05	8.98	31.52	2.85
93127699-c7ce-482e-a5fe-e028b4bba24a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(O(CH2)3CH3)(CO ₂) ₂] ₈	0	6020.68	8.89	35.27	2.85
bb1fd111-4c93-47f3-9af8-bea816dcfc93	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C56H76O12S4] ₄ [(C6H ₃)(C(H6O2)(C9H5O2))(CO ₂) ₂] ₈	0	8163.23	8.89	32.01	2.85
c53966d8-fa20-4e44-9135-287d742a3de2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H ₃)(C(H6O2)(C9H5O2))(CO ₂) ₂] ₈	0	6820.55	8.91	39.84	2.84
99b68d8c-e1f5-471e-80df-b9854b6d163	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(O(CH2)4CH3)(CO ₂) ₂] ₈	0	6132.89	8.89	35.26	2.84
56205ec0-411e-4d9a-9c27-6cb9d6c3506a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(O(CH2)13CH ₃)(CO ₂) ₂] ₈	0	7142.79	8.93	48.35	2.84
8ca883c7-4fa2-4567-ab02-b4d40b4c3bb2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3NHCO2C(CH3) ₃ (CO ₂) ₂] ₈	0	6364.88	8.89	35.26	2.84
6da19650-2ed3-45b9-8d42-372f47334f0b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O4S4] ₄ [(C6H ₃)(C2H4O2)(C9H5O2))(CO ₂) ₂] ₈	0	6757.43	8.99	31.85	2.84
fc6d8290-1e4b-4d37-8c44-c694lc58ebeff	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H3)NHCOC(CH3) ₃ (CO ₂) ₂] ₈	0	6236.88	8.89	35.26	2.84
04e19c84-c5aa-4ca7-8ffe-3d8cc2518261	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [(C6H ₃)(OCH2)(O)(CO ₂) ₂] ₈	0	5923.53	8.93	33.74	2.83
a616ba19-1a75-4aa3-8fa6-bc565c139373	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C48H2804S4] ₄ [(C6H ₃)(C(H6O2)(C9H5O2))(CO ₂) ₂] ₈	0	7077.27	8.9	35.29	2.83

