

Supplementary Information for

Collective Motions in the Primary Coordination Sphere: A Critical Functional Framework for Catalytic Activity of the Oxygen-Evolving Complex of Photosystem II

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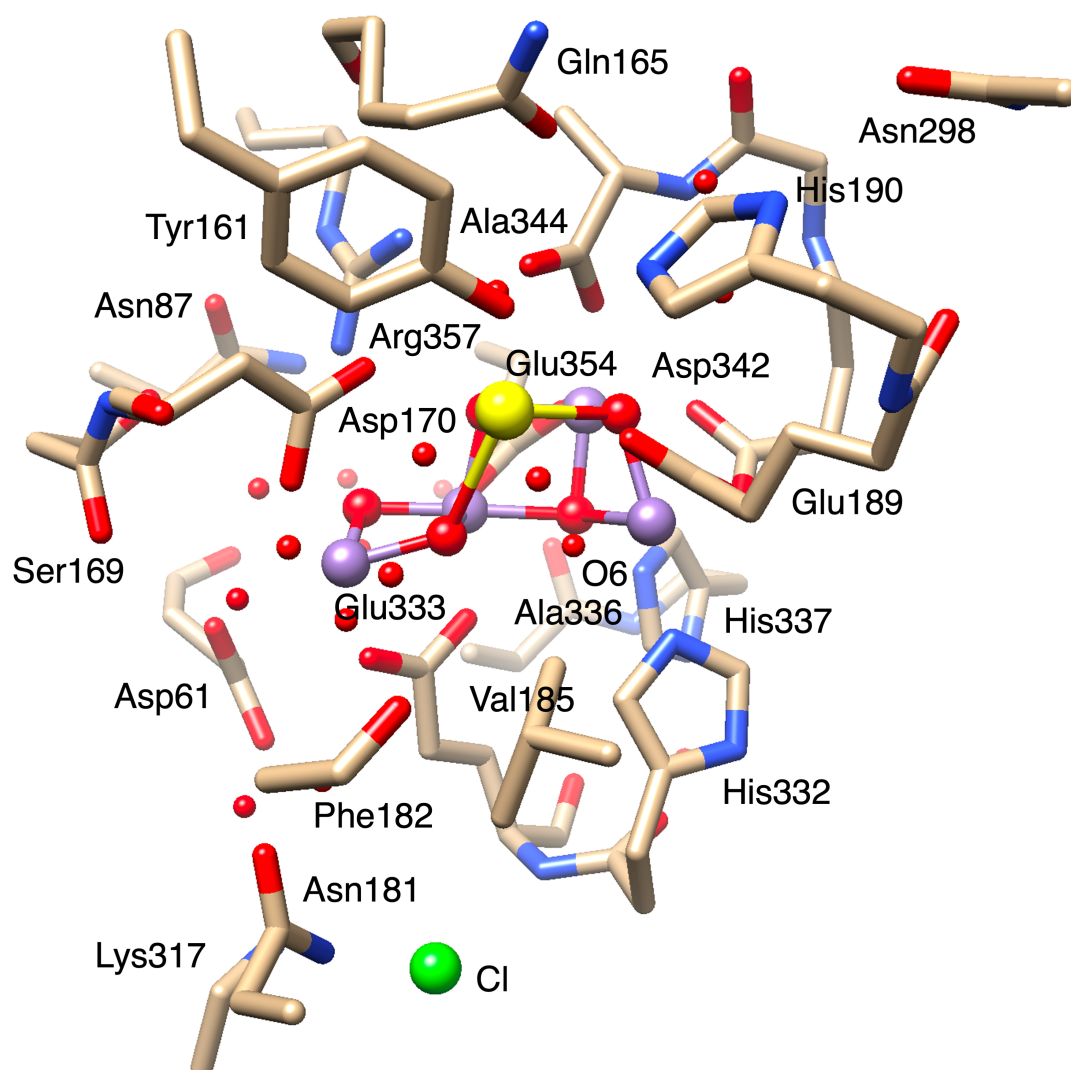


Fig. S1 Overall view of the OEC model employed in this study, with hydrogen atoms omitted for clarity.

Table S1 Alignment of fixed structural components during geometry optimization with corresponding PDB/DFT coordinates used for dataset preparation^a

entry	fixed components	
	backbone	side chain
1	6DHF (monomer A)	6DHF (monomer A)
2	6DHG (monomer A)	6DHG (monomer A)
3	6DHH (monomer A)	6DHH (monomer A)
4	6DHO (monomer A)	6DHO (monomer A)
5	6DHP (monomer A)	6DHP (monomer A)
6	6DHE (monomer A)	6DHE (monomer A)
7	6DHF (monomer B)	6DHF (monomer B)
8	6DHG (monomer B)	6DHG (monomer B)
9	6DHH (monomer B)	6DHH (monomer B)
10	6DHO (monomer B)	6DHO (monomer B)
11	6DHP (monomer B)	6DHP (monomer B)
12	6DHE (monomer B)	6DHE (monomer B)
13	6DHF (monomer A)	DFT optimized for closed cubane hydroxo–oxo
14	6DHF (monomer A)	DFT optimized for open cubane hydroxo–oxo
15	6DHF (monomer B)	DFT optimized for closed cubane hydroxo–oxo
16	6DHF (monomer B)	DFT optimized for open cubane hydroxo–oxo
17	6DHG (monomer A)	DFT optimized for closed cubane hydroxo–oxo
18	6DHG (monomer A)	DFT optimized for open cubane hydroxo–oxo
19	6DHG (monomer B)	DFT optimized for closed cubane hydroxo–oxo
20	6DHG (monomer B)	DFT optimized for open cubane hydroxo–oxo
21	6DHH (monomer A)	DFT optimized for closed cubane hydroxo–oxo
22	6DHH (monomer A)	DFT optimized for open cubane hydroxo–oxo
23	6DHH (monomer B)	DFT optimized for closed cubane hydroxo–oxo
24	6DHH (monomer B)	DFT optimized for open cubane hydroxo–oxo
25	6DHO (monomer A)	DFT optimized for closed cubane hydroxo–oxo
26	6DHO (monomer A)	DFT optimized for open cubane hydroxo–oxo
27	6DHO (monomer B)	DFT optimized for closed cubane hydroxo–oxo
28	6DHO (monomer B)	DFT optimized for open cubane hydroxo–oxo

29	6DHP (monomer A)	DFT optimized for closed cubane hydroxo–oxo
30	6DHP (monomer A)	DFT optimized for open cubane hydroxo–oxo
31	6DHP (monomer B)	DFT optimized for closed cubane hydroxo–oxo
32	6DHP (monomer B)	DFT optimized for open cubane hydroxo–oxo
33	6DHE (monomer A)	DFT optimized for closed cubane hydroxo–oxo
34	6DHE (monomer A)	DFT optimized for open cubane hydroxo–oxo
35	6DHE (monomer B)	DFT optimized for closed cubane hydroxo–oxo
36	6DHE (monomer B)	DFT optimized for open cubane hydroxo–oxo
37	6DHF (monomer A)	DFT optimized for closed cubane oxyl–oxo
38	6DHF (monomer A)	DFT optimized for open cubane oxyl–oxo
39	6DHF (monomer B)	DFT optimized for closed cubane oxyl–oxo
40	6DHF (monomer B)	DFT optimized for open cubane oxyl–oxo
41	6DHG (monomer A)	DFT optimized for closed cubane oxyl–oxo
42	6DHG (monomer A)	DFT optimized for open cubane oxyl–oxo
43	6DHG (monomer B)	DFT optimized for closed cubane oxyl–oxo
44	6DHG (monomer B)	DFT optimized for open cubane oxyl–oxo
45	6DHH (monomer A)	DFT optimized for closed cubane oxyl–oxo
46	6DHH (monomer A)	DFT optimized for open cubane oxyl–oxo
47	6DHH (monomer B)	DFT optimized for closed cubane oxyl–oxo
48	6DHH (monomer B)	DFT optimized for open cubane oxyl–oxo
49	6DHO (monomer A)	DFT optimized for closed cubane oxyl–oxo
50	6DHO (monomer A)	DFT optimized for open cubane oxyl–oxo
51	6DHO (monomer B)	DFT optimized for closed cubane oxyl–oxo
52	6DHO (monomer B)	DFT optimized for open cubane oxyl–oxo
53	6DHP (monomer A)	DFT optimized for closed cubane oxyl–oxo
54	6DHP (monomer A)	DFT optimized for open cubane oxyl–oxo
55	6DHP (monomer B)	DFT optimized for closed cubane oxyl–oxo
56	6DHP (monomer B)	DFT optimized for open cubane oxyl–oxo
57	6DHE (monomer A)	DFT optimized for closed cubane oxyl–oxo
58	6DHE (monomer A)	DFT optimized for open cubane oxyl–oxo
59	6DHE (monomer B)	DFT optimized for closed cubane oxyl–oxo
60	6DHE (monomer B)	DFT optimized for open cubane oxyl–oxo

61	6JLK (monomer A)	6JLK (monomer A)
62	6JLL (monomer A)	6JLL (monomer A)
63	6JLJ (monomer A)	6JLJ (monomer A)
64	6JLN (monomer A)	6JLN (monomer A)
65	6JLO (monomer A)	6JLO (monomer A)
66	6JLP (monomer A)	6JLP (monomer A)
67	6JLM (monomer A)	6JLM (monomer A)
68	6JLK (monomer B)	6JLK (monomer B)
69	6JLL (monomer B)	6JLL (monomer B)
70	6JLJ (monomer B)	6JLJ (monomer B)
71	6JLN (monomer B)	6JLN (monomer B)
72	6JLO (monomer B)	6JLO (monomer B)
73	6JLP (monomer B)	6JLP (monomer B)
74	6JLM (monomer B)	6JLM (monomer B)
75	6JLK (monomer A)	DFT optimized for closed cubane hydroxo–oxo
76	6JLK (monomer A)	DFT optimized for open cubane hydroxo–oxo
77	6JLK (monomer B)	DFT optimized for closed cubane hydroxo–oxo
78	6JLK (monomer B)	DFT optimized for open cubane hydroxo–oxo
79	6JLL (monomer A)	DFT optimized for closed cubane hydroxo–oxo
80	6JLL (monomer A)	DFT optimized for open cubane hydroxo–oxo
81	6JLL (monomer B)	DFT optimized for closed cubane hydroxo–oxo
82	6JLL (monomer B)	DFT optimized for open cubane hydroxo–oxo
83	6JLJ (monomer A)	DFT optimized for closed cubane hydroxo–oxo
84	6JLJ (monomer A)	DFT optimized for open cubane hydroxo–oxo
85	6JLJ (monomer B)	DFT optimized for closed cubane hydroxo–oxo
86	6JLJ (monomer B)	DFT optimized for open cubane hydroxo–oxo
87	6JLN (monomer A)	DFT optimized for closed cubane hydroxo–oxo
88	6JLN (monomer A)	DFT optimized for open cubane hydroxo–oxo
89	6JLN (monomer B)	DFT optimized for closed cubane hydroxo–oxo
90	6JLN (monomer B)	DFT optimized for open cubane hydroxo–oxo
91	6JLO (monomer A)	DFT optimized for closed cubane hydroxo–oxo
92	6JLO (monomer A)	DFT optimized for open cubane hydroxo–oxo

93	6JLO (monomer B)	DFT optimized for closed cubane hydroxo-oxo
94	6JLO (monomer B)	DFT optimized for open cubane hydroxo-oxo
95	6JLP (monomer A)	DFT optimized for closed cubane hydroxo-oxo
96	6JLP (monomer A)	DFT optimized for open cubane hydroxo-oxo
97	6JLP (monomer B)	DFT optimized for closed cubane hydroxo-oxo
98	6JLP (monomer B)	DFT optimized for open cubane hydroxo-oxo
99	6JLM (monomer A)	DFT optimized for closed cubane hydroxo-oxo
100	6JLM (monomer A)	DFT optimized for open cubane hydroxo-oxo
101	6JLM (monomer B)	DFT optimized for closed cubane hydroxo-oxo
102	6JLM (monomer B)	DFT optimized for open cubane hydroxo-oxo
103	6JLK (monomer A)	DFT optimized for closed cubane oxyl-oxo
104	6JLK (monomer A)	DFT optimized for open cubane oxyl-oxo
105	6JLK (monomer B)	DFT optimized for closed cubane oxyl-oxo
106	6JLK (monomer B)	DFT optimized for open cubane oxyl-oxo
107	6JLL (monomer A)	DFT optimized for closed cubane oxyl-oxo
108	6JLL (monomer A)	DFT optimized for open cubane oxyl-oxo
109	6JLL (monomer B)	DFT optimized for closed cubane oxyl-oxo
110	6JLL (monomer B)	DFT optimized for open cubane oxyl-oxo
111	6JLJ (monomer A)	DFT optimized for closed cubane oxyl-oxo
112	6JLJ (monomer A)	DFT optimized for open cubane oxyl-oxo
113	6JLJ (monomer B)	DFT optimized for closed cubane oxyl-oxo
114	6JLJ (monomer B)	DFT optimized for open cubane oxyl-oxo
115	6JLN (monomer A)	DFT optimized for closed cubane oxyl-oxo
116	6JLN (monomer A)	DFT optimized for open cubane oxyl-oxo
117	6JLN (monomer B)	DFT optimized for closed cubane oxyl-oxo
118	6JLN (monomer B)	DFT optimized for open cubane oxyl-oxo
119	6JLO (monomer A)	DFT optimized for closed cubane oxyl-oxo
120	6JLO (monomer A)	DFT optimized for open cubane oxyl-oxo
121	6JLO (monomer B)	DFT optimized for closed cubane oxyl-oxo
122	6JLO (monomer B)	DFT optimized for open cubane oxyl-oxo
123	6JLP (monomer A)	DFT optimized for closed cubane oxyl-oxo
124	6JLP (monomer A)	DFT optimized for open cubane oxyl-oxo

125	6JLP (monomer B)	DFT optimized for closed cubane oxyl-oxo
126	6JLP (monomer B)	DFT optimized for open cubane oxyl-oxo
127	6JLM (monomer A)	DFT optimized for closed cubane oxyl-oxo
128	6JLM (monomer A)	DFT optimized for open cubane oxyl-oxo
129	6JLM (monomer B)	DFT optimized for closed cubane oxyl-oxo
130	6JLM (monomer B)	DFT optimized for open cubane oxyl-oxo

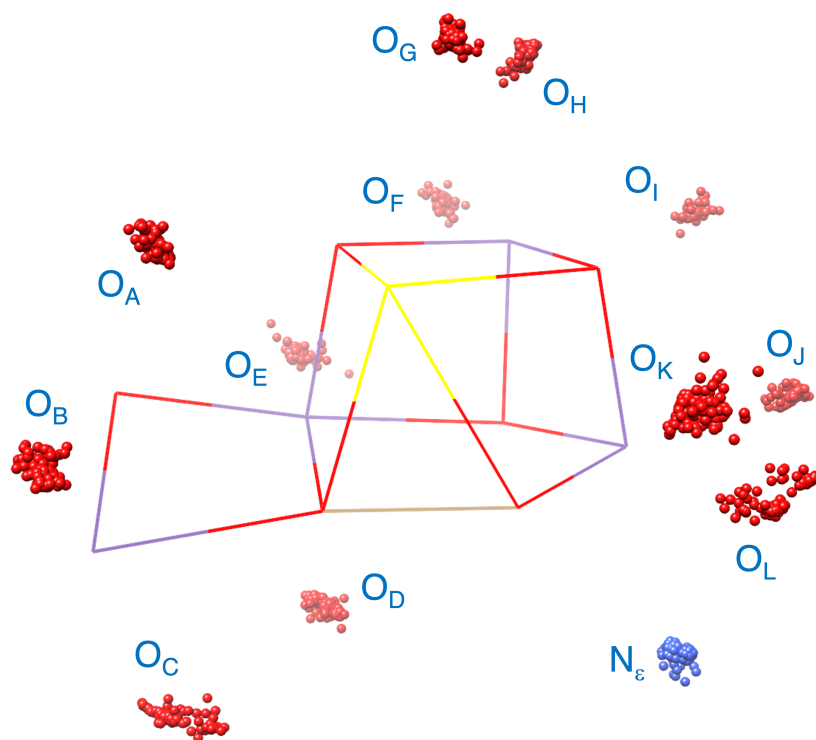


Fig. S2 Spatial sampling region of the coordinating atoms (O_A , O_B , ..., N_ϵ in Fig. 1C) for entries 1–130 listed in Table S1. Incorporating a diverse array of three-dimensional configurations prevents the model from overfitting to any specific pattern, thereby enhancing its flexibility and adaptability across varying conditions, a critical feature for elucidating how different ligand structural states influence the catalytic driving forces.

Classical CCA. Canonical correlation analysis (CCA) is a multivariate statistical technique designed to elucidate the relationships between two sets of variables measured on the same subjects [s1]. In our study, CCA was applied to a dataset comprising $N = 60$ entries (entries 1–60 in Table S1), using two primary data matrices as input. The first matrix, denoted as $\mathbf{X}$, consists of P measured distances between ligating atoms directly coordinated to three catalytic Mn ions (Mn_A , Mn_B , Mn_D). These distances, expressed as $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_P)$, are critical for characterizing the spatial configuration of the ligand environment. The second matrix, denoted as $\mathbf{Y}$, contains Q driving force variables, given by $\mathbf{Y} = (\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_Q)$, which correspond to the energetic driving forces associated with the closed-to-open interconversion. In our analysis, Q is set to 2, as our investigation focuses on the hydroxo–oxo and oxyl–oxo species, which are key intermediates in the catalytic cycle. Prior to performing CCA, the data were subjected to two preprocessing steps. First, distances between pairs of ligating oxygen atoms within the same carboxylate groups were removed from the $\mathbf{X}$ matrix, as these distances exhibit minimal variability and are thus less informative for capturing the dynamic behavior of the system. Consequently, the number of $\mathbf{X}$ variables is reduced to $P = 19$. Second, to eliminate bias due to differences in measurement scales, each column of the $\mathbf{X}$ and $\mathbf{Y}$ matrices was standardized via Z-score normalization. This transformation adjusts the variables so that each has a mean of zero and a standard deviation of one, as expressed by:

$$\tilde{X}_i^k = \frac{X_i^k - \bar{X}_i}{\sigma_{X_i}} \quad (\text{s1})$$

$$\tilde{Y}_i^l = \frac{Y_i^l - \bar{Y}_i}{\sigma_{Y_i}} \quad (\text{s2})$$

where $\bar{X}_i$ and $\bar{Y}_i$ represent the mean values of the i th variable in the $\mathbf{X}$ and $\mathbf{Y}$ datasets, while σ_{X_i} and σ_{Y_i} denote the corresponding standard deviations. The tilde symbol ($\sim$) signifies that the data have been standardized using the Z-score normalization. The objective of CCA is to derive linear combinations of the standardized variables from $\tilde{\mathbf{X}}$ ($N \times P$) and $\tilde{\mathbf{Y}}$ ($N \times Q$) that yield canonical variates capturing the maximum correlation between the two datasets while reducing their dimensionality. These canonical variates are defined as:

$$\mathbf{f} = \tilde{\mathbf{X}}\mathbf{a} = a_1\tilde{\mathbf{X}}_1 + a_2\tilde{\mathbf{X}}_2 + \dots + a_P\tilde{\mathbf{X}}_P \quad (\text{s3})$$

$$\mathbf{g} = \tilde{\mathbf{Y}}\mathbf{b} = b_1\tilde{\mathbf{Y}}_1 + b_2\tilde{\mathbf{Y}}_2 + \dots + b_Q\tilde{\mathbf{Y}}_Q \quad (\text{s4})$$

For the first canonical dimension, CCA searches for two weight vectors, $\mathbf{a} = (a_1, a_2, \dots, a_p)^T$ and $\mathbf{b} = (b_1, b_2, \dots, b_Q)^T$, that maximize the correlation between $\mathbf{f}$ and $\mathbf{g}$. Formally, the optimization problem is:

$$\begin{aligned} \rho^1 = \text{corr}(\mathbf{f}^1, \mathbf{g}^1) &= \max_{\mathbf{a}, \mathbf{b}} \text{corr}(\mathbf{f}, \mathbf{g}) = \frac{\text{cov}(\mathbf{f}, \mathbf{g})}{\sqrt{\text{var}(\mathbf{f})}\sqrt{\text{var}(\mathbf{g})}} \\ &\text{subject to } \text{var}(\mathbf{f}) = \text{var}(\mathbf{g}) = 1 \end{aligned} \quad (\text{s5})$$

The maximum correlation ρ^1 is referred to as the first canonical correlation, and the associated canonical variates $\mathbf{f}^1$ and $\mathbf{g}^1$ represent the most significant patterns of correlation between the standardized $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$ datasets. This optimization problem is mathematically equivalent to solving the following generalized eigenvalue problem:

$$\tilde{\mathbf{X}}^T \tilde{\mathbf{Y}} (\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}})^{-1} \tilde{\mathbf{Y}}^T \tilde{\mathbf{X}} \mathbf{a} = (\rho)^2 \tilde{\mathbf{X}}^T \tilde{\mathbf{X}} \mathbf{a} \quad (\text{s6})$$

$$\tilde{\mathbf{Y}}^T \tilde{\mathbf{X}} (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T \tilde{\mathbf{Y}} \mathbf{b} = (\rho)^2 \tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} \mathbf{b} \quad (\text{s7})$$

For the second dimension, CCA identifies the second canonical correlation (ρ^2) between a new pair of the canonical variates ($\mathbf{f}^2$ and $\mathbf{g}^2$), where $\rho^1 \geq \rho^2$ under the orthogonality conditions $\text{corr}(\mathbf{f}^1, \mathbf{f}^2) = \text{corr}(\mathbf{g}^1, \mathbf{g}^2) = 0$. This orthogonality ensures that the second set of variates captures unique and independent patterns of correlation not already explained by the first set. These theoretical concepts are visually depicted in Fig. S3, which illustrates how the canonical variates identify and separate distinct patterns of correlation across multiple dimensions.

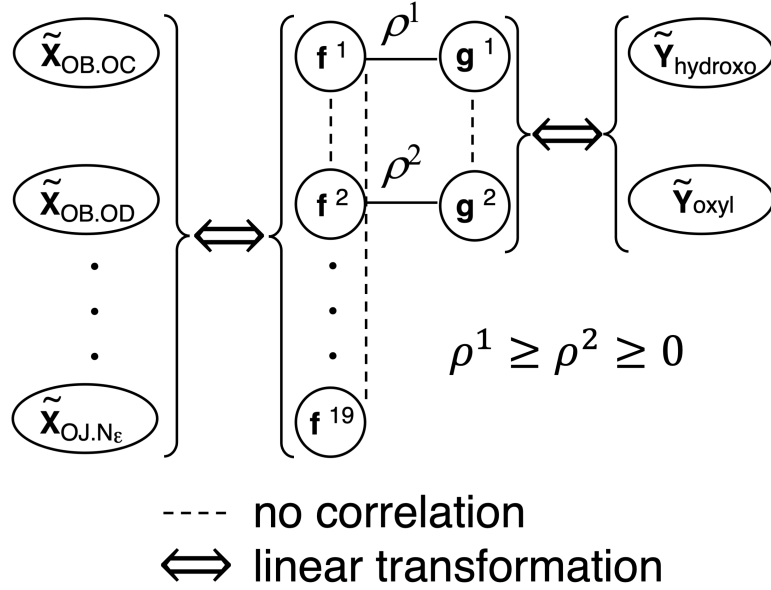


Fig. S3 Schematic illustration of classical canonical correlation analysis (CCA).

Regularized CCA. Despite its utility, CCA often encounters challenges when the number of variables exceeds the sample size ($N < P + Q$) or when there is substantial multicollinearity among variables within the standardized $\tilde{\mathbf{X}}$ or $\tilde{\mathbf{Y}}$ matrices. Under these conditions, the estimated inverses of $\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}}$ become unreliable, often resulting in canonical correlations that are artificially close to 1. These issues reduce the interpretability and stability of the canonical subspace, making it difficult to extract meaningful patterns. To mitigate these problems, a regularization step is introduced into the CCA procedure. Specifically, an l_2 -norm (ridge) penalty is applied by adding small constants to the diagonal elements of the variance-covariance matrices of $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$, ensuring that the matrices $\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}}$ become regular (well-conditioned) [s2–s4]. In addition to stabilizing matrix inversions, the ridge penalty effectively shrinks the coefficients of less influential variables in the loading vectors toward small but non-zero values. In the framework of regularized CCA (rCCA), the classical procedure is modified by replacing the original covariance matrices $\tilde{\mathbf{X}}^T \tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}}$ with their regularized counterparts, given by $\tilde{\mathbf{X}}^T \tilde{\mathbf{X}} + \lambda_1 \mathbf{I}_P$ and $\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} + \lambda_2 \mathbf{I}_Q$, where λ_1 and λ_2 are non-negative regularization parameters, and $\mathbf{I}_P$ and $\mathbf{I}_Q$ denote the $P \times P$ and $Q \times Q$ identity matrices. The generalized eigenvalue problems are then reformulated as follows:

$$\tilde{\mathbf{X}}^T \tilde{\mathbf{Y}} (\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} + \lambda_2 \mathbf{I}_Q)^{-1} \tilde{\mathbf{Y}}^T \tilde{\mathbf{X}} \mathbf{a} = (\rho)^2 (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}} + \lambda_1 \mathbf{I}_P) \mathbf{a} \quad (\text{s8})$$

$$\tilde{\mathbf{Y}}^T \tilde{\mathbf{X}} (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}} + \lambda_1 \mathbf{I}_P)^{-1} \tilde{\mathbf{X}}^T \tilde{\mathbf{Y}} \mathbf{b} = (\rho)^2 (\tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} + \lambda_2 \mathbf{I}_Q) \mathbf{b} \quad (\text{s9})$$

To determine the optimal regularization parameters λ_1 and λ_2 , we employed a leave-one-out cross-validation (LOOCV) approach [s5]. This technique involves iteratively leaving out one sample from the dataset to serve as the test set ($\mathbf{X}_{\text{test}}$ and $\mathbf{Y}_{\text{test}}$), while the remaining $N - 1$ samples constitute the training set ($\mathbf{X}_{\text{train}}$ and $\mathbf{Y}_{\text{train}}$). For each candidate pair (λ_1, λ_2) , rCCA is performed on $\mathbf{X}_{\text{train}}$ and $\mathbf{Y}_{\text{train}}$ using the corresponding regularized variance-covariance matrices. The resulting first canonical coefficients $\mathbf{a}^1_{\text{train}}$ and $\mathbf{b}^1_{\text{train}}$ obtained from $\mathbf{X}_{\text{train}}$ and $\mathbf{Y}_{\text{train}}$ are then used to project the left-out sample, yielding the predicted canonical variates $\mathbf{f}^1_{\text{test}} = \mathbf{X}_{\text{test}} \mathbf{a}^1_{\text{train}}$ and $\mathbf{g}^1_{\text{test}} = \mathbf{Y}_{\text{test}} \mathbf{b}^1_{\text{train}}$, along with the predicted canonical correlation $\rho(\lambda_1, \lambda_2) = \text{corr}(\mathbf{f}^1_{\text{test}}, \mathbf{g}^1_{\text{test}})$. The overall performance is assessed by averaging these individual canonical correlations over all N test samples, yielding the cross-validation score (CV-score) $\bar{\rho}(\lambda_1, \lambda_2)$. The optimal parameter set is chosen as the one that maximizes $\bar{\rho}(\lambda_1, \lambda_2)$. Below is an example of R code using the mixOmics package that implements this LOOCV procedure for rCCA [s5]:

```
cv_results <- tune.rcc(X_zscore, Y_zscore, grid1 = seq(0, 1, length = 50),
                      grid2 = seq(0, 0.01, length = 50), validation = "loo")
rcca_results <- rcc(X_zscore, Y_zscore, ncomp = 2, method = "ridge",
                   lambda1 = cv_results$opt.lambda1,
                   lambda2 = cv_results$opt.lambda2)
```

As illustrated in Table S2, our rCCA model, employing optimal λ_1 and λ_2 values of 0.5306122 and 0.008979592, clearly demonstrates a feature-specific shrinkage effect. This regularization diminishes the contributions of less influential variables, thereby allowing for more insightful inferences regarding variable importance and interrelationships.

Table S2 Regularization-induced feature-specific shrinkage ratios for the first canonical variate ($\mathbf{f}^1$)^a

$\tilde{\mathbf{X}}$ (feature)	canonical weight $ \mathbf{a} $ for $\mathbf{f}^1$		shrinkage ratio
	$\lambda_1 = 0$	$\lambda_1 = 0.5306122$	
OD.OE	0.212857	0.096927	0.455361
OB.OE	0.294184	0.100108	0.340290
OE.N _e	0.399447	0.133229	0.333534
OC.OJ	0.384229	0.086252	0.224480
OB.OC	0.637257	0.087876	0.137897
OJ.N _e	0.370406	0.045293	0.122279
OD.OJ	0.196719	0.017934	0.091167
OB.N _e	1.383960	0.102645	0.074168
OB.OL	1.944007	0.141392	0.072732
OD.N _e	2.154380	0.142070	0.065945
OD.OL	2.823092	0.164775	0.058367
OE.OL	1.960701	0.105147	0.053627
OJ.OL	1.914434	0.073911	0.038607
OC.OE	0.037234	0.001215	0.032633
OB.OD	0.472997	0.013898	0.029383
OC.OL	4.910672	0.078223	0.015929
OE.OJ	1.588235	0.022737	0.014316
OB.OJ	2.097310	0.023741	0.011320
OC.N _e	3.376998	0.016394	0.004855

^aThe parameter λ_2 was fixed at 0.008979592.

DNN model. We employed a supervised learning approach predicated on the hypothesis that a complex, nontrivial functional relationship exists between the input feature dataset, represented by the distance matrix, and the corresponding target variable dataset, represented by the energy matrix. In our study, the distance matrix ($\mathbf{X}$) consists of fixed-size vectors for $N = 130$ samples, each comprising $P = 19$ distances between ligating atoms that are directly coordinated to the three catalytic Mn ions (Mn_A , Mn_B , and Mn_D). Correspondingly, the energy matrix ($\mathbf{Y}$) comprises two catalytic driving forces associated with the hydroxo-oxo and oxyl-oxo species. To ensure consistency and promote efficient learning, both $\mathbf{X}$ and $\mathbf{Y}$ were independently normalized to the range $[0, 1]$ using min-max scaling, as defined below:

$$X_i^{\prime k} = \frac{X_i^k - \min_{i,k}(X_i^k)}{\max_{i,k}(X_i^k) - \min_{i,k}(X_i^k)} \quad (\text{s10})$$

$$Y_i^{\prime k} = \frac{Y_i^k - \min_{i,k}(Y_i^k)}{\max_{i,k}(Y_i^k) - \min_{i,k}(Y_i^k)} \quad (\text{s11})$$

The prime symbol (') denotes that min-max scaling has been applied. It is important to note that this data preprocessing procedure (resulting in $\mathbf{X}'$ and $\mathbf{Y}'$) differs from that used for rCCA, which involves Z-score normalization (yielding $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$). The key distinction lies in the underlying distance metric. The min-max scaling preserves the original Euclidean metric within $\mathbf{X}'$, ensuring that the relative distances, angles, and spatial configurations among data points in the transformed dataset closely mirror those of the original dataset. This preservation is particularly crucial when spatial relationships and structural patterns have direct physical or chemical significance, such as the three-dimensional configurations of amino acid side chains in the first coordination shell. In contrast, standardization via Z-score normalization (yielding $\tilde{\mathbf{X}}$) converts the original metric into a variant of the Mahalanobis distance, where the variance-covariance matrix is constrained to be diagonal (Table S3). While this standardization ensures that all variables contribute equally to the analysis regardless of their original scale, it may distort the inherent spatial relationships among data points. Such distortion can be problematic when the original spatial structure is closely linked to the underlying catalytic processes, as is the case in the OEC system.

After data preprocessing, the dataset was randomly split into training and test sets, with 90% of the data allocated for training and 10% for testing, using a 10-fold cross-validation approach.

We designed our deep neural network (DNN) with a three-layered architecture, represented as f , and systematically evaluated various node configurations for the hidden layers. Each node's output was processed through the ReLU (rectified linear unit) activation function [s6], thereby enabling the network to effectively capture and model the complex nonlinear relationships between the input feature space and the output target variables. To optimize the weights and biases of the DNN model, we used the momentum stochastic gradient descent (SGD) optimizer [s7,s8] to minimize the objective function defined as $L(f) = R(f, D) + \lambda\Omega(f)$, where $R(f, D)$ represents the fitting loss, quantified by the mean squared error relative to the given data D , and $\Omega(f)$ is a regularization term that penalizes model complexity, weighted by the coefficient λ . In our formulation, $\Omega(f)$ is defined as the squared l_2 -norm of the weight vector, expressed as $1/2 \sum_{i=1}^P \|w_i\|^2$. Focusing solely on minimizing the fitting loss $R(f, D)$ may cause the model to overfit, resulting in a configuration that is too finely tuned to the training data and loses its generalization ability. Incorporating a regularization term mitigates this risk by discouraging overly complex models. To identify the optimal model for predicting the two driving forces, we carried out an extensive hyperparameter search using Optuna [s9], which employs Bayesian optimization to efficiently traverse the hyperparameter landscape, achieving faster convergence compared to alternative approaches such as grid search. The hyperparameters explored included the number of nodes in each hidden layer (n_hidden1, n_hidden2, n_hidden3), the learning rate (lr) and momentum for the momentum SGD optimizer, and the weight decay coefficient λ in the l_2 -norm regularization term (rate). Overall model performance was evaluated by calculating the average mean absolute error ($\overline{\text{MAE}}$) across the ten individual test sets from the 10-fold cross-validation. The set of hyperparameters (n_hidden1, n_hidden2, n_hidden3, lr, momentum, and rate) that yielded the lowest $\overline{\text{MAE}}$ was identified as the optimal configuration, as summarized in Table S4.

In the context of machine learning, data scarcity is intrinsically linked to the dimensionality and complexity of the problem being addressed. The remarkably small optimal λ value (5.3×10^{-6}) underscores the importance of incorporating domain knowledge into the model, as this significantly enhances its generalization performance even when the available data are limited. This improvement is clearly demonstrated by the concurrent decline in both the training and testing loss curves, as detailed in Fig. S4D. To further validate the reliability of our DNN model's predictions and its robust generalization capability, we intentionally excluded samples corresponding to closed cubane coordination environments from the training set outlined in Table S1 and conducted repeated training trials using multiple random seeds on a restricted dataset of only 78 samples. As shown in Fig. S5, these trials consistently exhibited simultaneous reductions in training

and testing loss curves, which serves as a compelling indicator of stable generalization performance. This reproducible behavior substantiates that the performance of our deep neural network model, as shown in Fig. 8, cannot be attributed to any isolated outlier that significantly outperforms the average.

Table S3 Definitions of distance metrics^a

distance metric	Σ	example
Euclidean	$\begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$	$\mathbf{X}$ $\mathbf{X}'$ (min-max normalization)
	$\begin{pmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_P^2 \end{pmatrix}$	$\tilde{\mathbf{X}}$ (Z-score normalization)
Mahalanobis	$\begin{pmatrix} \sigma_1^2 & \cdots & \sigma_{1P} \\ \vdots & \ddots & \vdots \\ \sigma_{P1} & \cdots & \sigma_P^2 \end{pmatrix}$	

^aThe distance between two points $\mathbf{x}$ and $\mathbf{y}$ is given by the formula $d(\mathbf{x}, \mathbf{y})^2 = (\mathbf{x} - \mathbf{y})^T \Sigma^{-1} (\mathbf{x} - \mathbf{y})$, in which Σ represents the variance-covariance matrix.

Table S4 Search space for hyperparameters in the DNN model and optimal configuration identified by Optuna

	parameter ^a	search space	optimal value
node counts	n_hidden1	$\{x \in \mathbb{Z} \mid 3 \leq x \leq 120\}$	13
	n_hidden2	$\{x \in \mathbb{Z} \mid 3 \leq x \leq 120\}$	21
	n_hidden3	$\{x \in \mathbb{Z} \mid 3 \leq x \leq 120\}$	16
momentum SGD	lr	$\{x \in \mathbb{R} \mid 10^{-4} \leq x \leq 10^{-2}\}$	7.588980×10^{-3}
	momentum	$\{x \in \mathbb{R} \mid 0.5 \leq x \leq 1.0\}$	0.930036
weight decay	rate	$\{x \in \mathbb{R} \mid 10^{-6} \leq x \leq 10^{-3}\}$	5.299335×10^{-6}

^an_hidden1, n_hidden2, and n_hidden3 represent the number of nodes in the hidden layers; lr and momentum denote the learning rate and momentum in the momentum SGD; rate is the coefficient for the weight decay in the l_2 -norm term.

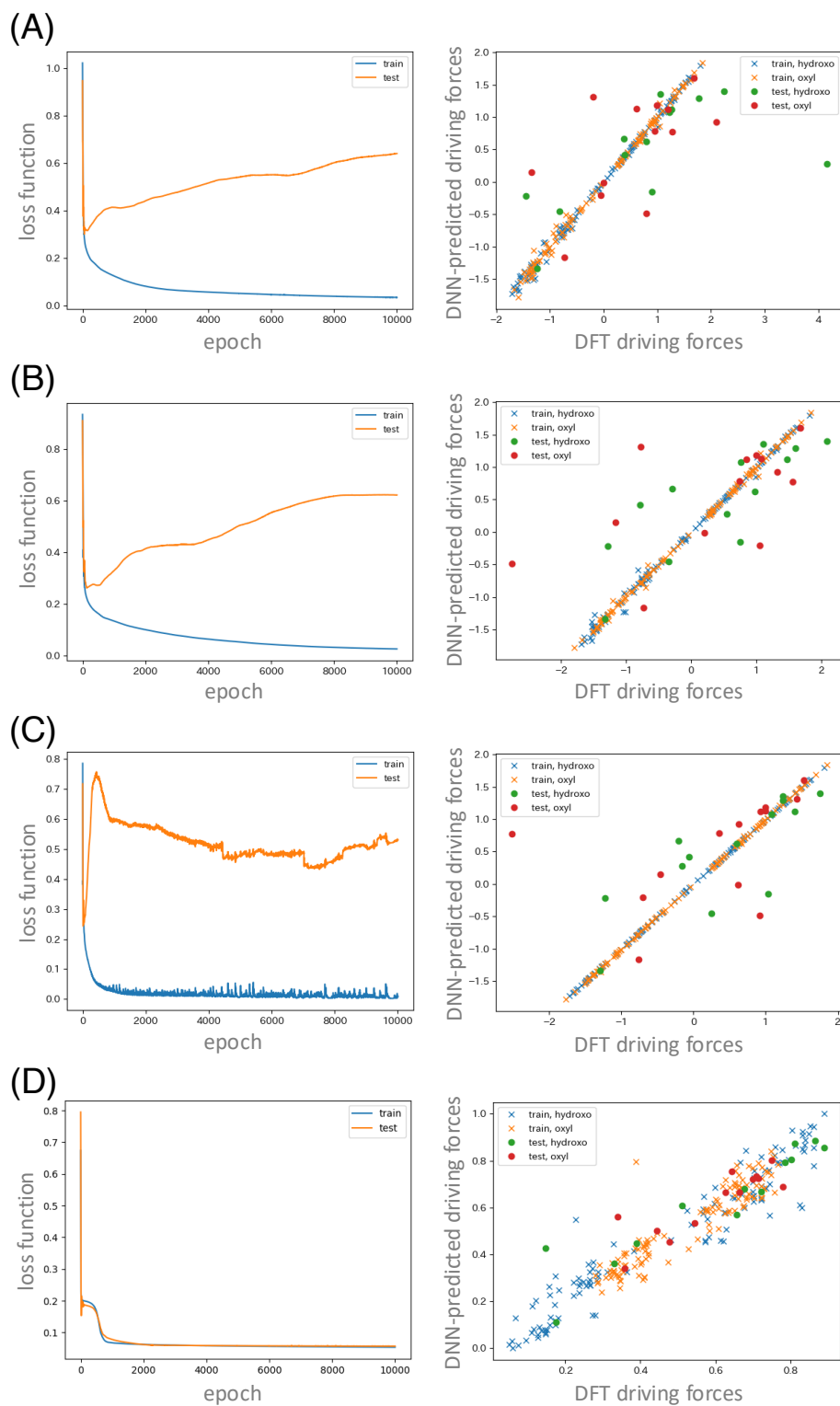


Fig. S4 Left column: Representative training and testing loss curves using the complete dataset of 130 samples listed in Table S1. Right column: Scatter plots comparing driving forces computed via DFT with those predicted by the DNN model. Panels A, B, and C are based on the standardized

(Z-score normalized) datasets ($\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Y}}$), while panel D is based on the min–max normalized datasets ($\mathbf{X}'$ and $\mathbf{Y}'$). The DNN model was optimized using momentum SGD in panel A, momentum SGD with l_2 -norm regularization in panels B and D, and Adam in panel C. All hyperparameters are consistent with those listed in Table S4, except in panel C, where alpha (learning rate coefficient) and beta1 (exponential decay rate of the first order moment) in the Adam optimizer were set to 0.0076 and 0.93.