Continued

Table 4: (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-4234-8847-5e9eaccd462	(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-ce91fc50bc9	(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-45ce-8eb6-a314837057d	(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-95b0-79250860890	(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-b499-49e5-9822-9a23979f15	(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
d19f5487-7fdf-4aa9-8650-beef0c90ff10	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3)C6H2(O16H33) 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-a775-b0e9259f61fb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3(CH3)) ₂ (CO2) ₂]8	0	4850.49	8.95	26.92	2.79
b8ea86b6-4599-41b4-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-3c157802613f	(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
d7fdf3c-b721-4bco-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
edc6e882-85cb-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-81e9334eedda	(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
b51e4a7-d66a-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-b4e-f62c2ea40291	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3OOCOCH2CH2)(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-279a236ce19	(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
c6a8a3f33-eecf-445a-7c3-9035142674ab	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3NH2)(CO2) ₂]8	0	4858.4	8.95	26.92	2.79
20b56845-5a89-49b5-928d-2e5534706577	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ ((C6H3)C(CH3) ₂ (CO2) ₂]8	0	5187.12	8.96	26.92	2.79
a4094753-071b-45bc-a742-d27b90088ba	(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
136c5bd-094f-461b-891-757dbe46ce0	(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-4c14-9e11-571aa391aaa	(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-cd5-4614-8795-8b2f4a3601b	(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 (C6H3C2S(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-e3fa-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
ad26421-ff00-4cd6-a52b-5c1ba049569	(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
0484c3f2-944c-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-fbb0a294ab83	(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
60d53b37-2907-4c92-aaa0-3b0a6d75336d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3OOCOCHCH2(CO2) ₂]8	0	5294.81	8.9	26.85	2.78
5c5a2d47-df4c-46a1-813c-9ea06c59850	(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-4244-83f2-4ab140a814f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H2O)(CH2CH2)(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
1f9da9c0-1b90-44e1-9f26-379f25e20299	(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-fa520a7cab	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ ((C6H3)NH2)(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(C3H3)(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-9175-477bf2ae6364	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(OCH2C2H)(CO2) ₂]8	0	5166.81	8.93	26.88	2.78
fd82da-a61d-4e95-9e13-535ad7ca65e0	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)C6H2(O16H3) ₃ (CO2) ₂]8	0	11113.35	8.94	60.77	2.78
7f80f7e-389b-4c97-a71a-dbbf81a4e089	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3)(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-b0b2-4f83-83c2-61c80bc8c748	(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 4: (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)] 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)(CH2)13CH3(CO2)] ₈	0	6437.23	8.92	48.16	2.77
8c0eedda-d7db-4174-bf63-84ac93a5d318	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ [C6H3NHCO2C(CH3)] ₃ (CO2)] ₈	0	5659.32	8.91	26.88	2.77
f9053291-df9a-47ed-aea7-7d130b942bb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(C3H6O2)(C9H5O2)](CO2)] ₈	0	6480.07	8.91	34.18	2.77
14e79c66-f935-421c-8803-bc81323b7dd	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(CH2)(C4N2H202CH3)](CO2)] ₈	0	5839.42	8.92	26.87	2.77
30579s80-c8e5-43fa-9132-05bb70b12554	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H12O12S4] ₄ (C6H3)(NHCOC(CH3)) ₃ (CO2)] 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)] ₈	0	5311.27	8.89	26.84	2.77
b0d19b68-9134-4b94-ab9-b93f7823e04	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ (C6H3N2C6H3)(CH3) ₂ (CO2)] 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)] ₈	0	5427.33	8.91	26.89	2.77
3aaabe34-a89f-46ad-ab76-56b1d47cb154	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [C6H3C25i(C3H7)] ₃ (CO2)] 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)] ₈	0	6031.89	8.89	35.53	2.76
0a049fd4-369c-4d0b-93a9-ebc23dfb12f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [C6H3CO2C2H4Si(CH3)](CO2)] ₈	0	5888.37	8.9	27.09	2.76
0d922a38-0965-4bc5-bbf7-8154d1a7d063	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(O)(CH2)3CH3(CO2)] ₈	0	6433.38	8.89	48.14	2.76