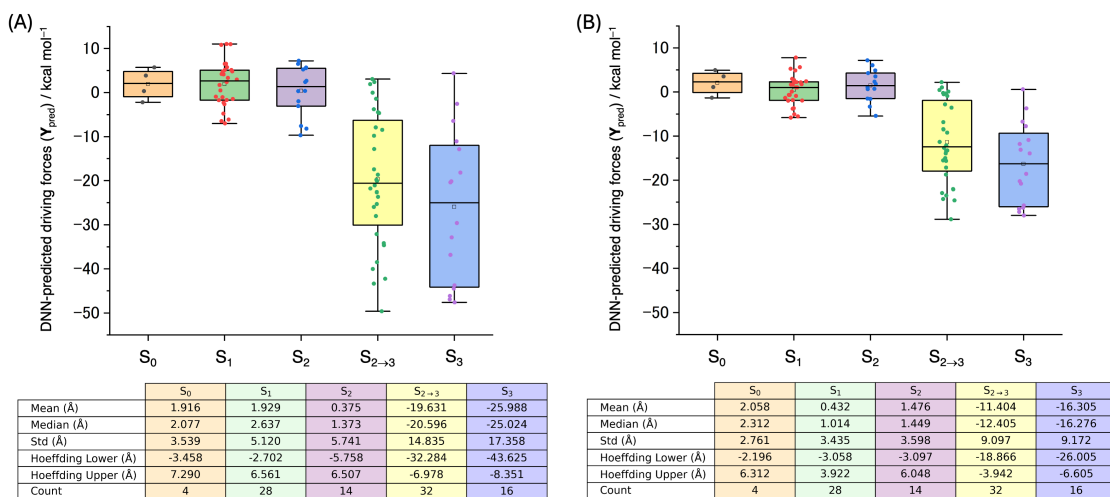


Fig. S5 (A) Box plots of the driving forces for the hydroxo–oxo species predicted by the DNN model trained on the full dataset of 130 samples listed in Table S1. The input data are identical to those listed in Fig. 2: 6DHP and 6JLP for S_0 ; 3WU2, 5B5E, 5B66, 4UB6, 4UB8, 5WS5, 6DHE, 6JLJ, 6JLM, 6W1O, 7RF2, 7COU, 7CJI, and 8IR5 for S_1 ; 6DHF, 6JLK, 6JLN, 6W1P, 7RF3, 7CJJ, and 8IRC for S_2 ; 6DHG, 6DHH, 6W1Q, 6W1R, 6W1T, 6W1U, 7RF4, 7RF5, 7RF6, 7RF7, 8IRD, 8IRE, 8IRF, 8IRG, 8IRH, and 8IRI for $S_{2 \rightarrow 3}$; and 5WS6, 6DHO, 6JLL, 6JLO, 6W1V, 7RF8, 8EZ5, and 8F4C for S_3 . For details regarding the box plot construction, see Fig. 7. Std denotes the standard deviation. For details regarding the derivation of the Hoeffding upper and lower bounds, see the caption of Fig. 2. (B) Box plots of the driving forces for the oxyl–oxo species predicted by the DNN model trained on the full dataset of 130 samples listed in Table S1. The input data remain the same as those described above.

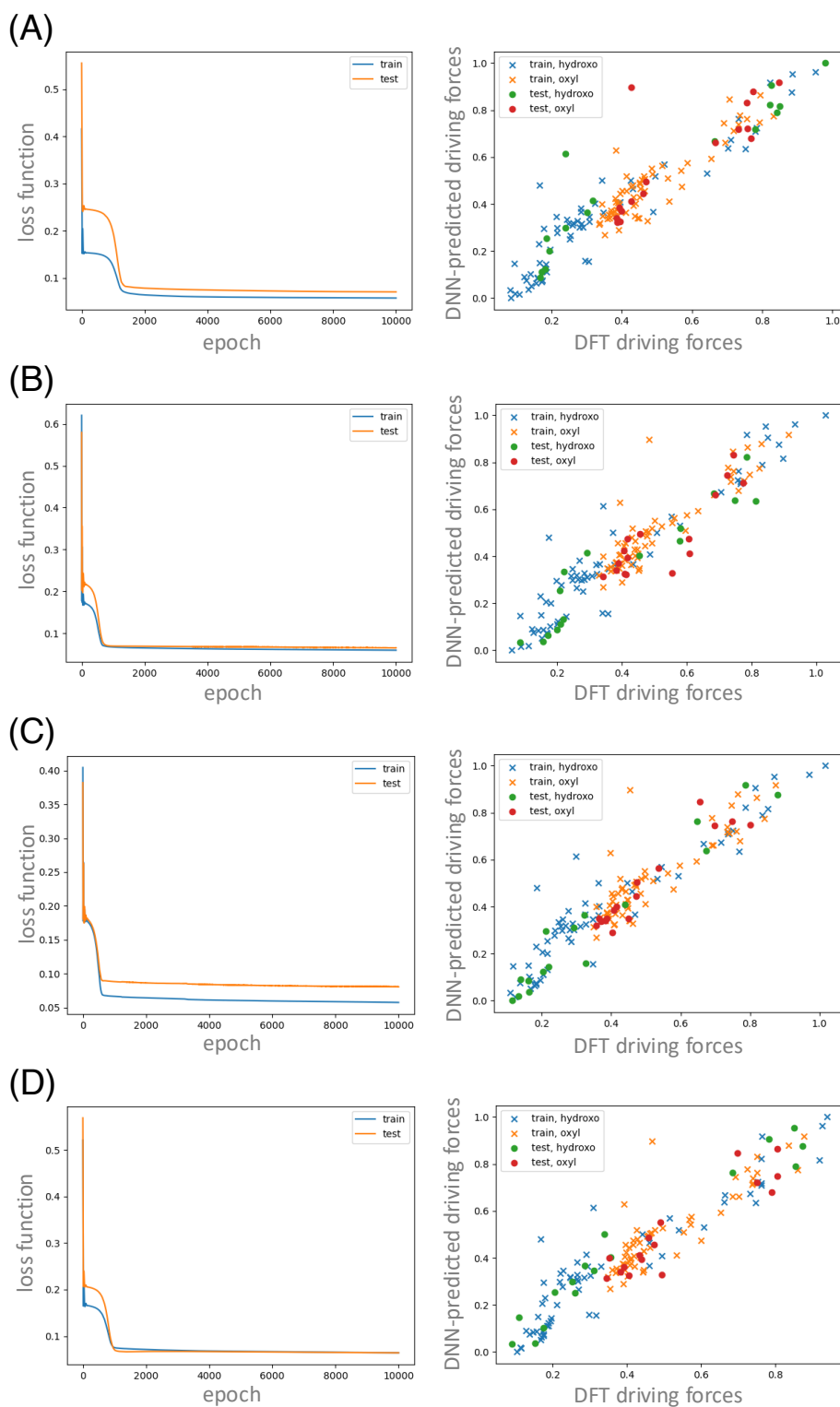


Fig. S6 Left column: Representative training and testing loss curves obtained under four different random seeds, 100 (panel A), 200 (panel B), 300 (panel C), and 400 (panel D), using a reduced dataset of 78 samples generated by excluding entries corresponding to closed cubane coordination

environments from Table S1. Right column: Scatter plots comparing driving forces computed via DFT with those predicted by the DNN model. Prior to training, the data were normalized using min–max scaling (yielding $\mathbf{X}'$ and $\mathbf{Y}'$). The DNN model was optimized using momentum SGD with l_2 -norm regularization, with hyperparameters as specified in Table S3. Note that we conducted over 100 repeated training trials using various random seeds, consistently confirming the behavior illustrated in this figure.

Table S5 Pairs of first ($\mathbf{f}^1$ and $\mathbf{g}^1$) and second ($\mathbf{f}^2$ and $\mathbf{g}^2$) canonical variates

	$\mathbf{f}^1$	$\mathbf{f}^2$	$\mathbf{g}^1$	$\mathbf{g}^2$
entry 1	-0.25422	-1.4614	0.03611	0.038675
entry 2	0.65474	-0.76507	0.54526	-0.35453
entry 3	0.41468	1.2214	0.54729	2.4825
entry 4	1.0515	0.74317	0.99513	0.17382
entry 5	-0.55841	-1.6988	-0.60875	-0.92533
entry 6	-0.41909	-0.72725	-0.38667	0.16383
entry 7	-1.1237	-0.85690	-0.92782	-1.5304
entry 8	-0.52185	-1.6731	-0.75445	-1.5351
entry 9	0.15316	-0.92975	0.16593	0.88290
entry 10	0.27531	-1.4485	0.52988	-0.51071
entry 11	-0.55954	-2.1526	-0.32303	-0.73838
entry 12	-1.2681	-1.5612	-1.46486	-0.68680
entry 13	-0.99336	0.57495	-1.52054	1.4199
entry 14	1.2906	-0.094069	1.43452	-0.12416
entry 15	-1.2467	1.3858	-1.47424	2.1746
entry 16	1.1620	0.44347	1.38133	-0.16448
entry 17	-0.89964	1.1764	-1.01102	-0.90867
entry 18	1.4520	0.28246	1.69291	-0.35219
entry 19	-1.1827	1.0980	-1.36886	-0.51822
entry 20	1.2497	0.34631	1.45993	-0.28614
entry 21	-1.2012	1.5272	-1.26574	1.5643
entry 22	1.3875	0.26066	1.23339	-0.33984
entry 23	-1.1610	0.74794	-1.35834	0.53130
entry 24	1.2608	0.086383	1.42669	0.056611
entry 25	-1.0900	0.98654	-1.06500	0.80577
entry 26	1.2616	0.28469	1.67469	0.40875
entry 27	-1.2375	0.66344	-1.10303	-0.11157
entry 28	1.1538	-0.17643	1.51445	-0.69156
entry 29	-1.2548	0.83654	-1.61753	0.74644
entry 30	1.2114	0.19270	1.43330	-0.0060248

entry 31	-1.2942	0.79897	-1.44631	-0.50030
entry 32	1.2208	-0.13736	1.24009	0.016804
entry 33	-1.3119	1.0358	-0.43541	-0.58357
entry 34	1.1594	-0.046743	0.16353	-0.80835
entry 35	-1.1228	-0.0027616	-0.49806	-1.1866
entry 36	0.69968	0.057326	-0.36320	-3.2620
entry 37	-0.64984	-0.33017	-0.62999	-0.99819
entry 38	0.90456	0.11917	0.74268	0.90281
entry 39	-0.84384	0.090695	-0.75752	-0.56157
entry 40	0.76499	0.42744	0.79776	0.64642
entry 41	-0.34135	-0.073296	-0.16969	-0.30407
entry 42	1.0519	0.46980	1.09309	0.45856
entry 43	-0.66096	-0.17820	-0.57850	0.82022
entry 44	0.85829	0.37938	0.70786	-0.091820
entry 45	-0.33501	0.17273	-0.40232	1.0988
entry 46	0.97487	0.49626	0.96472	1.4432
entry 47	-0.36314	-0.45109	-0.55678	0.59257
entry 48	0.85251	0.029055	0.65887	0.10581
entry 49	-0.57139	-0.041590	-0.33832	-0.079585
entry 50	0.88545	0.38019	0.83092	-0.063964
entry 51	-0.73084	-0.69679	-0.53339	0.74272
entry 52	0.76235	-0.22972	0.88127	0.15327
entry 53	-0.79141	-0.22417	-0.75014	-0.97750
entry 54	0.81403	0.16133	0.75874	-0.028657
entry 55	-0.81429	-0.58952	-0.93181	1.2891
entry 56	0.81665	-0.052313	0.54574	1.0429
entry 57	-0.78125	-0.40266	-0.79552	0.18530
entry 58	0.72552	0.22685	0.70181	-0.26166
entry 59	-1.0102	-0.70760	-1.12584	-0.96736
entry 60	0.12411	0.0059616	0.40477	-0.48853

Table S6 Ligand cavity sizes and DNN-predicted driving forces for various crystallographic models of PSII

PDB ID code		R^a	$Y_{\text{pred,hydroxo}}^b$	$Y_{\text{pred,oxy}}^b$
3WU2	monomer A	3.7735	-6.1256	-5.5377
3WU2	monomer B	3.7228	1.7000	-0.69278
5B5E	monomer A	3.6856	-4.7834	-3.8012
5B5E	monomer B	3.6816	-1.7589	-1.9764
5B66	monomer A	3.6806	-6.5122	-5.8107
5B66	monomer B	3.6924	-2.6450	-3.6987
4UB6	monomer A	3.6791	0.48619	-0.68674
4UB6	monomer B	3.7082	5.0975	2.2583
4UB8	monomer A	3.7068	-1.6924	-0.90274
4UB8	monomer B	3.7088	-2.2986	-1.8486
5WS5	monomer A	3.6703	4.8071	1.7563
5WS5	monomer B	3.6641	10.983	5.6256
5WS6	monomer A	3.6440	-11.116	-7.7784
5WS6	monomer B	3.6622	4.3447	0.57737
6DHP	monomer A	3.6366	-2.3111	-2.0965
6DHP	monomer B	3.6366	-2.2031	-1.3285
6DHE	monomer A	3.5785	3.8315	4.9364
6DHE	monomer B	3.6188	-7.0331	-5.0848
6DHF	monomer A	3.6589	11.013	7.7880
6DHF	monomer B	3.5749	-8.2135	-5.4319
6DHG	monomer A	3.6688	-23.691	-13.285
6DHG	monomer B	3.6110	-0.051777	1.0339
6DHH	monomer A	3.7048	-22.663	-15.657
6DHH	monomer B	3.6336	-12.848	-8.5108
6DHO	monomer A	3.7153	-32.871	-20.817
6DHO	monomer B	3.7103	-20.409	-11.824
6JLP	monomer A	3.6436	0.32348	1.0888
6JLP	monomer B	3.6429	5.7113	3.5344
6JLM	monomer A	3.6835	4.2085	1.6421

6JLM	monomer B	3.6860	10.830	5.2716
6JLN	monomer A	3.6843	-1.9782	0.62655
6JLN	monomer B	3.6348	5.5388	4.8696
6JLO	monomer A	3.7313	-12.889	-10.891
6JLO	monomer B	3.6827	-2.5760	-3.7423
6JLJ	monomer A	3.6732	6.4756	2.6953
6JLJ	monomer B	3.6895	5.7515	2.2255
6JLK	monomer A	3.6437	0.30361	1.0776
6JLK	monomer B	3.6429	5.6791	3.5201
6JLL	monomer A	3.7233	-18.205	-13.949
6JLL	monomer B	3.6868	-6.4518	-6.7356
6W1O	monomer A	3.6648	-1.0902	0.088022
6W1O	monomer B	3.6712	2.9120	2.3987
6W1P	monomer A	3.6132	-7.6150	-1.5764
6W1P	monomer B	3.5824	6.5095	7.1665
6W1Q	monomer A	3.6322	-18.659	-9.2535
6W1Q	monomer B	3.6641	-17.435	-8.4403
6W1R	monomer A	3.7825	-21.099	-12.698
6W1R	monomer B	3.7522	-43.393	-24.273
6W1T	monomer A	3.7358	-38.494	-23.478
6W1T	monomer B	3.6968	-32.151	-18.729
6W1U	monomer A	3.6609	-34.656	-22.091
6W1U	monomer B	3.6956	-21.789	-11.327
6W1V	monomer A	3.7257	-47.602	-27.993
6W1V	monomer B	3.6979	-36.843	-20.229
7RF2	monomer A	3.6594	4.7311	2.9510
7RF2	monomer B	3.6729	6.5309	4.8701
7RF3	monomer A	3.6139	-9.7054	-3.3251
7RF3	monomer B	3.6021	5.2341	6.0643
7RF4	monomer A	3.6317	-7.9115	-2.8232
7RF4	monomer B	3.6727	-8.4664	-3.5747
7RF5	monomer A	3.7560	-26.003	-15.527

7RF5	monomer B	3.7316	-49.640	-28.868
7RF6	monomer A	3.7233	-42.271	-24.596
7RF6	monomer B	3.6802	-40.065	-22.961
7RF7	monomer A	3.6470	-34.193	-22.024
7RF7	monomer B	3.6591	-28.042	-15.018
7RF8	monomer A	3.7421	-46.946	-26.561
7RF8	monomer B	3.7028	-43.780	-25.735
7CJI	monomer A	3.6917	5.0915	2.1548
7CJI	monomer B	3.6979	-0.97473	-1.3319
7COU	monomer A	3.6878	3.3260	1.0085
7COU	monomer B	3.7029	4.1130	1.6583
7CJJ	monomer A	3.6766	7.1909	4.2831
7CJJ	monomer B	3.6832	2.6467	1.8201
8IR5	monomer A	3.6775	2.3627	1.0191
8IR5	monomer B	3.6729	-1.4810	-1.9421
8IRC	monomer A	3.6449	0.36889	0.71366
8IRC	monomer B	3.6584	-3.0914	-1.5011
8IRD	monomer A	3.6482	-3.8241	-0.24264
8IRD	monomer B	3.6716	1.8977	0.41259
8IRE	monomer A	3.6288	-4.4690	-0.92964
8IRE	monomer B	3.6437	-1.4146	-0.37971
8IRF	monomer A	3.6431	-4.6812	0.056326
8IRF	monomer B	3.6451	2.3866	-0.49978
8IRG	monomer A	3.6740	3.0622	2.2129
8IRG	monomer B	3.6439	-9.8296	-6.8417
8IRH	monomer A	3.7223	-20.093	-12.111
8IRH	monomer B	3.6852	-19.801	-13.948
8IRI	monomer A	3.6896	-22.593	-13.407
8IRI	monomer B	3.6720	-25.303	-17.145
8EZ5	monomer A	3.7547	-44.496	-26.252
8EZ5	monomer B	3.7251	-46.169	-27.218
8F4C	monomer A	3.6967	-29.639	-18.603

8F4C	monomer B	3.6961	-20.157	-13.127
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^aCavity sizes evaluated using eqn (1) (R) are given in Å. ^bDNN-Predicted driving forces ($Y_{\text{pred,hydroxo}}$ and $Y_{\text{pred,oxy}}$) are given in kcal mol⁻¹.

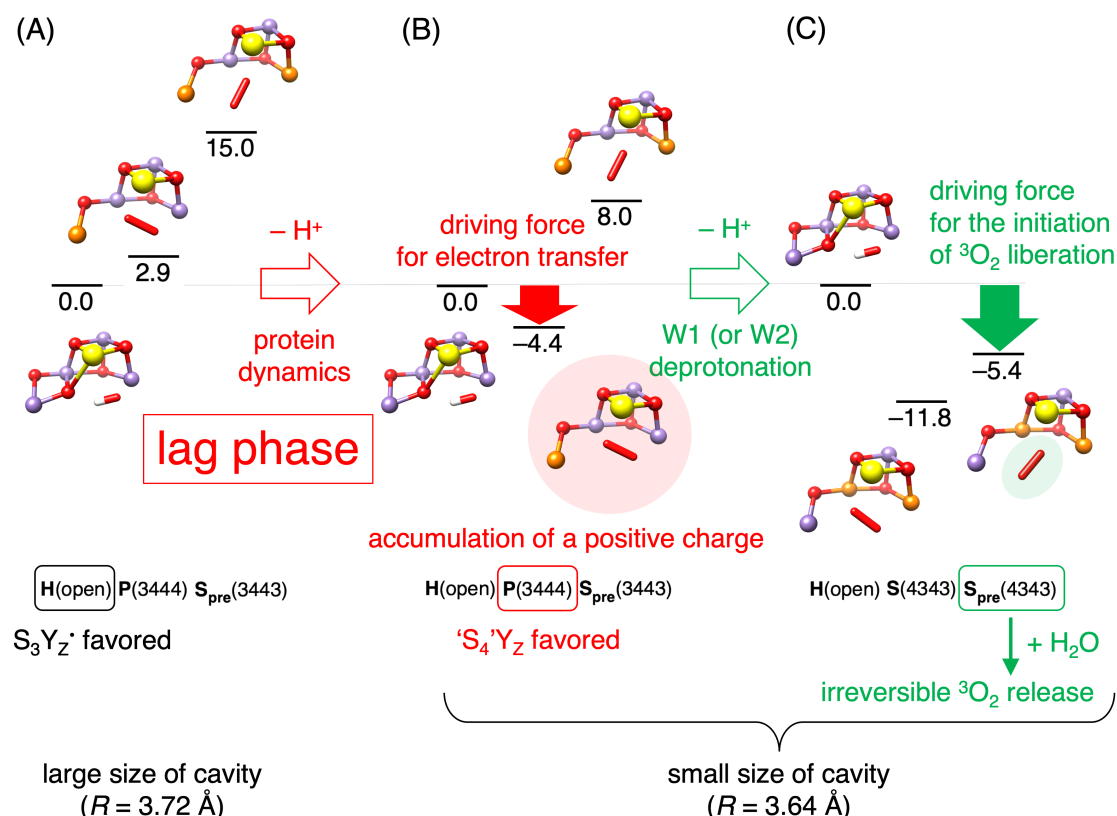


Fig. S7 Relative stabilities of $\mathbf{P}(3444)$ and $\mathbf{S}_{\text{pre}}(3443)$ in the $\text{'S}_4\text{'Y}_Z$ state relative to $\mathbf{H}(\text{open})$ in the $\text{S}_3\text{Y}_Z'$ state, evaluated at the IEFPCM-B3LYP($w_{\text{HF}}10\%$)-D4/BS2//B3LYP-D3(BJ)/BS1 level using the PDB coordinates 6JLL (A) and 6JLP (B, C). For panels A and B, the protonation states were set as follows: (W1, W2) = (H_2O , OH^-) for $\mathbf{H}(\text{open})$ and (W1, W2) = (H_2O , H_2O) for $\mathbf{P}(3444)$ and $\mathbf{S}_{\text{pre}}(3443)$. In panel C, (W1, W2) = (OH^- , OH^-) was assumed for $\mathbf{H}(\text{open})$ and (OH^- , H_2O) for $\mathbf{S}(4343)$ and $\mathbf{S}_{\text{pre}}(4343)$. Ligand cavity sizes (R) were determined from the experimental data using eqn (1). The accumulation of a positive charge in the Mn cluster is expected to facilitate deprotonation of a water ligand, either W1 or W2 at Mn_A , thereby initiating redox leveling within the Mn cluster. As a result, both $\mathbf{P}(3444)$ and $\mathbf{S}_{\text{pre}}(3443)$ become substantially stabilized relative to $\mathbf{H}(\text{open})$, with energy levels shifting from -4.4 and $8.0 \text{ kcal mol}^{-1}$ to even more negative values (-11.8 and $-5.4 \text{ kcal mol}^{-1}$). For details on the irreversible $^3\text{O}_2$ release following the formation of $\mathbf{S}_{\text{pre}}(4343)$, see ref [s10]. This cascade of events is consistent with the experimentally observed irreversible progression of the oxygen-evolving reaction [s11]. The following color codes are used: yellow, calcium; red, oxygen; white, hydrogen; purple, Mn^{IV} ; orange, Mn^{III} .

Table S7 Mulliken Spin Densities for All Structures in Fig. 9^a

	Mn _A	Mn _B	Mn _C	Mn _D	O1	O2	O3	O4	O5	O6 (or O6*)
PDB ID code: 6JLL										
H (open)	2.96	2.89	2.97	2.94	0.01	0.02	-0.02	0.10	0.00	0.05
O* (open)	3.83	2.91	2.95	2.72	0.02	0.01	-0.04	0.01	-0.24	-0.24
S (open)	3.83	3.62	2.93	3.62	0.02	0.04	-0.01	0.08	-0.14	-0.19
P (3444)	3.87	2.92	2.90	2.97	0.06	0.07	-0.01	0.12	-0.04	-0.05
S_{pre} (3443)	3.83	3.16	2.93	3.79	0.04	0.05	-0.02	-0.11	-0.68	-0.47
S (closed)	3.80	3.53	2.91	3.78	0.03	0.05	0.01	0.06	-0.21	-0.22
O* (closed)	2.73	2.90	2.95	3.77	0.02	0.03	-0.03	0.08	-0.28	-0.24
H (closed)	2.87	2.79	2.91	2.94	0.06	0.05	-0.02	0.20	-0.02	0.06
TS_{PT}	2.99	2.95	2.97	2.81	0.01	0.02	-0.03	0.06	0.01	0.19
TS_{oo}	3.81	2.77	2.90	2.40	0.05	0.04	-0.00	0.07	-0.12	-0.03
Mn^{IV}O*	2.96	2.95	2.97	2.83	0.03	0.03	-0.05	0.06	-0.00	-0.62
PDB ID code: 6JLP										
H (open)	2.95	2.88	2.97	2.93	0.00	0.03	-0.02	0.10	0.01	0.06
O* (open)	3.83	2.89	2.95	2.69	0.01	0.02	-0.04	0.01	-0.24	-0.20
S (open)	3.82	3.60	2.92	3.60	0.01	0.05	-0.01	0.07	-0.14	-0.20
P (3444)	3.87	2.91	2.89	2.97	0.05	0.08	-0.01	0.12	-0.03	-0.05

S_{pre} (3443)	3.82	3.09	2.92	3.77	0.04	0.05	-0.02	0.12	-0.43	-0.64
S (closed)	3.79	3.46	2.91	3.77	0.03	0.06	0.00	0.07	-0.19	-0.19
O* (closed)	2.75	2.92	2.93	3.74	0.01	0.04	-0.03	0.07	-0.28	-0.22
H (closed)	2.88	2.77	2.91	2.93	0.05	0.05	-0.02	0.21	-0.01	0.03
TS_{PT}	2.97	2.93	2.97	2.70	0.01	0.02	-0.03	0.08	0.02	0.31
TS_{oo}	3.84	2.84	2.95	2.42	0.02	0.02	-0.02	0.04	-0.16	-0.03
Mn^{IV}O*	2.93	2.93	2.97	2.84	0.02	0.04	-0.05	0.07	-0.03	-0.65

^aSpin densities were assessed using IEFPCM-B3LYP(*w*_{HF}15%)/BS2//B3LYP-D3(BJ)/BS1, except for **S**, **P**, and **S_{pre}**, which were assessed using IEFPCM-B3LYP(*w*_{HF}10%)/BS2//B3LYP-D3(BJ)/BS1.

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Cartesian coordinates for all structures in Fig. 9

All structures were optimized using the B3LYP-D3(BJ)/BS1 level of theory.

All amino acid residues in the first coordination sphere were fully relaxed.

Spherical-harmonic angular functions (keywords 5D and 7F in Gaussian 16) were used.

H(open)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.71554637 a.u.

Grimme-D3(BJ): -0.8635644929 a.u.

Grimme-D4: -0.8214333110 a.u.

IEFPCM-B3LYP(w_{HF} 10%)/BS2: -9414.54887479 a.u.

IEFPCM-B3LYP(w_{HF} 15%)/BS2: -9419.73399093 a.u.

Ca	27.554979	-36.448299	-59.195358
Mn	27.587187	-32.899357	-57.307362
Mn	27.378538	-33.073074	-60.077675
Mn	27.335079	-34.950943	-62.210323
Mn	24.887568	-35.488754	-61.071487
O	26.459309	-36.337067	-61.439968
O	28.284594	-34.509979	-60.749695
O	25.947437	-33.927498	-61.432163
O	28.529905	-32.379021	-58.937855
O	26.848431	-33.969879	-58.584976
O	25.113417	-35.547955	-59.312710
C	32.871857	-41.753975	-53.559959
C	31.526979	-41.339840	-52.923695
C	30.455347	-41.085621	-53.954361
C	30.024229	-42.158588	-54.786678
C	29.861082	-39.807636	-54.123871
C	29.064739	-41.973152	-55.747334
C	28.886734	-39.591602	-55.075504
C	28.460011	-40.671631	-55.941879
O	27.602814	-40.503384	-56.862907
H	31.666008	-40.445705	-52.308201

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H	30.166298	-38.982376	-53.485855
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H	28.417137	-38.620312	-55.202923
H	26.444868	-41.292107	-58.930470
H	33.647060	-41.940666	-52.807522
H	33.224892	-40.953159	-54.220818
H	32.769600	-42.661663	-54.164974
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C	22.645082	-44.870029	-58.346848
C	22.139990	-41.425869	-59.917000
C	22.529062	-42.903950	-59.745148
O	23.081059	-43.510983	-60.666977
C	23.865124	-44.868904	-57.372448
C	24.924582	-43.944378	-57.909744
C	25.186325	-42.609276	-57.705093
N	25.698418	-44.312859	-59.000984
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C	24.164364	-38.105202	-60.156975
O	25.190561	-38.290840	-59.486721
O	23.933277	-37.106125	-60.956596
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H	23.559320	-44.532745	-56.376453
H	24.811501	-41.899498	-56.984261
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H	22.997766	-27.995155	-59.038689
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C	29.949112	-31.870184	-64.759521
C	29.060719	-31.293364	-63.648186
C	28.317217	-32.300037	-62.799469
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O	27.987610	-31.935469	-61.623631
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H	30.446312	-32.777630	-64.392311
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H	24.540909	-28.475849	-55.255230
H	22.835197	-28.668297	-55.430058
H	23.515869	-27.114027	-55.504314
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C	23.467564	-36.054657	-56.734165
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H	33.238331	-28.200853	-60.433060
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H	32.386791	-31.148493	-62.244812
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H	35.440323	-28.949686	-59.495857
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H	26.006409	-39.581272	-56.745579
H	26.531624	-36.259888	-54.286949
H	26.944813	-34.897266	-54.997784
H	26.346382	-29.039871	-56.058727
H	25.615707	-30.201412	-55.215439
H	24.277245	-31.980387	-54.153561
H	23.792442	-31.508490	-55.553402
H	30.071604	-30.056461	-58.071693
H	29.900606	-31.401831	-58.781933
H	28.228605	-40.700108	-60.661598
H	26.910160	-40.146030	-61.278252
H	26.419001	-38.003159	-62.220234
H	26.288301	-38.962357	-63.464336
H	25.490223	-34.708267	-58.931923
H	25.843710	-32.857430	-55.723717
H	22.618822	-28.131384	-63.795128
H	21.675613	-27.994301	-65.046806
H	29.003717	-39.078213	-59.348881
H	26.106697	-37.501259	-56.799866
H	27.131063	-36.521172	-56.106510
H	24.609053	-37.759460	-53.406586
H	24.940563	-38.133392	-54.882347
H	30.941513	-27.459641	-62.208195
H	30.081741	-28.715322	-62.032883
H	29.257027	-27.762333	-65.435532
H	30.418098	-27.855288	-64.445358
H	29.782120	-29.878529	-60.133163
H	28.602495	-30.299881	-61.043644

O*(open)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.71977078 a.u.

Grimme-D3(BJ): -0.8681940879 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.73040665 a.u.

Ca	27.538170	-36.420451	-59.202501
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Mn	27.223505	-33.167524	-60.127719
Mn	27.315598	-34.979439	-62.253428
Mn	24.904985	-35.466712	-61.013748
O	26.459600	-36.349389	-61.444767
O	28.249523	-34.529926	-60.789144
O	25.942843	-33.921240	-61.491401
O	28.428050	-32.543264	-58.880144
O	26.592353	-34.113219	-58.796343
O	25.203037	-35.435462	-59.362068
C	32.872268	-41.753632	-53.559735
C	31.522921	-41.346285	-52.928592
C	30.455377	-41.108348	-53.966974
C	30.017951	-42.193930	-54.778564
C	29.874478	-39.828450	-54.168403
C	29.062030	-42.020992	-55.745749
C	28.906106	-39.624368	-55.127517
C	28.465962	-40.720101	-55.966925
O	27.600974	-40.563522	-56.881821
H	31.652138	-40.447183	-52.318049
H	31.186595	-42.144841	-52.253132
H	30.447853	-43.177718	-54.609964
H	30.191052	-38.996098	-53.545659
H	28.712535	-42.838904	-56.367794
H	28.449423	-38.652596	-55.293239
H	26.435177	-41.296274	-58.995207
H	33.646691	-41.940653	-52.807557
H	33.224681	-40.953393	-54.221122
H	32.769623	-42.661896	-54.165044

N	22.229954	-43.493044	-58.589923
C	22.645056	-44.870187	-58.346964
C	22.140028	-41.425936	-59.916943
C	22.529031	-42.904026	-59.745184
O	23.080981	-43.511072	-60.666955
C	23.870702	-44.866212	-57.378076
C	24.927737	-43.944425	-57.927180
C	25.190665	-42.607547	-57.734241
N	25.693398	-44.318491	-59.021727
C	26.347375	-43.265035	-59.502334
N	26.068194	-42.219873	-58.728683
C	23.367654	-40.504515	-59.853347
C	22.963395	-39.045996	-60.043074
C	24.129272	-38.066357	-60.053551
O	25.131746	-38.224565	-59.329291
O	23.919982	-37.089201	-60.869499
H	24.265485	-45.882968	-57.277036
H	23.570864	-44.525350	-56.381840
H	24.824203	-41.899908	-57.007448
H	26.974493	-43.216666	-60.376669
H	23.859158	-40.609923	-58.882416
H	24.092539	-40.803051	-60.617918
H	22.296678	-38.731150	-59.226260
H	22.404187	-38.912382	-60.973422
H	25.710594	-45.285334	-59.421785
H	21.790317	-45.469475	-58.011781
H	21.410026	-41.103473	-59.162692
H	21.824133	-42.956158	-57.837233
H	22.986995	-45.244703	-59.309940
H	21.661883	-41.356646	-60.899698
C	30.207596	-27.056342	-58.221030
C	31.049817	-26.377452	-59.299036
O	30.891858	-26.645045	-60.490237

C	28.734417	-27.272081	-58.571536
C	28.087164	-28.276692	-57.613219
O	28.837219	-29.188841	-57.125839
O	26.863715	-28.139136	-57.367353
H	28.657309	-27.688712	-59.581143
H	28.163897	-26.339969	-58.540816
H	30.321539	-26.532175	-57.265588
H	30.626467	-28.055893	-58.075333
H	31.842398	-25.666058	-58.987166
C	33.360045	-39.662980	-59.276005
C	34.284910	-38.551994	-59.789087
O	33.863993	-37.684997	-60.557952
C	32.183964	-39.075979	-58.491999
C	31.224970	-40.139010	-58.003966
C	30.666330	-40.970846	-59.146164
N	30.959890	-42.277015	-59.140944
O	29.993337	-40.446846	-60.032807
H	33.930263	-40.374257	-58.666864
H	32.985165	-40.194558	-60.159824
H	35.339502	-38.534242	-59.457101
H	32.547696	-38.504208	-57.630024
H	31.644777	-38.374028	-59.135647
H	30.372883	-39.657118	-57.516156
H	31.696030	-40.775926	-57.246010
H	31.424269	-42.712429	-58.358664
H	30.576683	-42.869485	-59.866439
N	31.861127	-33.865060	-54.797181
C	30.755139	-34.809043	-54.634167
C	30.847065	-35.632046	-53.351702
O	30.048608	-36.547303	-53.142530
C	32.921123	-31.674973	-54.669874
C	31.692959	-32.568708	-54.538572
O	30.608712	-32.091442	-54.197393

C	30.568118	-35.698547	-55.885100
C	29.659665	-35.087696	-56.962401
O	29.653329	-35.574106	-58.106733
O	28.901675	-34.145441	-56.538338
C	32.754084	-30.848242	-55.952786
O	32.578241	-31.739657	-57.038179
H	31.526121	-35.960191	-56.346432
H	30.087303	-36.639378	-55.594510
H	31.878083	-30.196748	-55.827329
H	33.636693	-30.208329	-56.098792
H	31.919886	-31.356924	-57.656798
H	33.836725	-32.279555	-54.687588
H	32.742204	-34.187388	-55.170836
H	29.842267	-34.209635	-54.562981
H	31.635459	-35.378062	-52.618724
H	32.961555	-31.018593	-53.796457
C	20.066002	-31.360041	-59.209994
C	21.173991	-30.598006	-59.933017
O	21.454996	-30.848973	-61.104041
N	21.791006	-29.658911	-59.210951
C	22.847959	-28.811034	-59.759061
C	22.427060	-28.168002	-61.088083
O	23.121927	-28.286946	-62.101932
C	20.593590	-32.720520	-58.680565
C	21.481436	-33.447650	-59.632821
C	22.810479	-33.775606	-59.564648
N	21.058599	-33.910202	-60.873679
C	22.104751	-34.478855	-61.511788
N	23.175183	-34.416560	-60.733908
C	24.173175	-29.568430	-59.905790
C	24.655653	-30.098473	-58.563687
C	25.705642	-31.173468	-58.676353
O	25.969803	-31.662501	-59.813574

O	26.231226	-31.529964	-57.577867
H	21.165657	-32.528558	-57.768314
H	19.738288	-33.343945	-58.390871
H	23.524567	-33.639835	-58.768389
H	22.075395	-34.946527	-62.482345
H	24.927475	-28.910898	-60.343434
H	24.028920	-30.393866	-60.601250
H	25.094054	-29.307257	-57.949111
H	23.833332	-30.539647	-57.986380
H	20.146209	-33.751486	-61.276183
H	19.254554	-31.479113	-59.935491
H	19.683354	-30.807589	-58.348100
H	21.628033	-29.638035	-58.203478
H	22.997745	-27.995139	-59.038710
H	21.472427	-27.609215	-61.093829
C	26.167966	-27.319888	-63.863040
C	26.355976	-28.187843	-65.123356
O	27.490383	-28.430080	-65.531635
N	25.270853	-28.651992	-65.739052
C	25.399962	-29.534989	-66.909885
C	26.545565	-28.132811	-62.614980
C	24.502052	-30.786892	-66.738078
C	24.510547	-31.342723	-65.340664
C	25.307706	-32.245209	-64.681569
N	23.580210	-30.918101	-64.398155
C	23.801486	-31.520118	-63.222084
N	24.845284	-32.333373	-63.378538
H	23.465334	-30.542515	-66.998435
H	24.824732	-31.558103	-67.445028
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H	27.590639	-28.445387	-62.673019
H	25.917110	-29.023869	-62.511156
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H	25.144046	-26.931613	-63.796042
H	25.162827	-28.998921	-67.835703
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H	24.349061	-28.333441	-65.471914
H	26.450790	-29.822825	-66.941380
C	25.287765	-36.661984	-66.406996
C	26.208252	-37.841717	-66.090232
O	25.791391	-38.795386	-65.435838
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C	28.319090	-38.973003	-66.568970
C	29.161104	-39.119131	-65.302960
O	29.792983	-40.154002	-65.087007
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C	29.792999	-38.160040	-63.151971
C	24.353617	-36.352080	-65.238497
C	25.020492	-35.752851	-63.993480
O	26.258147	-35.463284	-64.010214
O	24.253289	-35.578536	-63.003830
C	29.169921	-37.106749	-62.255786
O	29.183585	-37.246054	-61.022329
C	31.320946	-38.031341	-63.218404
O	28.668850	-36.107908	-62.908816
H	23.570007	-35.650504	-65.548523
H	23.848994	-37.264904	-64.908034
H	31.700978	-38.799751	-63.894893
H	31.611868	-37.044341	-63.592058
H	31.761861	-38.186445	-62.229450
H	24.739759	-36.922399	-67.321918
H	28.983654	-38.927584	-67.435495
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H	27.726090	-36.986729	-67.121141
H	27.697690	-39.866461	-66.648573
H	28.533251	-37.310369	-64.615264
H	29.539016	-39.122039	-62.698369
C	30.993967	-30.837988	-65.204981
C	29.948718	-31.870052	-64.755986
C	29.075993	-31.307054	-63.625631
C	28.307833	-32.317668	-62.799240
O	28.033905	-33.453023	-63.306139
O	27.957060	-31.963776	-61.627779
H	29.314125	-32.174280	-65.597311
H	30.446864	-32.784274	-64.406920
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H	29.688892	-30.743047	-62.919108
H	30.553397	-29.885772	-65.525818
H	31.616559	-31.222501	-66.020012
H	31.656692	-30.596549	-64.367581
C	36.822807	-32.169703	-62.941933
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C	34.910123	-33.861521	-62.779649
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N	33.154922	-33.948147	-61.044575
C	31.964930	-34.342053	-60.587549
N	31.545854	-35.605139	-60.767048
N	31.161080	-33.447478	-59.994734
H	35.286970	-32.207660	-61.429925
H	36.441572	-33.519178	-61.296033
H	34.258441	-33.271160	-63.438604
H	35.491434	-34.526674	-63.431579
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H	31.512893	-32.514772	-59.812106
H	36.297416	-31.688736	-63.775856
H	37.583575	-32.835097	-63.369913
H	37.340285	-31.386055	-62.378880
C	21.429798	-33.349485	-50.364030
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C	22.583235	-31.856176	-52.014595
N	21.690664	-31.117725	-52.716653
O	23.588045	-32.364073	-52.529077
H	21.762312	-31.207494	-50.110312
H	23.236735	-32.186050	-50.030950
H	20.832380	-30.807700	-52.284077
H	21.745403	-31.053755	-53.735174
H	21.355189	-33.672864	-49.320800
H	21.883973	-34.158170	-50.944298
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C	22.949263	-26.584982	-52.987103
C	23.450004	-27.918293	-53.542822
N	23.563943	-28.024522	-55.043119
H	21.934618	-26.353037	-53.329581
H	23.612140	-25.757942	-53.265713
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H	23.515860	-27.114030	-55.504330
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C	22.670972	-35.952504	-55.465287
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C	22.207414	-34.511535	-55.219708

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H	22.782337	-35.766029	-57.631630
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H	23.051401	-33.815266	-55.241519
H	20.906279	-36.796324	-54.497881
H	21.842200	-37.976313	-55.431495
H	20.820454	-36.793444	-56.270359
C	24.041082	-36.051471	-50.719070
C	23.149655	-37.272446	-50.955005
O	23.248771	-37.933860	-52.004990
H	23.648241	-35.395096	-49.938251
H	25.031127	-36.404744	-50.401163
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H	22.428167	-37.570669	-50.173541
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C	33.265695	-29.062784	-59.745624
C	33.102171	-30.354502	-60.525687
N	32.507975	-30.286451	-61.726843
O	33.498280	-31.431081	-60.036025
H	33.216391	-28.201157	-60.417462
H	32.385006	-29.012120	-59.093802
H	31.990223	-29.459153	-62.064128
H	32.330181	-31.158691	-62.208931
H	34.513906	-28.256649	-58.151766
H	35.440338	-28.949722	-59.495853
H	34.600100	-30.023889	-58.363119
C	23.583006	-48.235985	-60.182979
C	24.552942	-47.106781	-60.534821
N	24.365987	-46.509963	-61.704071
O	25.468020	-46.793168	-59.767118

H	24.128452	-49.014203	-59.646065
H	22.811284	-47.839025	-59.513646
H	23.093940	-48.667358	-61.061086
H	23.516470	-46.659859	-62.229937
H	24.828643	-45.621737	-61.862806
Cl	21.824387	-30.424360	-56.027601
O	25.389528	-37.801556	-53.985184
O	30.653207	-28.380997	-62.567618
O	30.197940	-27.578762	-65.298918
O	27.167180	-35.797298	-54.354542
O	25.852491	-29.198780	-55.200458
O	24.651492	-31.750350	-54.958500
O	30.429687	-30.738573	-58.597282
O	28.515258	-38.539531	-58.675960
O	27.069975	-36.922663	-56.846659
O	25.237319	-39.057491	-56.698576
O	27.246292	-40.743371	-60.597144
O	26.527114	-38.908556	-62.503816
O	26.299047	-33.634090	-55.875266
O	28.371653	-31.441769	-55.835687
O	22.492362	-28.398751	-64.732721
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H	28.064121	-39.213515	-58.139184
H	28.459299	-30.518523	-56.212933
H	29.168732	-31.642745	-55.301346
H	25.065575	-38.838002	-57.648366
H	26.079303	-39.558373	-56.707197
H	26.473720	-36.463535	-54.091935
H	27.996933	-36.069852	-53.922238
H	26.359623	-28.944980	-56.029287
H	25.695160	-30.167171	-55.212284
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H	23.875387	-31.546834	-55.519328

H	29.943967	-30.091072	-58.011326
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H	26.896829	-40.109629	-61.272824
H	26.394427	-37.982710	-62.203270
H	26.256240	-38.953753	-63.440295
H	26.676029	-34.201666	-55.165924
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H	22.623250	-28.126353	-63.793812
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H	28.993434	-39.014853	-59.384394
H	26.290457	-37.498077	-56.697886
H	27.136569	-36.355218	-56.044594
H	24.630102	-37.802723	-53.365968
H	25.065561	-38.164629	-54.831990
H	30.819677	-27.517590	-62.149701
H	29.976366	-28.784792	-61.964448
H	29.247703	-27.752624	-65.413608
H	30.369903	-27.882577	-64.388503
H	29.672159	-29.940249	-60.069229
H	28.523356	-30.356427	-61.022060

S(open)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.72771210 a.u.