b50fe756-6661-416f-a325-92d9191d5b0	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ (C6H3)C6H2(O)(C16H33)](CO2)] 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)] 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)] ₈	0	5714.35	8.84	32.26	2.75
ccf470f1-a4d6-4acf-bda6-49b54f14c6d7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ (C6H3(CH3))](CO2)] ₈	0	5194.12	8.84	32.26	2.75
c1d381bb-80fe-4452-9c60-fcb919764046	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3Br)](CO2)] ₈	0	5713.07	8.84	32.26	2.75
5edf6fb1-e349-44ce-81f3-42dac08bfc69	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(OC2H4)(2OH)(CO2)] ₈	0	5914.74	8.8	32.21	2.75
d6885041-7011-48d6-8a3d-32a0677cea68	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(O)(CH2)4CH3(CO2)] ₈	0	5423.48	8.89	26.84	2.75
0d418434-0603-4f47-bf54-9ccb73f0a67	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3CO2CH3)(CO2)] 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)] ₈	0	5546.53	8.85	32.25	2.75
81c1817e-fa60-41f8-809f-cc133eda075e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(N2(C6H4CH3))](CO2)] ₈	0	6026.99	8.85	32.25	2.75
8d9f68d-07f1-4159-bd4f-533c76daff0e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(OCH2CH3)](CO2)] ₈	0	5434.32	8.84	32.26	2.75
bd969362-3d5f-49b6-b455-06dfdc4a0388	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H2O)(CH2CHCH2)(CO2)] ₈	0	5522.35	8.84	32.25	2.75
d0f381c-d493-4c34-9cd6-62b4dca8ed2b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ (C6H3OCOCH2CH2)(CO2)] 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)] ₈	0	6412.01	8.81	32.21	2.75
6a73ee24-012c-4095-a73f-afc4cf6228c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(NO2)](CO2)] ₈	0	5441.89	8.84	32.26	2.75
dafeae44-88b8-46e5-a56b-5c74dead08d4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3NH2)](CO2)] ₈	0	5202.02	8.84	32.26	2.75
60a3e478-d72a-4ed6-9711-02de8cb00aa9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(OCH24OH)](CO2)] ₈	0	5562.32	8.84	32.25	2.75
45c01b83-8cf7-4ea9-a481-798e1198da99	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ [C6H3NHCOC2(CH3)](CO2)] ₈	0	5655.47	8.89	26.84	2.75
58719aba-4125-45e8-b8e6-d45f62d1ba9d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ ((C6H3)C(CH3))](CO2)] ₈	0	5530.75	8.85	32.25	2.75
8f28a216-a105-46a8-a50b-5881a2e42b2f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(OCH2C2H)(CO2)] ₈	0	5514.28	8.84	32.26	2.75
74521f159-2673-4c08-a911-07ff2b282ee	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(CH2)(C4N2H2O2CH3)](CO2)] 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)(CONCH6G5)](CO2)] ₈	0	6515.28	8.83	32.25	2.75
bc70f06b-f460-4c6f-90b4-fe27a9e9924	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(NHCOC(CH3))](CO2)] ₈	0	5527.47	8.89	26.84	2.75
0afa0d24-7837-4260-910b-2161444c733d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)CSi(CH3)](CO2)] ₈	0	6524.78	8.84	32.23	2.74
2849f7b7-f81f-4c9f-80c1-e8ed22b54775	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C0H44O12S4] ₄ (C6H3)(O)(CH2)11CH3](CO2)] ₈	0	6556.43	8.85	39.96	2.74
441c66ea-7a18-43e0-b0c0-a295fe80fee	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(C(H6O2)(C9H5O2))](CO2)] ₈	0	6827.54	8.83	34.19	2.74
a9b5b3c00-4201-4f54-8468-8bc8ed6782a3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(O)(CH2)3CH3](CO2)] ₈	0	5658.74	8.81	32.22	2.74
e29ed01f3-253e-4e45-9153-68183b4e7000	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C24H12O12S4] ₄ (C6H3)(C2H4O2)(C9H5O2)](CO2)] ₈	0	6367.86	8.89	31.61	2.74
dbe91f12-fd5c-429b-8e68-514c96381af	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(OCH24CH3)](CO2)] 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)(3OCH3)](CO2)] ₈	0	6379.36	8.81	35.53	2.73
172c8451-97ef-41a7-a859-a157be6183c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(NHCO2C(CH3))](CO2)] ₈	0	6002.94	8.8	32.21	2.73
8cdec12-d645-4cab-91ef-aa1ebc80acb8	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3CO2C2H4Si(CH3))](CO2)] ₈	0	6235.85	8.82	32.23	2.73
97e1f2e9-d157-4b7f-8d4f-3c4983bc9266	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(O)(CH2)13CH3](CO2)] 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)(NHCO(C(CH3)))](CO2)] ₈	0	5874.95	8.8	32.21	2.73
17819e36-6d37-4a70-9d88-76196555801f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Mg4C40H44O12S4] ₄ (C6H3)(C2H4O2)(C9H5O2)](CO2)] ₈	0	6715.33	8.81	32.24	2.71
bf47e1b0-c040-4f08-a10-61077c2679da	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H8024S8] ₄ (C6H3)(C6H202)(C9H5O2)](CO2)] ₈	-16	8085.43	8.72	39.72	2.7
2b2bc298-3f24-4648-90b3-bb4053ba3227	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H8024S8] ₄ (C6H3)(OC2H4)(3OH)(CO2)] ₈	-16	7188.41	8.74	33.56	2.69
65270415-e483-4833-9330-8ef5f4d0611f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C24H8024S8] ₄ (C6H3CH2CS3C4H9)(CO2)] ₈	-16	7429.86	8.7	29.95	2.68
81141fb7-c512-4e30-a732-dbd2fa4b0222	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S0412] ₄ (C6H3(CH3))](CO2)] ₈	0	5744.33	8.54	31.49	2.68