Grimme-D3(BJ): -0.8674297446 a.u.

Grimme-D4: -0.821937062 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.53252012 a.u.

Ca	27.620431	-36.475576	-59.210036
Mn	27.511307	-32.955940	-57.185356
Mn	27.236948	-33.089030	-60.179357
Mn	27.302342	-34.958336	-62.241756
Mn	24.882769	-35.411646	-61.003429

O	26.438073	-36.311676	-61.359925
O	28.257192	-34.499739	-60.806719
O	25.935513	-33.878391	-61.516785
O	28.359432	-32.674269	-58.745752
O	26.454242	-34.362927	-58.721594
O	25.366097	-35.138618	-58.992936
C	32.871996	-41.753955	-53.559982
C	31.526357	-41.348784	-52.921017
C	30.455536	-41.118358	-53.955621
C	30.016887	-42.211565	-54.756155
C	29.878717	-39.838843	-54.168733
C	29.063575	-42.045879	-55.726544
C	28.913110	-39.641923	-55.131585
C	28.472901	-40.745384	-55.960434
O	27.609681	-40.594877	-56.878099
H	31.656880	-40.447521	-52.314007
H	31.196964	-42.146817	-52.241635
H	30.444694	-43.194291	-54.576603
H	30.196732	-39.001787	-53.553013
H	28.711974	-42.868501	-56.341101
H	28.460268	-38.670491	-55.309842
H	26.440597	-41.298168	-58.985726
H	33.646852	-41.940495	-52.807513
H	33.224769	-40.953314	-54.221062
H	32.769652	-42.661870	-54.164894
N	22.229930	-43.493038	-58.589912
C	22.645015	-44.869958	-58.347023
C	22.139995	-41.425932	-59.916977
C	22.529027	-42.903896	-59.745143
O	23.081024	-43.511000	-60.666989
C	23.871315	-44.868152	-57.378624
C	24.929999	-43.947513	-57.926865
C	25.199832	-42.613298	-57.726444

N	25.689609	-44.317913	-59.026971
C	26.345537	-43.264170	-59.504145
N	26.074414	-42.222885	-58.722763
C	23.374964	-40.506505	-59.832151
C	22.978298	-39.033617	-59.894850
C	24.138084	-38.039274	-59.873595
O	25.184436	-38.241239	-59.218770
O	23.876782	-36.987785	-60.561452
H	24.264291	-45.885736	-57.278577
H	23.572653	-44.527521	-56.381950
H	24.839139	-41.908410	-56.994019
H	26.968138	-43.213346	-60.381579
H	23.894893	-40.685884	-58.887744
H	24.075817	-40.751613	-60.636869
H	22.337798	-38.783267	-59.035582
H	22.388193	-38.826008	-60.792042
H	25.705899	-45.284118	-59.428798
H	21.790342	-45.469567	-58.011814
H	21.409991	-41.103286	-59.162685
H	21.824140	-42.956159	-57.837257
H	22.986974	-45.244759	-59.309953
H	21.661918	-41.356398	-60.899668
C	30.207691	-27.056380	-58.221228
C	31.050602	-26.377645	-59.299155
O	30.890915	-26.644765	-60.490193
C	28.737063	-27.291032	-58.572778
C	28.097454	-28.305513	-57.617885
O	28.845055	-29.230208	-57.149729
O	26.877223	-28.164384	-57.356679
H	28.670659	-27.711044	-59.582100
H	28.153164	-26.367331	-58.544575
H	30.321197	-26.532067	-57.265682
H	30.626580	-28.055875	-58.075119

H	31.842489	-25.666269	-58.987052
C	33.360052	-39.662976	-59.276003
C	34.284900	-38.551990	-59.789093
O	33.863998	-37.685005	-60.557943
C	32.183969	-39.075972	-58.491998
C	31.224987	-40.139003	-58.003962
C	30.666333	-40.970855	-59.146133
N	30.959910	-42.277011	-59.140941
O	29.993283	-40.446907	-60.032871
H	33.930264	-40.374256	-58.666862
H	32.985165	-40.194559	-60.159823
H	35.339501	-38.534242	-59.457103
H	32.547693	-38.504205	-57.630023
H	31.644778	-38.374030	-59.135646
H	30.372885	-39.657114	-57.516157
H	31.696026	-40.775927	-57.246004
H	31.424270	-42.712430	-58.358662
H	30.576695	-42.869474	-59.866443
N	31.861031	-33.865033	-54.797195
C	30.755152	-34.809088	-54.634156
C	30.847047	-35.632036	-53.351715
O	30.048637	-36.547300	-53.142542
C	32.921172	-31.674982	-54.669870
C	31.692933	-32.568650	-54.538607
O	30.608715	-32.091357	-54.197404
C	30.566640	-35.697612	-55.882790
C	29.608618	-35.112715	-56.927776
O	29.641221	-35.549517	-58.092185
O	28.770393	-34.262841	-56.461009
C	32.749553	-30.857490	-55.959174
O	32.565222	-31.760651	-57.033856
H	31.519387	-35.923827	-56.371739
H	30.122659	-36.654507	-55.584988

H	31.876351	-30.202111	-55.835217
H	33.633284	-30.222493	-56.117569
H	31.888668	-31.398692	-57.645456
H	33.836706	-32.279587	-54.687587
H	32.742158	-34.187379	-55.170858
H	29.842192	-34.209650	-54.562933
H	31.635476	-35.378064	-52.618747
H	32.961527	-31.018613	-53.796454
C	20.066026	-31.360112	-59.210035
C	21.173975	-30.598063	-59.933009
O	21.454984	-30.848977	-61.104062
N	21.791017	-29.658949	-59.210924
C	22.848052	-28.811069	-59.759009
C	22.427094	-28.168044	-61.088058
O	23.121937	-28.286992	-62.101903
C	20.561091	-32.717679	-58.654402
C	21.451579	-33.450289	-59.590301
C	22.787019	-33.739637	-59.517641
N	21.045022	-33.909375	-60.836089
C	22.107863	-34.442104	-61.475147
N	23.173677	-34.356422	-60.691688
C	24.172131	-29.575374	-59.890745
C	24.647372	-30.087593	-58.535289
C	25.663318	-31.197209	-58.627872
O	25.964134	-31.651606	-59.769500
O	26.125455	-31.616720	-57.523427
H	21.121373	-32.525245	-57.735140
H	19.690764	-33.324362	-58.374595
H	23.487265	-33.587551	-58.712801
H	22.097488	-34.903770	-62.449205
H	24.931593	-28.929794	-60.337041
H	24.025383	-30.411061	-60.573684
H	25.119832	-29.294275	-57.947905

H	23.817638	-30.482988	-57.936913
H	20.130690	-33.769663	-61.241307
H	19.254515	-31.479140	-59.935492
H	19.683371	-30.807652	-58.348104
H	21.628028	-29.638063	-58.203465
H	22.997766	-27.995181	-59.038655
H	21.472446	-27.609231	-61.093830
C	26.167946	-27.319909	-63.863030
C	26.356009	-28.187751	-65.123226
O	27.490540	-28.430121	-65.531645
N	25.270834	-28.652015	-65.739042
C	25.399958	-29.535003	-66.909899
C	26.547598	-28.133984	-62.616044
C	24.494168	-30.782020	-66.750854
C	24.494050	-31.345426	-65.358675
C	25.284579	-32.257169	-64.705314
N	23.573310	-30.911461	-64.411649
C	23.796668	-31.516723	-63.237077
N	24.829853	-32.340965	-63.400553
H	23.460724	-30.528684	-67.015792
H	24.816279	-31.549790	-67.461763
H	26.126450	-32.847087	-65.031640
H	23.212508	-31.365865	-62.338794
H	22.920224	-30.129254	-64.555084
H	25.248323	-32.947285	-62.644255
H	27.591918	-28.448535	-62.678790
H	25.919121	-29.024672	-62.510787
H	26.436497	-27.531080	-61.708943
H	25.144043	-26.931615	-63.796043
H	25.162812	-28.998953	-67.835681
H	26.862476	-26.480672	-63.959520
H	24.349051	-28.333455	-65.471922
H	26.450794	-29.822835	-66.941353

C	25.287719	-36.661603	-66.407231
C	26.208187	-37.841730	-66.090316
O	25.791382	-38.795431	-65.435884
N	27.453084	-37.786117	-66.567317
C	28.319098	-38.972998	-66.568961
C	29.161086	-39.119149	-65.302940
O	29.792999	-40.153998	-65.087011
N	29.169946	-38.084850	-64.471918
C	29.793055	-38.160030	-63.151997
C	24.335993	-36.364349	-65.255051
C	24.974435	-35.769455	-63.996867
O	26.214940	-35.486071	-63.986205
O	24.183728	-35.593566	-63.028662
C	29.161617	-37.108933	-62.257121
O	29.196456	-37.246201	-61.020857
C	31.320419	-38.029785	-63.215670
O	28.631866	-36.127332	-62.904842
H	23.553968	-35.665318	-65.574436
H	23.830164	-37.282556	-64.941685
H	31.701880	-38.796997	-63.892727
H	31.611013	-37.042138	-63.587785
H	31.760009	-38.185934	-62.226392
H	24.739698	-36.922764	-67.321832
H	28.983669	-38.927566	-67.435483
H	25.873126	-35.761286	-66.621007
H	27.726091	-36.986727	-67.121134
H	27.697703	-39.866460	-66.648581
H	28.533210	-37.310385	-64.615254
H	29.539014	-39.122033	-62.698346
C	30.993891	-30.837915	-65.204877
C	29.951724	-31.881719	-64.795668
C	28.975021	-31.289872	-63.777724
C	28.241208	-32.279113	-62.905311

O	28.010938	-33.456128	-63.345475
O	27.873224	-31.868969	-61.763884
H	29.402023	-32.246589	-65.671891
H	30.445815	-32.761562	-64.362645
H	28.234624	-30.652647	-64.282067
H	29.505051	-30.620560	-63.096640
H	30.553347	-29.885873	-65.525921
H	31.616722	-31.222407	-66.020103
H	31.656578	-30.596656	-64.367590
C	36.822976	-32.169985	-62.941997
C	35.860587	-32.928381	-62.020899
C	34.894407	-33.842579	-62.784153
C	34.031061	-34.738085	-61.891851
N	33.148352	-33.945106	-61.037115
C	31.964646	-34.351777	-60.574761
N	31.556347	-35.616483	-60.767190
N	31.156040	-33.475047	-59.962979
H	35.295901	-32.207845	-61.419842
H	36.438471	-33.531786	-61.306447
H	34.241841	-33.237909	-63.429142
H	35.464430	-34.503136	-63.450652
H	34.667197	-35.391052	-61.282095
H	33.409133	-35.388151	-62.516541
H	33.438968	-33.002466	-60.734465
H	30.631218	-35.905432	-60.471244
H	32.242797	-36.346915	-60.907585
H	30.287967	-33.775532	-59.529717
H	31.486353	-32.534868	-59.778581
H	36.297424	-31.688558	-63.775823
H	37.583380	-32.835151	-63.369739
H	37.340285	-31.385869	-62.378955
C	21.429830	-33.349489	-50.364101
C	22.267938	-32.071175	-50.530108

C	22.573063	-31.845262	-52.003378
N	21.684398	-31.100387	-52.702644
O	23.574134	-32.359644	-52.519509
H	21.748785	-31.208667	-50.096807
H	23.229992	-32.177882	-50.022440
H	20.829826	-30.784237	-52.267087
H	21.735793	-31.036107	-53.721464
H	21.355204	-33.672788	-49.320812
H	21.883963	-34.158236	-50.944274
H	20.410131	-33.207136	-50.739066
C	22.949266	-26.584983	-52.987107
C	23.450012	-27.918296	-53.542820
N	23.563945	-28.024554	-55.043122
H	21.934621	-26.353037	-53.329583
H	23.612141	-25.757940	-53.265710
H	22.932582	-26.646274	-51.895112
H	22.797452	-28.738605	-53.233786
H	24.449225	-28.135115	-53.156954
H	24.540910	-28.475798	-55.255243
H	22.835198	-28.668296	-55.430054
H	23.515884	-27.114022	-55.504296
C	21.492958	-36.937031	-55.413947
C	22.670672	-35.954378	-55.447019
C	23.467332	-36.084728	-56.746206
C	22.201233	-34.509731	-55.237731
H	23.342545	-36.214491	-54.616303
H	23.808971	-37.112273	-56.900566
H	22.851811	-35.809114	-57.611687
H	24.346797	-35.434884	-56.749555
H	21.674954	-34.388628	-54.283070
H	21.512569	-34.205044	-56.036600
H	23.046083	-33.814253	-55.241400
H	20.906249	-36.796300	-54.497909

H	21.842185	-37.976343	-55.431456
H	20.820484	-36.793485	-56.270400
C	24.041085	-36.051480	-50.719067
C	23.149615	-37.272438	-50.955021
O	23.248800	-37.933828	-52.004968
H	23.648229	-35.395087	-49.938265
H	25.031122	-36.404743	-50.401149
H	24.166844	-35.500884	-51.655823
H	22.428202	-37.570688	-50.173540
C	34.536911	-29.067008	-58.887897
C	33.265277	-29.074134	-59.745114
C	33.113166	-30.374559	-60.514981
N	32.520501	-30.320527	-61.717267
O	33.519337	-31.442205	-60.014588
H	33.209048	-28.218060	-60.423381
H	32.384377	-29.023854	-59.092672
H	32.001768	-29.495703	-62.060333
H	32.345822	-31.197286	-62.192408
H	34.513853	-28.256701	-58.151783
H	35.440342	-28.949683	-59.495866
H	34.600089	-30.023910	-58.363206
C	23.583006	-48.235985	-60.182995
C	24.552968	-47.106973	-60.534849
N	24.365992	-46.509956	-61.704079
O	25.468091	-46.792834	-59.767017
H	24.128431	-49.014219	-59.646079
H	22.811284	-47.839029	-59.513643
H	23.093915	-48.667357	-61.061083
H	23.516466	-46.659847	-62.229930
H	24.828639	-45.621728	-61.862807
Cl	21.810102	-30.420313	-56.017483
O	25.382733	-37.858814	-53.969794
O	30.683818	-28.404886	-62.550137

O	30.191419	-27.569817	-65.265228
O	27.091077	-35.825103	-54.343619
O	25.851597	-29.204712	-55.188384
O	24.622252	-31.734474	-54.921662
O	30.378820	-30.853641	-58.605500
O	28.548325	-38.583638	-58.650638
O	27.100155	-36.960197	-56.839986
O	25.254356	-39.113217	-56.627894
O	27.239923	-40.731434	-60.594157
O	26.455339	-38.866264	-62.451190
O	26.220203	-33.650761	-55.788534
O	28.352881	-31.489390	-55.860929
O	22.494991	-28.383080	-64.735262
O	29.072932	-29.613035	-60.751982
H	28.069612	-39.241645	-58.117208
H	28.450418	-30.570059	-56.251548
H	29.142075	-31.683405	-55.310923
H	25.091641	-38.885081	-57.578402
H	26.096526	-39.613807	-56.639323
H	26.422877	-36.520973	-54.084945
H	27.932336	-36.063056	-53.914621
H	26.365241	-28.959882	-56.015707
H	25.681315	-30.170893	-55.195911
H	24.230154	-31.933173	-54.029879
H	23.853984	-31.540546	-55.496491
H	29.925859	-30.164165	-58.044113
H	29.692303	-31.570991	-58.631264
H	28.207702	-40.666041	-60.670755
H	26.878269	-40.086350	-61.252274
H	26.358323	-37.934930	-62.152707
H	26.221467	-38.899313	-63.397894
H	26.572018	-34.256027	-55.094780
H	25.615282	-32.945015	-55.405161

H	22.625468	-28.116196	-63.794930
H	21.685761	-27.949624	-65.045394
H	29.016015	-39.076709	-59.355553
H	26.331101	-37.548518	-56.691631
H	27.137475	-36.380224	-56.044586
H	24.614981	-37.845472	-53.361519
H	25.073975	-38.230490	-54.819491
H	30.849359	-27.533770	-62.148555
H	30.013996	-28.803678	-61.934101
H	29.243190	-27.752073	-65.383962
H	30.369447	-27.895807	-64.363832
H	29.657803	-30.044065	-60.087825
H	28.521226	-30.340680	-61.107844

P(3444)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.72411594 a.u.

Grimme-D3(BJ): -0.8631066026 a.u.

Grimme-D4: -0.814255938 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.55135900 a.u.

Ca	27.657880	-36.595768	-59.206465
Mn	27.517994	-32.971549	-57.219756
Mn	27.194815	-33.190063	-60.218779
Mn	27.301192	-35.006206	-62.284721
Mn	24.873250	-35.422014	-61.041331
O	26.411406	-36.314335	-61.349865
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O	25.920640	-33.908653	-61.594321
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C	22.594644	-31.844307	-52.000776
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$S_{\text{pre}}(3443)$

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.71100467 a.u.

Grimme-D3(BJ): -0.8641810152 a.u.

Grimme-D4: -0.821952374 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.52849344 a.u.

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O	26.364199	-36.347134	-61.362946
O	28.149554	-34.578686	-60.772925
O	25.901638	-33.890388	-61.596908
O	28.219799	-32.789450	-58.799315
O	25.673375	-34.148156	-57.996430
O	26.072051	-34.532930	-59.157819
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C	31.520152	-41.364279	-52.942688
C	30.460871	-41.085770	-53.990479
C	30.037193	-42.093266	-54.869298
C	29.864616	-39.824194	-54.119482
C	29.063455	-41.857607	-55.837401
C	28.880885	-39.574284	-55.076793
C	28.460858	-40.590424	-55.955160
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S(closed)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.71803500 a.u.

Grimme-D3(BJ): -0.8661114543 a.u.

Grimme-D4: -0.826074173 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.52189740 a.u.

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C	29.887428	-39.864730	-54.184976
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H	21.790288	-45.469406	-58.011798
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C	31.049433	-26.377714	-59.298858

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H	30.263747	-33.874333	-59.512888
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O	25.278950	-39.193356	-56.575601
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O*(closed)

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.69885426 a.u.

Grimme-D3(BJ): -0.8687135127 a.u.

IEFPCM-B3LYP(_wHF15%)/BS2: -9419.70841159 a.u.

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C	29.882483	-39.838365	-54.173292
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C	28.921281	-39.642433	-55.140917
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C	28.733171	-27.252155	-58.577586
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O	28.849702	-29.181829	-57.173245
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H	28.647749	-27.650164	-59.593344
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C	31.224986	-40.139032	-58.003935
C	30.666301	-40.970879	-59.146045
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H	33.930264	-40.374262	-58.666848
H	32.985164	-40.194567	-60.159810
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H	32.547684	-38.504204	-57.630017
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H	30.372900	-39.657108	-57.516176
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H	32.961535	-31.018593	-53.796467
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H	23.230720	-32.167433	-50.054765
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H(closed)

PDB ID code: 6JLL

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Grimme-D3(BJ): -0.8753900640 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.69774446 a.u.

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O	25.848913	-33.949403	-61.821647
O	27.874394	-33.195269	-58.778023
O	25.777461	-34.804451	-59.549298
O	25.867043	-34.007869	-57.014788
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H	32.985155	-40.194562	-60.159817
H	35.339509	-38.534246	-59.457102
H	32.547684	-38.504202	-57.630012
H	31.644777	-38.374037	-59.135644
H	30.372884	-39.657105	-57.516151
H	31.696020	-40.775923	-57.245989
H	31.424262	-42.712422	-58.358658
H	30.576709	-42.869445	-59.866454
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C	30.754867	-34.808877	-54.634127
C	30.847037	-35.632065	-53.351737
O	30.048646	-36.547309	-53.142521
C	32.921048	-31.674907	-54.670002
C	31.692986	-32.568622	-54.538560
O	30.608714	-32.091475	-54.197384
C	30.523007	-35.682092	-55.891604
C	29.435990	-35.145850	-56.844341
O	29.403621	-35.588686	-58.011497
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C	32.835776	-30.879778	-55.973422
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H	31.443138	-35.820253	-56.468145
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H	31.877580	-30.342758	-56.010070
H	33.645823	-30.135929	-56.006174
H	32.496496	-31.442299	-57.816453
H	33.836712	-32.279591	-54.687577
H	32.742191	-34.187385	-55.170873
H	29.842297	-34.209596	-54.562975
H	31.635517	-35.378093	-52.618743
H	32.961570	-31.018628	-53.796470
C	20.066079	-31.360100	-59.209960

C	21.173959	-30.598024	-59.933030
O	21.454981	-30.848982	-61.104064
N	21.790984	-29.658860	-59.210975
C	22.847912	-28.811259	-59.758989
C	22.427124	-28.167950	-61.088101
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H	23.447886	-30.478481	-67.105031
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H	26.379836	-27.534598	-61.706266
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C	29.159057	-37.120640	-62.269436
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H	35.359873	-32.201788	-61.352779
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H	34.161383	-33.080640	-63.355265
H	35.299137	-34.416454	-63.468788
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H	30.654353	-36.014861	-60.430352
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H	36.297448	-31.688580	-63.775881
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H	37.340319	-31.385881	-62.378975
C	21.430425	-33.349599	-50.364647
C	22.252923	-32.064122	-50.540336
C	22.512865	-31.842216	-52.021866
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H	21.737450	-31.208323	-50.089911
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H	22.835189	-28.668258	-55.430080
H	23.515896	-27.113983	-55.504282
C	21.493119	-36.937031	-55.413931
C	22.700949	-36.001117	-55.532953
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H	21.919203	-34.353933	-54.323524
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O	23.248686	-37.933480	-52.005203
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O	28.523662	-38.609745	-58.626590
O	26.641020	-36.846040	-57.108748
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O	27.266606	-40.791688	-60.633496

O	26.510936	-38.956913	-62.556873
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O	29.075220	-31.685586	-56.622965
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H	24.069277	-31.909861	-54.083410
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H	30.231888	-30.255109	-58.713287
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H	25.766986	-34.404128	-57.913415
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H	29.003063	-39.130591	-59.303750
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H	24.911277	-38.491328	-54.865264
H	30.105134	-27.982647	-61.278020
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H	29.078861	-27.909168	-64.723414
H	29.848582	-28.243295	-63.430894
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TS_{PT}

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.68394624 a.u.

Grimme-D3(BJ): -0.8645935808 a.u.

IEFPCM-B3LYP(*w*_{HF}15%)/BS2: -9419.70914033 a.u.

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O	28.305036	-34.470805	-60.782797
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O	28.511009	-32.330587	-58.951044
O	26.925055	-33.984763	-58.570231
O	25.002218	-35.363849	-59.301626
C	32.871853	-41.753973	-53.559964
C	31.526805	-41.342335	-52.922780
C	30.451582	-41.064918	-53.944878
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C	29.831196	-39.792376	-54.051964
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H	31.668689	-40.459041	-52.292380
H	31.181315	-42.149847	-52.261926
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C	22.645083	-44.870026	-58.346848
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O	23.875835	-37.071105	-60.969130
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H	22.201125	-38.710303	-59.517326
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C	28.112406	-28.336303	-57.663538
O	28.916257	-29.196865	-57.155961
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H	28.663983	-27.655710	-59.602240
H	28.148246	-26.360210	-58.507274
H	30.321633	-26.532183	-57.265523
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H	33.930268	-40.374259	-58.666862
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H	35.339505	-38.534243	-59.457102
H	32.547689	-38.504200	-57.630021
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H	30.372898	-39.657105	-57.516179
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H	31.424254	-42.712432	-58.358655
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C	32.921122	-31.674996	-54.669927
C	31.692984	-32.568617	-54.538597
O	30.608711	-32.091459	-54.197386
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O	29.752905	-35.521805	-58.143687
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C	32.769887	-30.845560	-55.949511
O	32.651683	-31.736914	-57.043555
H	31.467162	-36.074615	-56.295797
H	29.915176	-36.539065	-55.587434
H	31.872730	-30.218499	-55.847936
H	33.638921	-30.180730	-56.065435
H	32.062944	-31.330019	-57.712117
H	33.836715	-32.279555	-54.687584
H	32.742200	-34.187376	-55.170845
H	29.842253	-34.209656	-54.562961
H	31.635475	-35.378062	-52.618738
H	32.961558	-31.018589	-53.796451
C	20.066032	-31.360078	-59.210007
C	21.173984	-30.598029	-59.932995
O	21.455005	-30.849006	-61.104044
N	21.791002	-29.658923	-59.210936
C	22.847954	-28.811071	-59.759039
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O	23.121932	-28.286991	-62.101919
C	20.577053	-32.731564	-58.701349
C	21.442657	-33.451552	-59.677612
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C	24.182479	-29.571237	-59.883943
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C	25.719222	-31.200477	-58.674156
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H	21.162917	-32.564956	-57.792622
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H	19.683361	-30.807616	-58.348093
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H	26.430710	-27.526513	-61.708231
H	25.144047	-26.931623	-63.796032
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C	29.196151	-37.093579	-62.264682
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C	29.947500	-31.869636	-64.760257
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C	28.298895	-32.296282	-62.809773
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C	36.822876	-32.169884	-62.941978
C	35.871167	-32.934241	-62.025029
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H	35.566555	-34.547899	-63.432831
H	34.761805	-35.433818	-61.278874
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H	32.311324	-36.373042	-60.892569
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H	31.625897	-32.546874	-59.811790
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H	37.340337	-31.385916	-62.378946
C	21.429804	-33.349479	-50.364077
C	22.282313	-32.081170	-50.549727
C	22.579530	-31.858470	-52.029851
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H	23.247987	-32.198324	-50.051278
H	20.809612	-30.834654	-52.284876
H	21.719849	-31.060749	-53.739621
H	21.355189	-33.672862	-49.320795
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H	23.612137	-25.757944	-53.265715
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H	22.835201	-28.668297	-55.430057
H	23.515870	-27.114025	-55.504322
C	21.492928	-36.936826	-55.413905
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C	23.301125	-35.891915	-56.812929
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H	22.598574	-35.566772	-57.589835
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H	22.908320	-33.766599	-55.120967
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H	20.820528	-36.793636	-56.270481
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C	34.536764	-29.066812	-58.888018
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C	33.113323	-30.350618	-60.540145
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H	34.600135	-30.023950	-58.363260
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O	28.607813	-38.497809	-58.593025
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O	27.234313	-40.661101	-60.495147
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O	28.483728	-31.482062	-56.161164
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O	29.135268	-29.534979	-60.798652
H	28.046288	-39.120587	-58.097391
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H	25.911240	-39.584491	-56.765649
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H	26.715206	-34.630127	-55.528912
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H	23.805030	-31.576342	-55.576499
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H	29.912288	-31.385812	-58.765228
H	28.201581	-40.633865	-60.600486
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H	25.874158	-32.945539	-55.666399
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H	24.596269	-37.786915	-53.536907
H	24.869796	-38.150760	-55.032414
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H	30.061808	-28.726005	-62.027628
H	29.255016	-27.761162	-65.434456
H	30.410637	-27.858114	-64.439249
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TSoo

PDB ID code: 6JLL

B3LYP-D3(BJ)/BS1: -9420.71157970 a.u.

Grimme-D3(BJ): -0.8691869349 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.71785136 a.u.

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Mn	27.309365	-34.997942	-62.264734
Mn	24.922088	-35.424570	-61.001308
O	26.468428	-36.343593	-61.424134
O	28.256446	-34.536817	-60.803322
O	25.970537	-33.894840	-61.521781
O	28.375656	-32.641920	-58.858716
O	26.497194	-34.198943	-58.880071
O	25.300926	-35.281009	-59.309954
C	32.872258	-41.753641	-53.559747
C	31.524517	-41.347176	-52.925331
C	30.455011	-41.112429	-53.961654
C	30.016434	-42.201105	-54.768321
C	29.875261	-39.832820	-54.167055
C	29.059683	-42.031450	-55.735073
C	28.906319	-39.631943	-55.126064
C	28.464390	-40.731044	-55.960004
O	27.597154	-40.577428	-56.873065
H	31.654408	-40.447097	-52.316369
H	31.191255	-42.145372	-52.247971
H	30.446125	-43.184346	-54.596068
H	30.193073	-38.998511	-53.547557
H	28.708363	-42.851479	-56.353278
H	28.450584	-38.660463	-55.295974
H	26.437325	-41.297347	-58.986880
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H	32.769622	-42.661895	-54.165037
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C	22.645059	-44.870179	-58.346966

C	22.140032	-41.425951	-59.916949
C	22.529032	-42.904011	-59.745196
O	23.080985	-43.511070	-60.666953
C	23.870526	-44.867820	-57.377746
C	24.928827	-43.946632	-57.925434
C	25.195819	-42.611443	-57.727529
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C	26.346261	-43.264354	-59.501469
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C	23.371917	-40.500234	-59.842077
C	22.972620	-39.026541	-59.922823
C	24.138226	-38.036248	-59.944751
O	25.164774	-38.209919	-59.245017
O	23.913453	-37.045267	-60.723211
H	24.264118	-45.885124	-57.277235
H	23.570770	-44.527287	-56.381366
H	24.832024	-41.905374	-56.997828
H	26.970496	-43.213754	-60.377728
H	23.894756	-40.666281	-58.896713
H	24.071614	-40.754339	-60.645263
H	22.352974	-38.763156	-59.052400
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H	25.707703	-45.284243	-59.424854
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H	22.986992	-45.244706	-59.309941
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C	30.207590	-27.056397	-58.220874
C	31.049631	-26.377331	-59.298997
O	30.891866	-26.645167	-60.490459
C	28.734778	-27.281260	-58.570061
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O	28.839170	-29.224572	-57.151822
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H	28.660831	-27.686777	-59.584381
H	28.156133	-26.354693	-58.527926
H	30.321522	-26.532161	-57.265624
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C	31.693003	-32.568806	-54.538573
O	30.608700	-32.091416	-54.197391
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H	33.633517	-30.214364	-56.108173
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H	29.842273	-34.209632	-54.562989
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H	32.961608	-31.018627	-53.796492
C	20.065992	-31.360056	-59.209991
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N	21.791008	-29.658895	-59.210963
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O	25.972241	-31.667031	-59.842986
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H	23.530498	-33.575915	-58.757656
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H	24.931171	-28.906918	-60.332397
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H	21.628034	-29.638032	-58.203478
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H	21.472424	-27.609217	-61.093831
C	26.167968	-27.319898	-63.863039
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C	25.399966	-29.534987	-66.909862
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C	25.308844	-32.244161	-64.691847
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C	23.803180	-31.525951	-63.228958
N	24.849664	-32.335056	-63.388367
H	23.462928	-30.535827	-67.002885
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H	25.270461	-32.937430	-62.632799
H	27.591265	-28.445086	-62.674056
H	25.917313	-29.023407	-62.510383

H	26.431973	-27.529809	-61.708196
H	25.144044	-26.931625	-63.796034
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H	26.862474	-26.480656	-63.959495
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C	26.208240	-37.841715	-66.090229
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C	25.012231	-35.784818	-63.970554
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C	29.172845	-37.109567	-62.256914
O	29.192297	-37.246149	-61.022741
C	31.321440	-38.033760	-63.219790
O	28.668984	-36.115224	-62.912612
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C	36.822803	-32.169699	-62.941974
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C	34.907412	-33.858110	-62.779213
C	34.044062	-34.748781	-61.881798
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C	31.963758	-34.353219	-60.586433
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N	31.151340	-33.467705	-59.991867
H	35.288725	-32.207305	-61.427567
H	36.441457	-33.520745	-61.297431
H	34.254926	-33.265819	-63.435679
H	35.486709	-34.522384	-63.433853
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H	30.269111	-33.755297	-59.579389

H	31.487083	-32.529023	-59.810338
H	36.297422	-31.688725	-63.775848
H	37.583558	-32.835117	-63.369867
H	37.340287	-31.386044	-62.378887
C	21.429801	-33.349488	-50.364029
C	22.274748	-32.075772	-50.537919
C	22.580609	-31.852769	-52.013410
N	21.684792	-31.116981	-52.713944
O	23.587276	-32.356011	-52.529211
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H	20.825435	-30.811279	-52.280365
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H	24.540892	-28.475778	-55.255176
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C	22.670625	-35.952661	-55.466278
C	23.426833	-36.062606	-56.793477
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O	27.108655	-35.799259	-54.353946
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O	24.637680	-31.758380	-54.962066
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O	28.531082	-38.565629	-58.658970
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H	26.077821	-39.575780	-56.665247
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H	26.253413	-38.940783	-63.423503
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H	25.638861	-32.957691	-55.497107
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H	29.003501	-39.048201	-59.367210
H	26.299422	-37.515205	-56.697483
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H	29.245627	-27.752699	-65.404470
H	30.364890	-27.889911	-64.376885
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Mn^{IV}O•

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.69937057 a.u.

Grimme-D3(BJ): -0.8573140942 a.u.

IEFPCM-B3LYP(_wHF15%)/BS2: -9419.72566153 a.u.

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O	26.464632	-36.371561	-61.454705
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O	26.795227	-34.019069	-58.625569
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C	28.914711	-39.551799	-55.103004
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O	23.900385	-37.113804	-60.991735
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O	30.608741	-32.091123	-54.197541
C	30.537378	-35.676966	-55.898408
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O	32.622656	-31.773019	-57.030096
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C	20.066144	-31.360034	-59.209937
C	21.173925	-30.597990	-59.933039
O	21.455025	-30.849010	-61.104063
N	21.790960	-29.658839	-59.210971
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O	23.121873	-28.287007	-62.101896
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C	24.589628	-30.215139	-58.573535
C	25.698975	-31.225279	-58.710556
O	25.989262	-31.686661	-59.846843
O	26.248478	-31.587892	-57.616980
H	21.168530	-32.526436	-57.765336
H	19.752567	-33.351769	-58.397653
H	23.526461	-33.656423	-58.738303
H	22.094791	-34.977858	-62.460490
H	24.961098	-28.881306	-60.230027
H	24.076310	-30.333220	-60.662359
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H	23.749671	-30.755904	-58.119283
H	20.173416	-33.758817	-61.275571
H	19.254577	-31.479166	-59.935497

H	19.683283	-30.807625	-58.348097
H	21.628013	-29.638056	-58.203473
H	22.997791	-27.995218	-59.038628
H	21.472471	-27.609173	-61.093809
C	26.167979	-27.320181	-63.862891
C	26.355836	-28.187221	-65.124076
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N	25.270803	-28.651505	-65.739434
C	25.400008	-29.535004	-66.909756
C	26.541223	-28.133292	-62.613779
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C	25.311373	-32.244301	-64.670983
N	23.582167	-30.918583	-64.392525
C	23.796964	-31.520197	-63.216319
N	24.843484	-32.333201	-63.368324
H	23.467687	-30.550307	-66.992273
H	24.829791	-31.562675	-67.436636
H	26.161530	-32.825033	-64.992077
H	23.198457	-31.377093	-62.325500
H	22.922672	-30.140525	-64.542962
H	25.241512	-32.936632	-62.614614
H	27.583790	-28.454856	-62.672111
H	25.904128	-29.018201	-62.506998
H	26.432275	-27.527571	-61.708305
H	25.144078	-26.931723	-63.795940
H	25.162751	-28.998999	-67.835656
H	26.862465	-26.480584	-63.959499
H	24.349086	-28.333512	-65.471818
H	26.450835	-29.822798	-66.941414
C	25.287879	-36.662178	-66.406809
C	26.208269	-37.841752	-66.090210
O	25.791384	-38.795394	-65.435730

N	27.453129	-37.786125	-66.567353
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C	29.793166	-38.159999	-63.152037
C	24.366592	-36.348047	-65.225934
C	25.044015	-35.736251	-63.993012
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C	29.187457	-37.099281	-62.258068
O	29.224488	-37.201561	-61.026207
C	31.323483	-38.041762	-63.220584
O	28.665880	-36.099734	-62.914310
H	23.569750	-35.657110	-65.525448
H	23.878074	-37.263818	-64.877866
H	31.691068	-38.815165	-63.897941
H	31.624791	-37.058284	-63.595777
H	31.764258	-38.203986	-62.233231
H	24.739743	-36.922304	-67.321965
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H	28.533232	-37.310373	-64.615265
H	29.539004	-39.122088	-62.698339
C	30.993907	-30.837890	-65.204982
C	29.951581	-31.874615	-64.757960
C	29.077070	-31.315736	-63.625378
C	28.318739	-32.331860	-62.799482
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H	29.317181	-32.178272	-65.599389

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H	28.353015	-30.591177	-64.026703
H	29.686096	-30.746514	-62.919257
H	30.553349	-29.885889	-65.525936
H	31.616799	-31.222418	-66.020079
H	31.656594	-30.596634	-64.367575
C	36.822858	-32.169690	-62.942016
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C	34.131119	-34.812750	-61.885594
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C	32.059432	-34.416446	-60.580823
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N	31.237120	-33.511001	-60.017861
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H	36.451938	-33.492383	-61.276963
H	34.306773	-33.354179	-63.466414
H	35.586776	-34.561646	-63.421891
H	34.779162	-35.439982	-61.263190
H	33.517335	-35.487127	-62.491443
H	33.513261	-33.061560	-60.770698
H	30.731884	-35.965510	-60.428745
H	32.342101	-36.421453	-60.857700
H	30.436471	-33.834643	-59.487074
H	31.623924	-32.596039	-59.806474
H	36.297457	-31.688660	-63.775870
H	37.583335	-32.835236	-63.369625
H	37.340389	-31.385916	-62.378976
C	21.430005	-33.349526	-50.364389
C	22.285797	-32.081544	-50.539622
C	22.600177	-31.852133	-52.013428
N	21.678836	-31.158509	-52.725981
O	23.636455	-32.303527	-52.518836

H	21.779653	-31.208769	-50.111042
H	23.245456	-32.199783	-50.030376
H	20.796654	-30.903049	-52.305560
H	21.741575	-31.097967	-53.743104
H	21.355103	-33.672848	-49.320737
H	21.883952	-34.158213	-50.944199
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C	22.949254	-26.584996	-52.987121
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H	23.612124	-25.757940	-53.265714
H	22.932573	-26.646278	-51.895111
H	22.797481	-28.738632	-53.233804
H	24.449234	-28.135097	-53.156960
H	24.540681	-28.476428	-55.255142
H	22.835228	-28.668223	-55.430152
H	23.515897	-27.113954	-55.504282
C	21.493001	-36.937123	-55.413928
C	22.654452	-35.934102	-55.451453
C	23.380460	-35.983015	-56.796101
C	22.170660	-34.510459	-55.147637
H	23.373623	-36.219271	-54.673218
H	23.710005	-36.996410	-57.031339
H	22.713872	-35.659753	-57.605656
H	24.265859	-35.338381	-56.810510
H	21.695627	-34.445969	-54.161040
H	21.433121	-34.178979	-55.891312
H	23.002708	-33.799036	-55.161735
H	20.906207	-36.796234	-54.497951
H	21.842190	-37.976335	-55.431460
H	20.820533	-36.793481	-56.270413
C	24.041087	-36.051545	-50.719049

C	23.149606	-37.272559	-50.955038
O	23.248940	-37.933653	-52.005058
H	23.648232	-35.395076	-49.938283
H	25.031129	-36.404729	-50.401156
H	24.166845	-35.500893	-51.655843
H	22.428170	-37.570673	-50.173506
C	34.536587	-29.066975	-58.887763
C	33.272498	-29.065188	-59.757075
C	33.101821	-30.364506	-60.526015
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H	33.239284	-28.211125	-60.439464
H	32.386160	-28.997364	-59.115824
H	32.080688	-29.453567	-62.112107
H	32.379128	-31.163344	-62.232454
H	34.513867	-28.256736	-58.151837
H	35.440459	-28.949591	-59.495883
H	34.600270	-30.024023	-58.363383
C	23.583026	-48.235988	-60.183014
C	24.552998	-47.107123	-60.534867
N	24.365968	-46.509919	-61.704136
O	25.468029	-46.792844	-59.766966
H	24.128444	-49.014197	-59.646083
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H	23.093908	-48.667324	-61.061074
H	23.516461	-46.659825	-62.229902
H	24.828659	-45.621730	-61.862814
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O	25.396980	-37.505105	-53.898188
O	30.753845	-28.340367	-62.615792
O	30.212139	-27.598578	-65.352346
O	27.246306	-35.647384	-54.339008
O	25.848060	-29.235999	-55.247651

O	24.691381	-31.775393	-54.970586
O	30.564106	-30.713223	-58.699065
O	28.312246	-38.643407	-58.838689
O	27.202488	-36.768332	-56.840574
O	25.361511	-38.736273	-56.472375
O	27.500716	-41.262525	-61.135131
O	26.647686	-38.970317	-62.621739
O	26.379163	-33.607120	-55.950281
O	28.390386	-31.568210	-56.174163
O	22.488319	-28.412889	-64.735331
O	29.122839	-29.553801	-60.795300
H	28.005925	-39.268894	-58.142959
H	28.492080	-30.604436	-56.525807
H	29.151854	-31.808261	-55.598616
H	25.034056	-38.651221	-57.391323
H	26.086295	-39.410004	-56.512765
H	26.507794	-36.264996	-54.060682
H	28.052298	-35.971540	-53.895646
H	26.341455	-29.054111	-56.097625
H	25.649922	-30.198105	-55.200321
H	24.324882	-31.965704	-54.064307
H	23.900801	-31.574943	-55.514122
H	30.075715	-30.085855	-58.098824
H	29.912783	-31.448440	-58.772691
H	28.427295	-41.004403	-60.998903
H	27.112910	-40.526186	-61.650254
H	26.437451	-38.088262	-62.262666
H	26.329183	-38.987160	-63.544201
H	26.780427	-34.172675	-55.243980
H	25.765425	-32.918843	-55.553554
H	22.611839	-28.124901	-63.800843
H	21.678238	-27.991831	-65.060812
H	28.877978	-39.157291	-59.452179

H	26.497115	-37.437664	-56.654166
H	27.261779	-36.236156	-56.016270
H	24.652480	-37.634097	-53.275176
H	25.160505	-37.955802	-54.734180
H	30.924727	-27.476712	-62.200396
H	30.063308	-28.731781	-62.024701
H	29.256959	-27.762399	-65.434681
H	30.410071	-27.867071	-64.436213
H	29.764618	-29.917591	-60.143783
H	28.571697	-30.320223	-61.044454

H(open)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.71498323 a.u.