Continued

Table 4: (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)
f7161bf0-3bbaa-49c5-b367-ebfe2b79f2b3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[C6H3N2C6H3(CH3)2(CO2)2]8	-16	7060.45	8.75	29.92	2.68
918cf1f11-4f09-4d91-a846-4ff0583e700c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C4H4O12S4]4[(C6H3(CH3)(CO2)2]8	0	5851.48	8.53	31.45	2.67
304a020a-7384-48de-8fb1-6fe5ccce70a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3NH2)(CO2)2]8	-16	6123.28	8.76	29.92	2.66
55cbad87-3205-4754-8bfc-102101b4a71	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)C6H2(OC1H3)3(CO2)2]8	-16	12382.08	8.78	60.67	2.66
49f6fa87-0084-4cf7-93c0-2d59062a2693	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]4[(C6H3(CH3))(CO2)2]8	-16	6115.37	8.76	29.92	2.65
0a41b4d4-8a80-4ea5-a02-ce1777d6ea76	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	-16	6948.24	8.76	29.92	2.65
93345b1e-7997-4b22-a9f3-056aa3f7c2f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OCH2CH3)(CO2)2]8	-16	6355.58	8.76	29.92	2.65
d14e4641-b05f-4e26-acaa-7ae5c57a42ffc	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	-16	6467.79	8.77	29.92	2.65
3306ef05-d2b4-4931-8246-ce94fb2fad	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3CO2CH3(CO2)2]8	-16	6467.45	8.73	29.9	2.65
e1cd0d60-eaf4-4fab-ab2-4ff19b98af54	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3(NO2))(CO2)2]8	-16	6363.14	8.76	29.92	2.65
48085b7b-849b-45a1-b22e-5ecc125c012c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H2O)(CH2CHCH2)(CO2)2]8	-16	6443.6	8.77	29.92	2.65
9897a1f-5ad2-4038-944e-f15712981018	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]4[(C6H3O)COCHCH2(CO2)2]8	-16	6563.53	8.73	29.89	2.65
404e6fa0-591b-4066-8697-faledc6bc242	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]4[(C6H3)(OCH2CH2)(CO2)2]8	-16	6435.54	8.76	29.92	2.65
8b5e05d-3200-4cc0-9092-16092151	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)C(C6H3)(CO2)2]8	-16	6452	8.77	29.92	2.65
02527590-024f-4170-9cc1-e24ba3163fc9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]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}	[Co4C4H8O24S8]4[(C6H3)(C2H4O2)(CONHC6H5)(CO2)2]8	-16	7436.53	8.74	32.12	2.65
4994cab-eab1-49c3-9053-c9f4494ea683	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OCH2)1CH3(CO2)2]8	-16	7477.69	8.76	39.83	2.64
608373c7-dd21-40b8-89a1-319e62974db	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3C2Si(C3H7)(CO2)2]8	-16	7446.04	8.75	29.9	2.64
f21dc008-821b-42bc-8-6bb2cf6bd62	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OC2H4)(C3CH)(CO2)2]8	-16	7300.62	8.72	35.37	2.64
3e8a01b-2e19-41f4-b9b7-d6816b81115f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3NH2)(CO2)2]8	0	5752.24	8.54	31.49	2.64
9be03ff-07ca-446f-9ca6-8877e08bf988	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(C3H6O2)(C9H5O2))(CO2)2]8	-16	7748.8	8.74	34.07	2.64
19570eb7-f6df-4832-bf62-f437e9f3769	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(CH2)3CH3(CO2)2]8	-16	6580	8.73	29.89	2.64
cb445570-242d-4785-92fd-0d866d8244d1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OCH2)4CH3(CO2)2]8	-16	6692.21	8.72	29.89	2.63
3e0660b2-0c20-49fa-58d2-b62357fd69f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C4H4O412S4]4[(C6H3NH2)(CO2)2]8	0	5859.38	8.53	31.45	2.63
62546655-cd3-4df3-b9d4-247e7e562783	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3CO2C2H4Si(C3)(CO2)2]8	-16	7157.1	8.73	29.9	2.63
61853735-3222-47cf-86d1-5a605df29434	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)(OCH2)1CH3(CO2)2]8	-16	7702.11	8.73	48.04	2.63
dc07d72-572d-45f-98af-2084221b681b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3NHCO2C2CH3)(CO2)2]8	-16	6924.2	8.72	29.88	2.63
7def83e-9007-45e2-8664-03a2fa02195a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]4[(C6H3)NHCOC(CH3)(CO2)2]8	-16	6796.2	8.72	29.88	2.63
1d4e3707-9be4-461b-9388-a81c38ba0d74	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C4H8O24S8]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}	[Ni4C4H4S4O12]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7714.39	8.49	39.54	2.53
91e15a85-89f1-432d-8e4a-5c5928a84f4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3)(OC2H4)(3)(OH)(CO2)2]8	0	6817.37	8.52	33.31	2.53
23baa8d0-f4bb-4f8b-b923-afb2492b0d64	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3CH2C2Si4C9H)(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}	[Zn4C4H4O412S4]4[(C6H3)((C6H12O2)(C9H5O2))(CO2)2]8	0	7821.53	8.47	39.53	2.52
db5a0c9f-8d5c-431b-9d4-28ad0aee5c8f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C4H4O412S4]4[(C6H3)CH2C2Si4C9H(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}	[Zn4C4H4O412S4]4[(C6H3)(OC2H4)(3)(OH)(CO2)2]8	0	6924.51	8.5	33.3	2.51
c263e2eb-f30e-4d63-aadf-75447ea2641	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3N2C6H3(C3)(CO2)2]8	0	6689.41	8.52	31.49	2.51
610fd487-aaaf-4808-a8cc-9b968aae21	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C4H4O412S4]4[(C6H3N2C6H3(C3)(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}	[Ni4C4H4S4O12]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}	[Ni4C4H4S4O12]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}	[Ni4C4H4S4O12]4[(C6H3)(OC2H4)2(OH)(CO2)2]8	0	6464.95	8.49	31.46	2.49
2998f839-6d2f-43cf-9b57-3d7e4585386	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3)(OCH2CH2CH3)(CO2)2]8	0	6096.75	8.54	31.49	2.49
2f6bea4f-6aab-4435-9cc0-b89cc58f4128	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3)(N2(C6H4CH3))(CO2)2]8	0	6577.2	8.54	31.49	2.49
a8d308dc-2246-4007-a53d-87e8809dd4e4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3)(OCH2CH3)(CO2)2]8	0	5984.54	8.54	31.49	2.49
72918148-cfbf-49fd-b567-6d802b7db15c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H2O)(CH2CH2CH2)(CO2)2]8	0	6072.56	8.54	31.49	2.49
75e2f13d-219a-4a4d-90f4-059fb7d15946	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3)CH2CS2(C6H5)(CO2)2]8	0	6962.22	8.5	31.46	2.49
91e14889-66d5-4f10-9b12-be456b1ade83	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3O)COCHCH2(CO2)2]8	0	6192.49	8.51	31.47	2.49
979dc45e-c73f-4d4f-a040-7f79a4b3a999	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C4H4S4O12]4[(C6H3(NO2))(CO2)2]8	0	5992.1	8.54	31.49	2.49

Continued

Table 4: (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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(C(CH ₃) ₃)(CO ₂) ₂) ₈	0	6080.96	8.54	31.49	2.49
ae0c0f90-f368-4823-93c5-702c0d135d82	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(OC2H4OH)(CO ₂) ₂) ₈	0	6112.53	8.54	31.49	2.49
dfc71108-3445-4892-aae8-ed34c6b7d04b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(OCH2C2H)(CO ₂) ₂) ₈	0	6064.5	8.54	31.49	2.49
9c18057a-ea3f-f418-9e39-dc19c81fec3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(C6H ₂ (OC16H3) ₃ (CO ₂) ₂) ₈	0	12011.04	8.54	60.52	2.49
7d16ead4-1971-43b6-827a-fbeb80b32aeb	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(C2H4O2)(CONHC6H5)(CO ₂) ₂) ₈	0	7065.49	8.51	31.91	2.49
71fabde5-8032-46e5-9bc0-97992f3f5bae	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3Br)(CO ₂) ₂) ₈	0	6370.43	8.53	31.45	2.48
6bb0c0e59-7790-4ba3-9e03-86db27af799d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(O(CH ₂) ₁₁ CH ₃ (CO ₂) ₂) ₈	0	7106.65	8.53	39.63	2.48
72d2428f-2a1d-44f3-8c6c-f9b0393bcfa3f	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3S03)(CO ₂) ₂) ₈	0	6371.71	8.53	31.45	2.48
6f2e029c-c533-4f89-a63b-96e4cbd5ac9b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(OCH2CH3)(CO ₂) ₂) ₈	0	6091.68	8.53	31.45	2.48
983633dd-6318-48f0-8893-706b6cbf4c76	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(OC2H4)(OH)(CO ₂) ₂) ₈	0	6572.1	8.48	31.41	2.48
d3d4250d-29ab-47a0-9f16-d73776a03716	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(OCH2C2H3)(CO ₂) ₂) ₈	0	6203.89	8.53	31.45	2.48
4376ae09-4683-43d0-99d3-4e90a08121b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(N2(C6H4CH3))(CO ₂) ₂) ₈	0	6684.35	8.53	31.45	2.48
16c909ac-1ef4-c13-bf47-ce38ea49be8c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H2O)(CH2CHCH2)(CO ₂) ₂) ₈	0	6179.71	8.53	31.45	2.48
269005a9-aad7-4a46-ac5-9c0859e5faaf	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3OCOCHCH2)(CO ₂) ₂) ₈	0	6299.64	8.49	31.42	2.48
e2988e6c-cb66-4e38-b863-846eba9e6ba1	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(CH2CS2(C6H5)(CO ₂) ₂) ₈	0	7069.37	8.49	31.42	2.48
fcacc268-6ef6-49e5-88a2-bb9b66077112	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3OC2CH3)(CO ₂) ₂) ₈	0	6096.41	8.51	31.47	2.48
9234a073-e3ea-4a22-94c9-888c6b9a7c06	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(NO2)(CO ₂) ₂) ₈	0	6099.25	8.53	31.45	2.48
4c5012f2-e2a0-4f6c-96a8-ba65f2e826	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(N2(C6H4CH3))(CO ₂) ₂) ₈	0	7377.76	8.51	33.87	2.48
9e75eac7-163e-47d4-972e-559130ea77c7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(OC2H4OH)(CO ₂) ₂) ₈	0	6219.68	8.53	31.45	2.48
998a7f73-5df5-47e8-9ae7-54c2d7ae0bc	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H ₃)(OCH2C2H)(CO ₂) ₂) ₈	0	6171.64	8.53	31.45	2.48
af5ab7d-8617-4c46-92d5-52a9bed96e7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(C(CH ₃) ₃)(CO ₂) ₂) ₈	0	6188.11	8.53	31.45	2.48
a4f71d09-9864-4343-bf14-c6c2b596c808	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(C6H2(OC16H3) ₃ (CO ₂) ₂) ₈	0	12118.19	8.52	60.51	2.48
2b35c4b2-42fc-4e6b-ba26-711dfa62e9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)(O(CH ₂) ₃ CH ₃)(CO ₂) ₂) ₈	0	6208.96	8.5	31.46	2.48
4439f5f9-9144-4f7f-b5ad-2d2b8ce2b574	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H ₃)(CH ₂)(C4N2H20CH3)(CO ₂) ₂) ₈	0	6737.11	8.53	31.49	2.48
c7a97273-20e1-4466-912a-561a4a8ca921	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(C2H4O2)(CONHC6H5)(CO ₂) ₂) ₈	0	7172.64	8.5	31.9	2.48
c766725f-fd06-40ac-8b92-da4dc305749c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3C2S(C3H7)(CO ₂) ₂) ₈	0	7075	8.52	31.48	2.47