Grimme-D3(BJ): -0.8682220820 a.u.

Grimme-D4: -0.826528876 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.54422448 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.72893223 a.u.

Ca	27.411311	-36.616864	-59.207151
Mn	27.484089	-33.011745	-57.394659
Mn	27.304411	-33.208423	-60.162874
Mn	27.276304	-35.131247	-62.247688
Mn	24.802783	-35.555549	-61.087355
O	26.355876	-36.458752	-61.437208
O	28.215839	-34.662934	-60.800407
O	25.896945	-34.047829	-61.506790
O	28.439118	-32.496722	-59.019787
O	26.772167	-34.092139	-58.666783
C	32.875999	-42.005011	-53.570989
C	31.542768	-41.585029	-52.913103
C	30.459539	-41.294505	-53.920244
C	29.993225	-42.344973	-54.762780
C	29.884017	-40.003986	-54.055100

C	29.021936	-42.123910	-55.703562
C	28.899827	-39.751117	-54.986705
C	28.444688	-40.805818	-55.868910
O	27.588845	-40.599335	-56.783719
H	31.702716	-40.706397	-52.280592
H	31.200422	-42.393743	-52.252470
H	30.414721	-43.339092	-54.638756
H	30.210495	-39.196532	-53.405538
H	28.652034	-42.911955	-56.352011
H	28.446855	-38.768462	-55.084680
H	26.463647	-41.439212	-58.705329
H	33.647042	-42.214280	-52.820299
H	33.239796	-41.198964	-54.219086
H	32.759925	-42.901520	-54.190660
N	22.171862	-43.550198	-58.611852
C	22.573108	-44.926980	-58.372077
C	22.292831	-41.390736	-59.755020
C	22.685115	-42.866904	-59.634119
O	23.416007	-43.386167	-60.478968
C	23.745897	-44.973946	-57.338713
C	24.859897	-44.079308	-57.807564
N	25.653538	-44.438853	-58.886648
C	25.155137	-42.760077	-57.554886
C	26.344482	-43.386869	-59.313959
N	26.074282	-42.364162	-58.507464
C	23.477433	-40.460440	-59.532663
C	23.025711	-39.016220	-59.720575
C	24.178780	-38.079079	-59.978051
O	25.264077	-38.214936	-59.382576
O	23.881180	-37.180565	-60.863125
H	24.098386	-46.006287	-57.237777
H	23.400605	-44.641783	-56.354552
H	24.784478	-42.066828	-56.816790

H	26.980553	-43.319787	-60.180026
H	23.888661	-40.587591	-58.529427
H	24.267163	-40.711517	-60.247270
H	22.326486	-38.927917	-60.556810
H	22.500397	-38.651998	-58.826385
H	25.617328	-45.370192	-59.355255
H	21.701093	-45.525168	-58.082598
H	21.465380	-41.137973	-59.077532
H	21.651525	-43.060597	-57.898336
H	22.962994	-45.296073	-59.319699
H	21.938218	-41.259529	-60.782701
C	30.100032	-27.195115	-58.252085
C	30.953958	-26.518829	-59.342104
O	30.765734	-26.791374	-60.528851
C	28.627826	-27.403729	-58.614319
C	27.981585	-28.457638	-57.709626
O	28.752393	-29.362038	-57.229780
O	26.749436	-28.375433	-57.499863
H	28.047126	-26.479906	-58.545881
H	28.556582	-27.776327	-59.641843
H	30.208923	-26.666587	-57.297644
H	30.495831	-28.206039	-58.103353
H	31.755403	-25.814284	-59.042770
C	33.267211	-39.896015	-59.264965
C	34.165868	-38.776008	-59.774109
O	33.748163	-37.952986	-60.587890
C	32.104056	-39.337968	-58.462958
C	31.184453	-40.419072	-57.969455
C	30.542903	-41.173125	-59.108782
O	29.962770	-40.566875	-60.015406
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H	33.853407	-40.606402	-58.668682
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H	30.371879	-39.967825	-57.391314
H	31.703549	-41.100723	-57.284325
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N	31.634008	-34.046104	-54.926028
C	30.534083	-35.004948	-54.799241
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O	29.788559	-36.715575	-53.303755
C	32.676010	-31.843001	-54.776032
C	31.446120	-32.745858	-54.696782
O	30.343906	-32.272062	-54.419176
C	30.352854	-35.860749	-56.063208
C	29.533599	-35.162901	-57.153603
O	29.512939	-35.626919	-58.306775
O	28.858996	-34.150831	-56.738609
C	32.553401	-30.992534	-56.042849
O	32.477367	-31.868351	-57.152647
H	31.300300	-36.194853	-56.500559
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H	33.418077	-30.316972	-56.122806
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H	29.607188	-34.419132	-54.768747
H	31.420766	-35.608996	-52.791934
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C	19.958959	-31.402198	-59.197966
C	21.056982	-30.633091	-59.935021
O	21.315996	-30.875925	-61.117048

N	21.704895	-29.711855	-59.220976
C	22.770898	-28.889114	-59.803928
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O	23.051887	-28.379041	-62.141911
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N	20.965410	-33.881414	-60.932172
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C	24.087182	-29.668751	-59.962395
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C	25.645222	-31.291161	-58.777151
O	25.927218	-31.785001	-59.905639
O	26.200194	-31.608139	-57.680129
H	21.112615	-32.569920	-57.787054
H	19.675632	-33.392317	-58.375197
H	23.382834	-33.767378	-58.771997
H	21.967831	-34.886471	-62.566715
H	23.951226	-30.446071	-60.712003
H	24.864929	-28.997937	-60.335727
H	23.697731	-30.835174	-58.170779
H	24.861306	-29.540237	-57.929720
H	20.069374	-33.668516	-61.346631
H	19.154141	-31.558532	-59.923780
H	19.562061	-30.836949	-58.350412
H	21.583688	-29.705173	-58.207628
H	22.953480	-28.066472	-59.097796
H	21.396679	-27.692379	-61.153220
C	26.060950	-27.439164	-63.994973
C	26.238873	-28.320864	-65.238354
O	27.365458	-28.589049	-65.638145
N	25.134894	-28.740876	-65.847333

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C	26.456485	-28.225556	-62.735062
C	24.301132	-30.880590	-66.758745
C	24.367791	-31.438835	-65.360731
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C	25.193098	-32.337130	-64.727710
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H	25.199010	-33.043124	-62.668806
H	23.259908	-30.604056	-66.961829
H	24.561537	-31.660836	-67.481368
H	26.038376	-32.908400	-65.078221
H	23.150400	-31.499241	-62.314441
H	22.797705	-30.250827	-64.517716
H	27.502422	-28.534478	-62.796749
H	25.832782	-29.117354	-62.606974
H	26.346725	-27.606834	-61.838752
H	25.034412	-27.057195	-63.919880
H	25.028173	-29.151676	-67.926950
H	26.743663	-26.591833	-64.109645
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C	25.249046	-36.850051	-66.374717
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C	28.278079	-39.145888	-66.603986
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C	24.316953	-36.579744	-65.195485
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O	24.191307	-35.680931	-63.008451
C	29.075802	-37.369530	-62.254871
O	29.054184	-37.513130	-61.024993
C	31.260280	-38.270254	-63.189750
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C	36.633865	-32.318812	-63.030927
C	35.665028	-33.067277	-62.113639

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C	33.956760	-34.976938	-61.929528
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H	33.354523	-35.671233	-62.525067
H	34.610382	-35.583624	-61.290545
H	33.326254	-33.204897	-60.864477
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H	32.157204	-36.570467	-60.889332
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C	22.470818	-31.987868	-52.103768
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C	22.526858	-36.120886	-55.438486
C	23.358594	-36.211131	-56.719820
C	21.995179	-34.695135	-55.240987
H	23.193217	-36.352368	-54.598023
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H	21.306452	-34.421903	-56.052681
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C	23.894780	-36.253918	-50.766971
C	23.014125	-37.490276	-50.984081
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H	35.227058	-29.106385	-59.504373
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O	30.063102	-27.687491	-65.411237
O	27.218428	-40.878310	-60.460006
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H	29.024431	-31.917123	-55.591062
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H	24.156179	-32.090470	-54.236472
H	23.655837	-31.554710	-55.609783
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H	29.916859	-28.836722	-62.095146
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H	26.166297	-39.148387	-63.398792
H	26.288795	-38.157901	-62.180536
H	29.116843	-27.890506	-65.508689
H	30.260084	-27.958348	-64.495126
H	28.183139	-40.774069	-60.550077
H	26.832005	-40.285077	-61.146031
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H	24.905270	-38.198756	-54.869108
H	28.455208	-30.428108	-61.130728
H	29.611557	-29.983414	-60.203578
H	26.216961	-29.160163	-56.136310
H	25.447269	-30.305023	-55.286548
H	29.772124	-31.515693	-58.875019

H	29.919874	-30.176588	-58.143574
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O*(open)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.72315300 a.u.

Grimme-D3(BJ): -0.8693098939 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.73066271 a.u.

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O	26.331269	-36.486007	-61.471669
O	28.170985	-34.701531	-60.844474
O	25.887116	-34.049078	-61.582236
O	28.337176	-32.666949	-58.975483
O	26.516802	-34.246920	-58.884188
C	32.875869	-42.004849	-53.571014
C	31.552289	-41.587711	-52.901092
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C	30.023709	-42.321746	-54.777096
C	29.826449	-40.026212	-53.955461
C	29.009782	-42.105576	-55.673198
C	28.789026	-39.783871	-54.829381
C	28.328255	-40.828480	-55.717665
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H	31.217034	-42.397393	-52.237459
H	30.498522	-43.297425	-54.718720
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O	23.415912	-43.386205	-60.478997
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C	24.111332	-38.033448	-59.907062
O	25.186458	-38.137622	-59.275831
O	23.820910	-37.145644	-60.791268
H	24.061367	-46.074033	-57.282961
H	23.388076	-44.737276	-56.339940
H	24.906609	-42.297274	-56.472732
H	27.020487	-43.170957	-60.012010
H	23.894395	-40.599322	-58.516624
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H	21.701194	-45.525094	-58.082628
H	21.465373	-41.137980	-59.077516
H	21.651549	-43.060604	-57.898372

H	22.963064	-45.295992	-59.319775
H	21.938187	-41.259516	-60.782676
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O	30.765737	-26.791388	-60.528821
C	28.625253	-27.380958	-58.617156
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H	28.070517	-26.439469	-58.582325
H	28.547770	-27.785419	-59.631768
H	30.208924	-26.666567	-57.297674
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C	31.446115	-32.745888	-54.696785
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H	23.735613	-30.695729	-58.083903
H	24.992583	-29.465681	-58.012132
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H	19.154173	-31.558536	-59.923801
H	19.562069	-30.836943	-58.350418
H	21.583661	-29.705164	-58.207640
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C	26.060951	-27.439178	-63.994971
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H	25.840537	-29.121309	-62.610330
H	26.345880	-27.609621	-61.838565
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S(open)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.73210808 a.u.

Grimme-D3(BJ): -0.8724787702 a.u.

Grimme-D4: -0.825850392 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.53182455 a.u.

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C	24.139933	-37.996222	-59.719294
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H	21.651515	-43.060593	-57.898288
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C	28.626665	-27.401189	-58.614887
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H	35.054118	-32.331929	-61.566433
H	35.357439	-34.713329	-63.480739
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H	33.285700	-35.606710	-62.556024
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P(3444)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.73828791 a.u.

Grimme-D3(BJ): -0.8696849288 a.u.

Grimme-D4: -0.820343775 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.55735967 a.u.

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C	29.991709	-42.315296	-54.832827
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C	29.010999	-42.061760	-55.789650
C	28.912454	-39.763627	-55.059401
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C	28.626279	-27.396889	-58.617703
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C	35.667405	-33.065836	-62.111094
C	34.807654	-34.100458	-62.846137
C	33.976943	-34.987278	-61.916730
N	33.060142	-34.177686	-61.115617
C	31.905064	-34.601461	-60.604098
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N	31.078212	-33.707482	-60.035440
H	36.240583	-33.572269	-61.321588
H	35.029034	-32.338301	-61.598676
H	35.453158	-34.761521	-63.438348
H	34.140821	-33.594475	-63.557984
H	33.386635	-35.696160	-62.506454
H	34.632354	-35.578121	-61.265368
H	33.318403	-33.215190	-60.863147
H	30.648778	-36.179511	-60.310761
H	32.228668	-36.606676	-60.854925
H	30.260077	-34.030711	-59.529942
H	31.434389	-32.775406	-59.850741
H	36.134987	-31.864972	-63.896464
H	37.413819	-32.989542	-63.415234
H	37.127341	-31.514010	-62.475214
C	21.341748	-33.479432	-50.427044
C	22.176241	-32.199561	-50.600980
C	22.491834	-31.973670	-52.073492
O	23.506006	-32.467180	-52.585907
N	21.595552	-31.243043	-52.778098

H	21.648884	-31.335567	-50.180319
H	23.133853	-32.296631	-50.083090
H	21.667671	-31.151819	-53.792139
H	20.737670	-30.929641	-52.347489
H	21.198191	-33.755646	-49.376029
H	21.841701	-34.308728	-50.933585
H	20.348877	-33.367192	-50.877807
C	22.829042	-26.739967	-53.012966
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H	23.548798	-25.923957	-53.149312
H	22.695307	-26.887611	-51.937103
H	22.623132	-28.852898	-53.494532
H	24.280059	-28.335976	-53.197378
H	24.509034	-28.513341	-55.323440
H	23.666485	-26.985878	-55.450066
H	22.815118	-28.453559	-55.612557
C	21.383493	-37.147762	-55.429465
C	22.538238	-36.132874	-55.460106
C	23.334190	-36.234362	-56.765320
C	22.032100	-34.701143	-55.242231
H	23.224571	-36.379084	-54.639715
H	23.703461	-37.252060	-56.917842
H	22.708488	-35.966936	-57.628364
H	24.203098	-35.568849	-56.764778
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H	21.336431	-34.407402	-56.040450
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H	32.178506	-29.229798	-59.089727
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H	31.881723	-29.571739	-62.124708
H	32.230408	-31.264589	-62.305848
H	34.310335	-28.434132	-58.141650
H	35.226950	-29.106255	-59.504407
H	34.409182	-30.198900	-58.368416
C	23.503040	-48.366016	-60.280031
C	24.430075	-47.194180	-60.602025
O	25.310967	-46.857861	-59.808801
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H	24.076807	-49.135546	-59.760927
H	23.028261	-48.794879	-61.167454
H	22.718783	-48.011794	-59.601121
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H	24.662301	-45.662089	-61.890932
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O	28.186410	-31.640481	-56.042223
O	30.244435	-30.966372	-58.755169
O	26.132333	-33.802042	-55.913264
O	22.380871	-28.467709	-64.764551

O	28.457052	-38.809626	-58.622391
O	26.486238	-39.088376	-62.567433
O	24.554047	-31.881225	-55.005442
O	30.522115	-28.494849	-62.635148
O	27.020481	-35.830189	-54.351148
O	30.057660	-27.698166	-65.363539
O	27.405257	-41.332451	-60.956064
O	27.002340	-36.885758	-56.875339
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O	28.886497	-29.701346	-60.826344
O	25.720300	-29.331222	-55.282562
H	28.291442	-30.712397	-56.415767
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H	27.856087	-36.141299	-53.954211
H	26.317002	-36.493691	-54.088367
H	24.176340	-32.071223	-54.102876
H	23.777133	-31.648584	-55.555593
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H	29.841402	-28.890340	-62.033795
H	25.531526	-33.089759	-55.527388
H	22.536286	-28.194904	-63.829118
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H	26.207861	-39.114629	-63.501997
H	26.280674	-38.197600	-62.227981
H	29.112896	-27.888893	-65.494193
H	30.222489	-27.992621	-64.448869
H	28.321751	-41.031226	-60.824035
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H	28.351493	-30.456320	-61.134323
H	29.507933	-30.104837	-60.176624
H	26.229297	-29.120988	-56.120335
H	25.514835	-30.292899	-55.254079
H	29.589315	-31.700251	-58.819907
H	29.774064	-30.314435	-58.162502
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$S_{\text{pre}}(3443)$

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.72151352 a.u.

Grimme-D3(BJ): -0.8698745630 a.u.

Grimme-D4: -0.825583359 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.53246835 a.u.

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Mn	27.094127	-33.330917	-60.285536
Mn	27.198927	-35.213430	-62.313756
Mn	24.748723	-35.487507	-61.095783
O	26.263456	-36.475159	-61.405180
O	28.085791	-34.740752	-60.820856
O	25.872849	-34.012176	-61.693649
O	28.113286	-32.908025	-58.871832
O	26.009968	-34.681048	-59.251412
C	32.875909	-42.004866	-53.571051
C	31.532841	-41.610043	-52.936556
C	30.462500	-41.311094	-53.966534
C	29.997901	-42.313529	-54.830430
C	29.896283	-40.035885	-54.094594

C	29.019401	-42.057597	-55.788417
C	28.909433	-39.764654	-55.042740
C	28.456453	-40.772417	-55.913704
O	27.535933	-40.500997	-56.858457
H	31.672952	-40.731918	-52.295039
H	31.197444	-42.421430	-52.276508
H	30.400124	-43.321184	-54.741996
H	30.215778	-39.237946	-53.428893
H	28.675154	-42.851312	-56.446070
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H	26.852105	-41.624493	-57.535991
H	33.646954	-42.214322	-52.820266
H	33.239866	-41.199002	-54.219105
H	32.759976	-42.901552	-54.190722
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C	22.573063	-44.926919	-58.372055
C	22.292992	-41.391025	-59.755172
C	22.685113	-42.866798	-59.634078
O	23.415955	-43.386103	-60.478957
C	23.692145	-45.077041	-57.309367
C	24.850439	-44.187864	-57.616877
N	25.629409	-44.339398	-58.754076
C	25.266993	-43.018960	-57.038829
C	26.454765	-43.292714	-58.877681
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C	23.503311	-40.472256	-59.500558
C	23.067386	-39.011655	-59.616951
C	24.172576	-37.974979	-59.689387
O	25.292248	-38.126285	-59.170298
O	23.789440	-36.903377	-60.310924
H	24.001507	-46.128749	-57.289644
H	23.313465	-44.826886	-56.312733
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H	27.085229	-43.057146	-59.724596
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H	22.435545	-38.730264	-58.761631
H	25.579456	-45.164392	-59.373410
H	21.701036	-45.525168	-58.082671
H	21.465427	-41.137755	-59.077576
H	21.651517	-43.060586	-57.898329
H	22.962978	-45.296108	-59.319702
H	21.938142	-41.259406	-60.782740
C	30.099839	-27.195480	-58.251899
C	30.953514	-26.518912	-59.342060
O	30.765908	-26.791388	-60.528713
C	28.628544	-27.385840	-58.623309
C	27.972465	-28.420027	-57.709537
O	28.720000	-29.361503	-57.270047
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H	28.062135	-26.452732	-58.565172
H	28.558861	-27.766465	-59.647542
H	30.208998	-26.666644	-57.297635
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C	32.104041	-39.337926	-58.462960
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H	30.371879	-39.967850	-57.391301
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H	31.029926	-42.990149	-58.288811
H	30.187997	-43.041224	-59.811549
N	31.633944	-34.046234	-54.926126
C	30.533540	-35.004809	-54.799345
C	30.611089	-35.835129	-53.515540
O	29.788502	-36.715473	-53.303707
C	32.675740	-31.843116	-54.775986
C	31.446063	-32.746027	-54.696706
O	30.344008	-32.271617	-54.419325
C	30.358761	-35.868896	-56.064411
C	29.430477	-35.216836	-57.090429
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H	33.600045	-32.435154	-54.776553
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H	29.607174	-34.419097	-54.768608
H	31.420850	-35.609090	-52.792002
H	32.676949	-31.200642	-53.889979
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C	21.056992	-30.633112	-59.934967
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C	21.392253	-33.458761	-59.577698
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C	22.045531	-34.396528	-61.491613
N	23.116211	-34.339744	-60.707175
C	24.075566	-29.688372	-59.962999
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H	21.065982	-32.525838	-57.719957
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C	31.261379	-38.270924	-63.185599
O	28.511582	-36.405552	-62.916587
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H	31.683245	-38.447390	-62.192851
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H	28.894095	-39.126426	-67.506645
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H	37.413832	-32.989535	-63.415239
H	37.127316	-31.514021	-62.475192
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C	22.162716	-32.189769	-50.582618
C	22.475644	-31.943812	-52.049272
O	23.496754	-32.423841	-52.561286
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H	23.120728	-32.281938	-50.064755
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C	23.328886	-28.032914	-53.642895
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H	22.623122	-28.852889	-53.494534
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H	22.815069	-28.453505	-55.612529
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C	22.552712	-36.155019	-55.463187
C	23.359805	-36.327997	-56.750878
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C	23.503038	-48.366016	-60.280030
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H	29.824928	-28.904457	-62.016631
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H	26.340566	-37.540705	-56.691668
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S(closed)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.72560760 a.u.