d6972f23-bfc6-448a-01-da5818e0b6c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(OCH2C2H)(CO ₂) ₂) ₈	0	7213.79	8.51	39.62	2.47
5b924e46-e54e-4475-949e-3e8165784d5	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)(OC2H4)(OCH(C3)(CO ₂) ₂) ₈	0	6929.58	8.5	35.12	2.47
71be972b-ac8a-49c3-93d8-7a7e1694909	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3C2O2CH3)(CO ₂) ₂) ₈	0	6203.55	8.49	31.43	2.47
b78a7fb-c647-4850-b18e-6df963014c7	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)(O(CH ₂) ₃ CH ₃)(CO ₂) ₂) ₈	0	7331.07	8.5	47.87	2.47
bb77420c-f427-4340-9ae7-c1608011e4f2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(C3H6O2)(C9H5O2)(CO ₂) ₂) ₈	0	7484.9	8.5	33.86	2.47
f65105f1-7108-4f4e-a4d1-af0451b1f302	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3CO2C2H4S)(CH ₃)(CO ₂) ₂) ₈	0	6786.06	8.51	31.47	2.47
20583e67-3304-4c5e-9ede-8733e43d9b30	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(CH ₂)(C4N2H20CH3)(CO ₂) ₂) ₈	0	6844.25	8.52	31.45	2.47
92a9fce962c-692c-442a-b74e-0866e7b4678a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3C2S(C3H7)(CO ₂) ₂) ₈	0	7182.14	8.51	31.44	2.46
4500393b-5a67-4698-b9b7-ebd2b83c5873	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)(O(CH ₂) ₄ CH ₃)(CO ₂) ₂) ₈	0	6321.17	8.49	31.46	2.46
71482eea-a5f3-4316-be1c-f18c18da77c8	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(OC2H4)(OCH ₃)(CO ₂) ₂) ₈	0	7036.72	8.48	35.11	2.46
88a39c2b-04ab-483f-ba0f-3c61385e46fe	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3CO2C2H4S)(CH ₃)(CO ₂) ₂) ₈	0	6893.21	8.49	31.43	2.46
a8e0b2fc-c50c-4b04-95cc-6a152768b2fa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3NHC02C)(CH ₃)(CO ₂) ₂) ₈	0	6553.16	8.49	31.46	2.46
6794f4c1-b7ad-465f-8243-931f03618aa3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(O(CH ₂) ₃ CH ₃)(CO ₂) ₂) ₈	0	6316.1	8.49	31.42	2.46
f2defdf5b-7235-4abb8-907a-d858d49154	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)(NHCO(C)(CH ₃)(CO ₂) ₂) ₈	0	6425.16	8.49	31.46	2.46
faah29dc-ec54-4d69-98a5-ab819c2c7185	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(O(CH ₂) ₄ CH ₃)(CO ₂) ₂) ₈	0	6428.31	8.48	31.42	2.45
a4d57914-d751-4e99-8907-4cea076aa8c4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(O(CH ₂) ₃ CH ₃)(CO ₂) ₂) ₈	0	7438.21	8.48	47.86	2.45
556e791f-a21a-4d94-86c1-ed87d9b29d3d	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3NHC02C)(CH ₃)(CO ₂) ₂) ₈	0	6660.3	8.48	31.41	2.45
0ad2849c-a372-4856-ba4-09d03d47b78c	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)NHCOC(CH ₃)(CO ₂) ₂) ₈	0	6532.31	8.48	31.42	2.45
12b94e3a-5823-43e5-85c6-3f62523fa95e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Ni4C40H44S4O12] ₄ ((C6H3)((C2H4O2)(C9H5O2))(CO ₂) ₂) ₈	0	7265.55	8.5	31.49	2.45
d8edc269-e631-44cd-865b-ff42d46539b	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Zn4C40H44O12S4] ₄ ((C6H3)(C2H4O2)(C9H5O2)(CO ₂) ₂) ₈	0	7372.69	8.48	31.45	2.44
84847434-1aa2-4e91-94bc-d2d0ce5752da	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3(CH ₃))(CO ₂) ₂) ₈	0	5748.17	7.8	31.42	2.21
e3cf0b44-1259-4b0f-85e3-sab91de7533e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3NH2)(CO ₂) ₂) ₈	0	5756.08	7.8	31.42	2.14
5690964-a500-473d-8164-23bd36291194	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3)(C6H1202)(C9H5O2)(CO ₂) ₂) ₈	0	7718.23	7.74	39.04	2.05
31f2494b-7f14-43b5-98b-a34d9af0457a	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3)(OC2H4)(OH)(CO ₂) ₂) ₈	0	6821.21	7.77	32.62	2.05
6794980b-3c65-4ca2-8e8e-1f8a666ad098	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3CH2CS3C4H9)(CO ₂) ₂) ₈	0	7062.66	7.73	31.39	2.04
60a7406a-9a00-427a-a441-fab60f5af304	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H2O)(CH2CHCH2)(CO ₂) ₂) ₈	0	6076.4	7.8	31.42	2.03

Continued

Table 4: (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-pyramidal) ₄ (2-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-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(N2(C6H4CH3))(CO2) ₂ [8]	0	6581.04	7.79	31.42	2.01
3ca9a2f8-686e-40de-a5c8-f1062bbe4969	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(OC2H42(OH))(CO2) ₂ [8]	0	6468.79	7.74	31.38	2.01
ebcc31d4-6f34-4fac-96a0-48f37598a5e	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(NO2)(CO2) ₂ [8]	0	5959.94	7.8	31.42	2.01
d76ee113-a16d-4e02-988d-71eac2dbf6cf	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)OCOCHCH2(CO2) ₂ [8]	0	6196.33	7.76	31.39	2.01
3c88ab7d-d630-4256-b179-14d5cd471aa	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)C6H2(OC16H33) ₃ (CO2) ₂ [8]	0	12014.88	7.79	60.09	2.01
af0d13ec-2d1d-43a7-aace-ddacfcc4be6	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(OC2H4OH)(CO2) ₂ [8]	0	6116.37	7.8	31.42	2.01
60123b4a-1ab3-4d24-9612-f584b5505ac3	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ ((C6H3)C(CH3) ₂)(CO2) ₂ [8]	0	6084.8	7.8	31.42	2.01
4f228dc-60d1-4875-b52c-3dbc020133e7	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3SO ₃)(CO2) ₂ [8]	0	6268.4	7.8	31.42	2.01
fa01491c-36a4-4c0a-b788-88cbcd08fd4	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(C2H4O2)(CONHC6H5)(CO2) ₂ [8]	0	7069.33	7.77	31.41	2.01
8e62fa5a-dec7-46ef-a195-9d79f64fe2	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)O(CH2) ₁₁ CH3(CO2) ₂ [8]	0	7110.49	7.78	39.07	2
cc2e2e30-4dec-402b-b403-2e9ad264ec10	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3CO2C2H3)(CO2) ₂ [8]	0	6100.25	7.76	31.4	2
3210f2cc-b48b-4b6d-acce-0f14659a697e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)((C3H6O2)(C9H5O2))(CO2) ₂ [8]	0	7381.6	7.77	33.34	2
a920d17e-0ecb-4fa3-9e0f-816b7352438	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(CH2)(C4N2H2O2CH3)(CO2) ₂ [8]	0	6740.95	7.78	31.41	2
dea37fb3-4575-4006-b886-129b1ac4da1	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(OC2H4) ₃ (OCH3)(CO2) ₂ [8]	0	6933.42	7.75	34.42	1.99
f1fb29b6-pf9-422a-9a5b-0ff724842967	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)O(C2H4O2C2H4Si(C3H3)(CO2) ₂ [8]	0	6789.9	7.76	31.4	1.99
e1f9f801-808a-4e09-8010-50a6f44034d7	(4-pyramidal) ₄ (2-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-pyramidal) ₄ (2-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-d782322a9ed	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(O(CH2) ₁₃ CH3)(CO2) ₂ [8]	0	7334.91	7.75	47.41	1.98
6dbec1ff-cb5e-442f-aef2-4e04e556cd3e	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3NHCO2C(C3H3)(CO2) ₂ [8]	0	6557	7.74	31.38	1.98
0283cd73-a838-4f79-9829-5ee727d2d649	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)NHCO(C3H3)(CO2) ₂ [8]	0	6429	7.75	31.39	1.98
d7466a81-bd09-4314-ab30-000284fc4727	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[Co4C40H44O12S4] ₄ (C6H3)(C2H4O2)(C9H5O2)(CO2) ₂ [8]	0	7269.39	7.75	31.42	1.97
4f26e7a2-24bf4-f428-9b3-672e9afc9d9	(4-pyramidal) ₄ (2-bent) ₈ _D _{4h}	[V5O9] ₆ (C14N2H10)(Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	-6	9321.74	21.97	42.65	11.49
6939469-dca9-4a24-b5d3-99fa5ed2a1e	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[V4O8] ₆ (C14N2H10)(Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	8920.09	21.38	39.06	11.15
4a74f863-9b8f-4ad2-bf9-82c2f4ee6f14	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Mg4C56H76O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	13929.53	20.43	53.19	10.66
d8732a5c-26a1-4928-b83d-b37a72164ee0	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Fe4C40H44S4O4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	12571.98	20.32	52.63	10.58
f8069cab-7057-4468-8eef-dd3217e6b963	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C56H76O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	14760.66	20.26	52.8	10.57
7f2547f0-be4a-442f-8609-ed170e64bf	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Ni4C56H76O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	14754.85	20.24	52.75	10.56
90dc4c8-b819-4a10-9d7f-6cb9bf70f52d	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C40H44O4S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	12646.14	20.26	52.47	10.54
4d4bf944-db3e-4321-8f71-034c71eaed1	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C48H28O4S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	13125.9	20.21	55.89	10.5
abaeec66-9ff8-4da3-b105-4d38164319a0	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C24H12O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	12067.56	20.11	47.99	10.44
82ea5975-4515-4f57-ac7d-881c2bc5bc3	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Ni4C48H12O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	12061.79	20.09	47.94	10.42
cb35d857-3c7e-4c18-8d0e-052b8561ff0	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Mg4C40H44O4S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	12583	19.97	53.49	10.38
a78615d-e880-405a-be61-22241231dddd	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C24H8O24S8] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	-24	13964.88	19.87	51.06	10.29
e127cb9b-2b7e-4ffa-bd0c-s1257b048e	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Ni4C40H44S4O12] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	13408.32	19.57	51.96	10.12
e56026fd-115f-4cd4-a9f3-302065542340	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Zn4C40H44O12S4] ₆ (C14N2H10)Co(OH)2(C6H4) ₂ (CO2) ₂ [12]	0	13569.04	19.55	51.91	10.11
97c771e2-f3ca-47ea-85c3-9384a2fc8b2f	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[V5O9] ₆ (C8H8)(C6H4) ₂ (CO2) ₂ [12]	-6	6525.02	17.6	36.82	9.78
1a2e9246-6408-4ada-81d0-23fb9bab4fa	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ _O _h	[V4O8] ₆ (C6H4N) ₂ (CO2) ₂ [12]	0	5209.45	20.83	30.85	8.96
c777c9ad-aab2-4492-bbbb-b5c874bd465b	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Mg4C56H76O12S4] ₆ (C8H8)(C6H4) ₂ (CO2) ₂ [12]	0	11132.81	16.07	47.43	8.92
7518bf1f-3c02-4821-b5b-68ce31a79be	(4-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Fe4C40H44S4O4] ₆ (C8H8)(C6H4) ₂ (CO2) ₂ [12]	0	975.26	15.98	46.97	8.85
afdf65214-3481-4bf1-9a85-1d1614431c47	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ _O _h	[Co4C48H28O4S4] ₆ (C8H8)(C6H4) ₂ (CO2) ₂ [12]	0	10329.18	15.88	50.24	8.78

Continued

Table 4: (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-pyramidal) ₆ (2-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-6f6c3ba965c58	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-l9d4084926e	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C24H18O24S8]6[(C8H8)(C6H4)2(CO2)2]12	-24	11168.16	15.52	45.32	8.57
ee819b5-e8ff-4e4d-88ab-c0a56c64d4cf	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C56H76O12S4]6[(C6H4N)2(CO2)2]12	0	10218.89	19.83	44.92	8.53
eb7b0325-af96-440d-8930-2fd84afe9491	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C56H76O12S4]6[(C6H4N)2(CO2)2]12	0	11050.02	19.66	44.53	8.45
02d98ea-460d-4b88-be04-a7396ea0f1b9	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H44O4S4]6[(C6H4N)2(CO2)2]12	0	8935.5	19.67	44.35	8.42
b779cc44-7412-4fc7-90d8-47b6a9306cb8	(4-pyramidal) ₆ (2-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-aea729e7973	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H28O4S4]6[(C6H4N)2(CO2)2]12	0	9415.26	19.64	47.8	8.38
ed0a09e3-67e7-45b4-b097-dc9fb4fe1f6d8	(4-pyramidal) ₆ (2-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-008166e066	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C24H12O12S4]6[(C6H4N)2(CO2)2]12	0	8356.92	19.54	39.8	8.33
b413a8b9-709e-4693-ab36-a5dd92a1f05	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Ni4C24H12O12S4]6[(C6H4N)2(CO2)2]12	0	8351.15	19.52	39.74	8.31
c0986d30-17dc-a8a8-0806-0340e3fd3b11	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C40H44O12S4]6[(C6H4N)2(CO2)2]12	0	8872.36	19.38	45.23	8.27
80f13aba-fb15-45cd-aef9-58104ac02007	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C24H18O24S8]6[(C6H4N)2(CO2)2]12	-24	10254.24	19.3	42.81	8.2
0dad802c-5b4a-4ba8-a9fa-aea729e7973	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Ni4C40H44S4O12]6[(C6H4N)2(CO2)2]12	0	9697.68	19	43.85	8.05
80ce05a8-1b18-4ba9-9440-e823e1f81da2	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H44O12S4]6[(C8H8)(C6H4)2(CO2)2]12	0	10617.36	14.24	45.92	7.84
4982t707-19bf4-4fa8-ba7d-527019681baa	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H44O12S4]6[(C6H4N)2(CO2)2]12	0	9703.44	18.03	43.46	7.58
5078ae79-2315-4ab9-9e57-ddd8a19d7689	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[V509]6[(C14H8)(C6H4)2(CO2)2]12	-6	7389.02	15.73	37	6.79
2285aa8d-85da-41ba-876f-230ccb6bd655	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[V408]6[(C14H8)(C6H4)2(CO2)2]12	0	6987.37	15.15	33.54	6.46
a9de1c09-7cef4445-8177-fed2bca0944	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C56H76O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11996.81	14.29	47.58	6
4f2982b9-9d40-4842-a15d-2384d2b344d7	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Fe4C40H44S4O4]6[(C14H8)(C6H4)2(CO2)2]12	0	10639.26	14.18	47.12	5.92
a8efdb74-4a9c-45b0-ad97-76c059377e03	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C56H76O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	12827.94	14.13	47.19	5.91
12edcdf-b0de-4587-8fe0-4e194e8d70c9	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C48H28O4S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11193.18	14.07	50.4	5.84
66494e67-438b-479f-b35b-5119bae7d755	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C44H12O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10134.84	13.93	42.45	5.78
89791d5-c463-4542-875b-2946c1d8999b	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Ni4C24H12O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10129.07	13.91	42.4	5.77
b715238e-1b9d-4f7-9852-a15471cd2a2	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	10650.28	13.87	47.85	5.73
adc3138f-775f-4f6e-b182-fc16029498eba	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C44H18O24S8]6[(C14H8)(C6H4)2(CO2)2]12	-24	12032.16	13.71	45.48	5.65
09b3a394-c3b0-49ac-a001-c61c41caa93	(4-pyramidal) ₆ (2-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-ea8f80627e49	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Zn4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11636.32	13.4	46.42	5.47
3931be65-9841-4194-boe0-05690edfd55	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H44O12S4]6[(C14H8)(C6H4)2(CO2)2]12	0	11481.36	12.47	46.08	4.97
144f304f-39b0-4f59-a27-385fa26520	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[V509]6[(C10H6)(C6H4)2(CO2)2]12	-6	6789.02	17.81	37.13	4.6
97f6a41c-d98d-4514-8575-5028875f84f3	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[V408]6[(C10H6)(C6H4)2(CO2)2]12	0	6387.37	17.25	33.68	4.29
d7215cf4-627c-481e-b4f1-5d19b7e5642	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C56H76O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	11396.81	16.47	47.68	3.84
38622766-7769-4924-d24-7f7e0b88f0f8	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Ni4C56H76O12S4]6[(C10H6)(C6H4)2(CO2)2]12	0	12222.13	16.29	47.24	3.74
19915f07-9519-444f-8aac-d8abcdhf25c	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C40H44O4S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10113.42	16.3	47.07	3.74
9220284b-25fc-475f-af59-31f0c08c0ca	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C40H44O4S4]6[(C10H6)(C6H4)2(CO2)2]12	0	10050.28	16.09	47.94	3.61
89729dea-cha1-4650-826b-634656fd206	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C44H18O24S8]6[(C10H6)(C6H4)2(CO2)2]12	-24	11432.16	15.89	45.58	3.52
0b4ee1ba-a498-4476-a088-76c79540e3a4	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-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-af9956cc6d6db	(4-pyramidal) ₆ (2-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-pyramidal) ₆ (2-linear) ₁₂ .O _h	[V408]6[(C14H8)(CO2)2]12	0	5161.57	6.97	24.9	2.74
be5f6046-c68f-4048-bd5f-eeb09a2bb	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Mg4C56H76O12S4]6[(C14H8)(CO2)2]12	0	10171.01	6.06	35.72	2.24

Continued

Table 4: (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-7716e8652a5	(4-pyramidal) ₆ (2-linear) ₁₂ .O _h	[Co4C56H76O12S4]6[(C14H8)(CO2)2]12	0	11002.14	5.91	35.33	2.15
ace563f6-3cfa-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-dea0-48f6-9116-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
4bc8ab4-bf6b-42fd-b089-9974f51e443	(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-ad1ec8ad9be	(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-4a68-8079-3bbc8d21bee	(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-aea7f975031	(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-a974-6c6b90e4c69	(5-pyramidal) ₁₂ (2-linear) ₃₀ .I _h	[WV5O11]12[(C6H4N)2(CO2)2]30	-12	15421.7	35.68	46.55	9.05
6aacfd83-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-f68ed5855186	(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

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

²The MOP formulae are written in plain text format

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