Grimme-D3(BJ): -0.8714945030 a.u.

Grimme-D4: -0.826773395 a.u.

IEFPCM-B3LYP($w_{\text{HF}}10\%$)/BS2: -9414.52474781 a.u.

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O	28.056323	-32.936268	-58.781581
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C	32.876137	-42.004800	-53.570846
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C	29.989117	-42.423269	-54.719839
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C	28.628985	-27.404963	-58.621565
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H	22.695307	-26.887608	-51.937104
H	22.623121	-28.852900	-53.494530
H	24.280049	-28.336001	-53.197376
H	24.509036	-28.513285	-55.323495

H	23.666510	-26.985855	-55.449966
H	22.815055	-28.453488	-55.612528
C	21.383088	-37.147964	-55.429174
C	22.547023	-36.141548	-55.441792
C	23.376394	-36.258971	-56.723721
C	22.055775	-34.701655	-55.244864
H	23.207280	-36.389983	-54.598523
H	23.752151	-37.278661	-56.851592
H	22.771925	-36.013488	-57.607064
H	24.238808	-35.584794	-56.714917
H	21.493790	-34.588844	-54.309684
H	21.394009	-34.400798	-56.068147
H	22.895568	-33.999116	-55.215563
H	20.787215	-37.026528	-54.516315
H	21.757023	-38.178115	-55.458683
H	20.720950	-36.999627	-56.292565
C	23.894679	-36.253914	-50.766974
C	23.014234	-37.490239	-50.984077
O	23.104030	-38.144514	-52.023108
H	23.630577	-35.704429	-49.859721
H	24.940155	-36.578480	-50.697779
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H	32.975695	-28.379569	-60.385793
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H	32.201003	-31.302921	-62.271599
H	34.310282	-28.434160	-58.141630

H	35.227017	-29.106350	-59.504392
H	34.409131	-30.198872	-58.368381
C	23.503049	-48.365927	-60.279982
C	24.430074	-47.194064	-60.601906
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H	24.076813	-49.135516	-59.760876
H	23.028353	-48.794876	-61.167457
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O	30.473062	-28.553766	-62.578219
O	26.980937	-35.940053	-54.270119
O	30.032235	-27.665974	-65.279424
O	27.183316	-40.814545	-60.463310
O	27.217622	-37.241329	-56.679019
O	25.277549	-38.003572	-53.934050
O	28.863794	-29.765978	-60.784068
O	25.742670	-29.272063	-55.238768
H	28.219983	-30.763671	-56.425121
H	28.876762	-31.869553	-55.466035
H	25.146439	-38.979046	-57.497332
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H	23.812009	-31.601951	-55.519734
H	30.642248	-27.684621	-62.173813
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H	25.545554	-33.002621	-55.260524
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H	29.097466	-27.880404	-65.443245
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H	27.164128	-36.562514	-55.966381
H	26.425083	-37.794464	-56.533542
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H	29.446927	-30.225761	-60.138726
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H	25.548531	-30.235415	-55.200776
H	29.434401	-31.824365	-58.685010
H	29.713905	-30.403229	-58.144577
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O*(closed)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.69823148 a.u.

Grimme-D3(BJ): -0.8722538912 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.70382741 a.u.

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O	26.268151	-36.475050	-61.448146
O	28.061583	-34.733405	-60.867456
O	25.875151	-34.007028	-61.850543
O	27.917887	-32.975784	-58.842043
O	25.845363	-34.587854	-59.503198
C	32.876079	-42.004847	-53.570937
C	31.539975	-41.598132	-52.912681
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C	29.997623	-42.410295	-54.744350
C	29.892769	-40.048813	-54.106808
C	29.040828	-42.212552	-55.705106
C	28.924320	-39.818567	-55.058967
C	28.475239	-40.896637	-55.915318
O	27.632219	-40.705495	-56.844250
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H	28.673909	-43.017383	-56.334185
H	28.478865	-38.839849	-55.214927
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H	33.646973	-42.214402	-52.820286
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H	32.759939	-42.901490	-54.190761
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C	22.573182	-44.927165	-58.371973
C	22.292952	-41.391096	-59.755170

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O	23.415947	-43.386116	-60.478963
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C	24.864662	-44.080134	-57.826410
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C	26.332943	-43.397237	-59.352207
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C	23.484497	-40.445950	-59.517164
C	23.036345	-38.988930	-59.612120
C	24.147460	-37.950595	-59.658454
O	25.246756	-38.110010	-59.071736
O	23.809679	-36.903847	-60.310779
H	24.104252	-46.003687	-57.240656
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H	24.785130	-42.058562	-56.858045
H	26.964323	-43.340157	-60.222566
H	23.913502	-40.624081	-58.528477
H	24.262036	-40.655488	-60.257956
H	22.423359	-38.830598	-60.504358
H	22.401455	-38.730056	-58.752044
H	25.618399	-45.384887	-59.364869
H	21.701002	-45.525040	-58.082663
H	21.465442	-41.137879	-59.077503
H	21.651448	-43.060572	-57.898352
H	22.962984	-45.296045	-59.319726
H	21.938082	-41.259374	-60.782715
C	30.099776	-27.195567	-58.251780
C	30.953796	-26.518918	-59.342160
O	30.765831	-26.791298	-60.528712
C	28.632078	-27.391684	-58.636919
C	27.957983	-28.443592	-57.755013
O	28.682880	-29.401706	-57.318387

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C	33.267256	-39.896008	-59.264993
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C	32.104048	-39.337924	-58.462954
C	31.184384	-40.419085	-57.969398
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C	30.611026	-35.835117	-53.515555
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C	32.675896	-31.843003	-54.775682
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O	30.344078	-32.271284	-54.419574
C	30.367706	-35.860009	-56.063277
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H	24.861253	-29.059005	-60.358938
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H	19.561952	-30.836998	-58.350395
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C	26.060940	-27.439192	-63.994984
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C	29.063132	-37.387045	-62.261172
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O	28.064544	-33.699933	-63.373954
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H	20.348783	-33.367233	-50.877756
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C	23.328915	-28.032900	-53.642899
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H	22.695305	-26.887609	-51.937104
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H	24.280052	-28.335994	-53.197375
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H	22.815047	-28.453484	-55.612511
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C	23.894682	-36.253917	-50.766972
C	23.014210	-37.490229	-50.984091
O	23.104104	-38.144542	-52.023116
H	23.630584	-35.704431	-49.859715
H	24.940154	-36.578484	-50.697782
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H	22.300084	-37.786013	-50.192023
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C	33.052891	-29.255857	-59.730690
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H	31.755102	-29.623425	-62.048262
H	32.172072	-31.297198	-62.262493
H	34.310287	-28.434152	-58.141629
H	35.227030	-29.106338	-59.504388
H	34.409135	-30.198870	-58.368395
C	23.503030	-48.365919	-60.279976
C	24.430040	-47.194019	-60.601902
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H	24.076817	-49.135526	-59.760882
H	23.028352	-48.794888	-61.167461
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O	30.363368	-28.597826	-62.525619
O	27.069881	-35.960308	-54.268575
O	30.022764	-27.670640	-65.229301
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H	29.357631	-30.261107	-60.102036
H	26.260242	-29.010573	-56.111615
H	25.619484	-30.139637	-55.132163
H	29.380005	-31.878716	-58.683187
H	29.682313	-30.456739	-58.149671
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H(closed)

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.70203925 a.u.

Grimme-D3(BJ): -0.8721255844 a.u.

Grimme-D4: -0.830173817 a.u.

IEFPCM-B3LYP($w_{\text{HF}}15\%$)/BS2: -9419.71137981 a.u.

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Mn	24.874376	-35.444330	-61.120030
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O	28.032077	-34.799214	-60.895466

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C	31.532564	-41.637322	-52.913229
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C	30.019361	-42.469646	-54.775511
C	29.824461	-40.141257	-54.059927
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C	28.834501	-39.923133	-54.991645
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H	30.121512	-39.327950	-53.403004
H	28.706653	-43.083876	-56.371528
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C	23.488472	-40.437322	-59.553270
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H	21.701063	-45.525120	-58.082714
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C	28.616725	-27.317239	-58.618888
C	27.959901	-28.428815	-57.802710
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C	29.300695	-35.290863	-57.032823
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H	23.879541	-30.541694	-60.620033
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H	35.226989	-29.106361	-59.504408
H	34.409151	-30.198899	-58.368416
C	23.503081	-48.365994	-60.280065
C	24.430148	-47.194422	-60.602080
O	25.310896	-46.857814	-59.808749
N	24.242877	-46.578806	-61.769129
H	24.076810	-49.135519	-59.760919
H	23.028250	-48.794842	-61.167444
H	22.718773	-48.011782	-59.601097
H	23.421153	-46.765528	-62.325777
H	24.662327	-45.662083	-61.890950
Cl	21.648126	-30.249622	-56.072112
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O	28.844740	-31.860344	-56.752436
O	30.607321	-31.236289	-58.764936
O	26.840485	-32.791465	-55.345702
O	22.390410	-28.374392	-64.768444

O	28.498269	-38.721868	-58.472670
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O	29.800394	-28.972157	-61.782413
O	27.430369	-37.221647	-54.722185
O	29.777359	-27.781783	-64.405740
O	27.230078	-40.882538	-60.522365
O	26.457618	-36.760809	-57.088732
O	25.332383	-38.479059	-53.783310
O	27.643600	-29.851638	-60.383346
O	25.689837	-29.368246	-55.202718
H	28.573913	-30.904147	-56.955677
H	29.142377	-31.931936	-55.812518
H	25.383084	-38.325183	-56.829633
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H	26.651122	-37.554878	-54.192289
H	23.985818	-32.025532	-54.160432
H	23.543124	-31.544849	-55.583660
H	30.015814	-28.086522	-61.424547
H	29.013917	-29.278960	-61.262869
H	25.866804	-32.630609	-55.282248
H	22.554584	-28.139177	-63.823709
H	21.615337	-27.870406	-65.058942
H	28.971178	-39.204821	-59.182379
H	27.999965	-39.396823	-57.973607
H	26.212392	-39.193720	-63.505887
H	26.260649	-38.197142	-62.289549
H	28.953439	-28.009120	-64.873063
H	29.750198	-28.315303	-63.592684
H	28.195421	-40.785900	-60.608293
H	26.848362	-40.297138	-61.216159
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H	26.083990	-35.852184	-56.954760
H	24.534700	-38.226096	-53.280445
H	25.044500	-38.776929	-54.677143
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H	27.976690	-30.031015	-59.479430
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H	25.393035	-30.309442	-55.214854
H	30.123391	-31.750106	-58.081857
H	30.078160	-30.414145	-58.777651
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H	25.580983	-34.339139	-58.125785

TS_{PT}

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.68151705 a.u.

Grimme-D3(BJ): -0.8658347187 a.u.

IEFPCM-B3LYP(*w*_{HF}15%)/BS2: -9419.70271192 a.u.

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Mn	27.230046	-35.126229	-62.291564
Mn	24.781533	-35.542631	-61.048079
O	26.328748	-36.462099	-61.481521
O	28.194952	-34.671454	-60.835007
O	25.906201	-34.032804	-61.545322
O	28.469975	-32.511197	-59.123541
O	26.800602	-34.070740	-58.641666
C	32.876016	-42.005030	-53.570989
C	31.556657	-41.582685	-52.894428
C	30.455727	-41.254007	-53.868803
C	30.013855	-42.245200	-54.789771
C	29.822690	-39.984932	-53.877380
C	28.989988	-41.994973	-55.665742

C	28.773506	-39.710267	-54.728210
C	28.308268	-40.716596	-55.657691
O	27.333972	-40.506096	-56.438960
H	31.736155	-40.721583	-52.243034
H	31.211919	-42.399570	-52.244188
H	30.489802	-43.222021	-54.775839
H	30.152642	-39.213701	-53.187387
H	28.636988	-42.749024	-56.362431
H	28.266484	-38.749735	-54.706767
H	26.700024	-41.555405	-57.853619
H	33.647078	-42.214286	-52.820304
H	33.239756	-41.198956	-54.219060
H	32.759964	-42.901534	-54.190658
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C	22.573119	-44.927002	-58.372113
C	22.292814	-41.390740	-59.755019
C	22.685115	-42.866889	-59.634144
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C	26.415624	-43.296143	-59.025055
N	26.185695	-42.420932	-58.043811
C	23.473460	-40.462805	-59.536538
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C	24.131294	-38.085609	-60.066990
O	25.241718	-38.246973	-59.520600
O	23.801924	-37.148089	-60.884534
H	24.043338	-46.093149	-57.287413
H	23.353079	-44.778858	-56.325826
H	24.873909	-42.357898	-56.345430
H	27.058982	-43.110544	-59.869790

H	23.865716	-40.567795	-58.520635
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H	22.308924	-38.995317	-60.633012
H	22.451456	-38.646540	-58.917416
H	25.591742	-45.224247	-59.385066
H	21.701074	-45.525145	-58.082592
H	21.465379	-41.137990	-59.077517
H	21.651508	-43.060597	-57.898347
H	22.963004	-45.296066	-59.319683
H	21.938216	-41.259517	-60.782691
C	30.100043	-27.195143	-58.252059
C	30.953935	-26.518829	-59.342121
O	30.765745	-26.791362	-60.528829
C	28.621569	-27.359504	-58.613432
C	27.947456	-28.349358	-57.662105
O	28.709656	-29.226442	-57.133825
O	26.713013	-28.243889	-57.462472
H	28.081837	-26.408755	-58.581933
H	28.530839	-27.766430	-59.626143
H	30.208924	-26.666570	-57.297653
H	30.495831	-28.206032	-58.103363
H	31.755405	-25.814284	-59.042773
C	33.267244	-39.896020	-59.264962
C	34.165867	-38.776002	-59.774113
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C	32.104067	-39.337971	-58.462987
C	31.184389	-40.419127	-57.969475
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O	29.962540	-40.566463	-60.014789
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H	31.538889	-38.640034	-59.088138
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H	31.703524	-41.100751	-57.284352
H	31.029814	-42.990160	-58.288740
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O	29.788569	-36.715575	-53.303749
C	32.676005	-31.843007	-54.776038
C	31.446123	-32.745838	-54.696773
O	30.343903	-32.272060	-54.419171
C	30.392383	-35.907846	-56.033302
C	29.567349	-35.293361	-57.164343
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C	20.526882	-32.750348	-58.677406
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O	25.903649	-31.807042	-59.905459
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H	23.758681	-30.793649	-58.113691
H	24.937675	-29.494784	-57.953442
H	20.012675	-33.801233	-61.266430
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H	19.562043	-30.836933	-58.350415
H	21.583723	-29.705108	-58.207618
H	22.953459	-28.066445	-59.097826
H	21.396662	-27.692385	-61.153232
C	26.060950	-27.439174	-63.994978
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C	25.232005	-29.660102	-66.975872

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H	31.686673	-38.449639	-62.199632
H	24.687082	-37.083828	-67.289685
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H	29.482877	-39.405393	-62.730808
C	30.860760	-30.949035	-65.312070
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O	27.997356	-33.634211	-63.375056
O	27.853262	-32.099363	-61.742659
H	29.186639	-32.278318	-65.719008
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N	21.576642	-31.239603	-52.787382
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C	23.014134	-37.490276	-50.984069
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H	23.630609	-35.704471	-49.859690
H	24.940184	-36.578446	-50.697844
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C	33.076034	-29.219531	-59.762070
C	32.927704	-30.485657	-60.584942

O	33.299743	-31.582829	-60.120846
N	32.373008	-30.377854	-61.802356
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H	33.044918	-28.340930	-60.412663
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H	32.204380	-31.236666	-62.311129
H	34.310320	-28.434142	-58.141601
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H	34.409052	-30.198853	-58.368408
C	23.503036	-48.365997	-60.280005
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H	22.718774	-48.011799	-59.601119
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H	24.662286	-45.662083	-61.890927
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O	28.741968	-31.642463	-56.513905
O	30.381497	-30.677482	-58.752019
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O	22.383720	-28.504750	-64.758252
O	28.034926	-38.922895	-58.846634
O	26.418713	-39.069603	-62.549183
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O	26.061900	-36.534179	-57.497768
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O	27.217346	-40.847912	-60.606825
O	26.704533	-33.438458	-55.959893
O	25.226555	-37.696974	-54.161270

O	28.876942	-29.644479	-60.866315
O	25.699212	-29.355216	-55.311956
H	28.520695	-30.655647	-56.570040
H	29.151970	-31.896211	-55.654505
H	25.080690	-38.993836	-57.854317
H	25.958321	-39.400024	-56.632966
H	26.240597	-36.251122	-54.701583
H	26.756705	-34.782049	-55.415038
H	24.174784	-32.091418	-54.277594
H	23.654514	-31.580564	-55.649061
H	30.700842	-27.608314	-62.229130
H	29.832149	-28.862731	-62.075690
H	25.401287	-35.966102	-58.342811
H	22.540734	-28.222764	-63.825569
H	21.560953	-28.082158	-65.047540
H	28.900283	-39.108655	-59.263491
H	27.456234	-39.544390	-59.353866
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H	29.112956	-27.886591	-65.507718
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H	26.829141	-40.304996	-61.340723
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H	25.617264	-37.380896	-57.260528
H	24.540188	-37.791022	-53.469159
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H	28.387890	-30.449407	-61.128565
H	29.513889	-29.955782	-60.182741
H	26.212010	-29.106872	-56.139864
H	25.443347	-30.306545	-55.353548
H	29.763923	-31.445129	-58.834091
H	29.894070	-30.109275	-58.100933

O	25.005414	-35.448076	-59.367922
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TS_{oo}

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.71898653 a.u.

Grimme-D3(BJ): -0.8701064002 a.u.

IEFPCM-B3LYP(*w*_{HF}15%)/BS2: -9419.72303442 a.u.

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Mn	27.151314	-33.323007	-60.260843
Mn	27.242861	-35.183992	-62.303849
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O	26.340466	-36.484293	-61.454266
O	28.181843	-34.704290	-60.856399
O	25.910865	-34.033180	-61.604503
O	28.295492	-32.743982	-58.952455
O	26.448633	-34.323308	-58.949860
C	32.875869	-42.004848	-53.571014
C	31.553317	-41.588056	-52.899389
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C	30.023519	-42.325392	-54.772302
C	29.824658	-40.029232	-53.952298
C	29.007273	-42.111606	-55.666260
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H	31.719592	-40.711404	-52.265336
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H	30.500020	-43.300246	-54.713929
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C	22.572946	-44.927108	-58.371920
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C	23.731257	-45.030181	-57.338029
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C	25.234865	-42.892054	-57.311875
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N	26.174755	-42.416448	-58.204970
C	23.476503	-40.452267	-59.511231
C	22.993440	-39.005158	-59.614072
C	24.108800	-38.006715	-59.833575
O	25.193089	-38.118771	-59.209251
O	23.811636	-37.101422	-60.686361
H	24.062478	-46.073303	-57.283173
H	23.389511	-44.736127	-56.340471
H	24.908067	-42.295569	-56.475640
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H	21.465372	-41.137979	-59.077517
H	21.651549	-43.060604	-57.898372
H	22.963064	-45.295992	-59.319775

H	21.938188	-41.259517	-60.782677
C	30.099974	-27.195174	-58.252016
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C	28.625336	-27.389336	-58.614916
C	27.959196	-28.406039	-57.682402
O	28.690006	-29.345781	-57.219355
O	26.737799	-28.254325	-57.431734
H	28.063481	-26.452502	-58.572162
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H	30.208932	-26.666560	-57.297673
H	30.495861	-28.206032	-58.103371
H	31.755410	-25.814268	-59.042763
C	33.267210	-39.896020	-59.264976
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O	29.788554	-36.715564	-53.303777
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C	31.446113	-32.745890	-54.696784
O	30.343927	-32.272005	-54.419192
C	30.402672	-35.906411	-56.044157
C	29.495424	-35.316618	-57.127393
O	29.504273	-35.815029	-58.267339
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O	32.414223	-31.881452	-57.149859
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H	33.415881	-30.345321	-56.159014
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N	20.976859	-33.925347	-60.870986
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C	22.020577	-34.485204	-61.522493
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H	23.459299	-33.652977	-58.788817
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H	23.905086	-30.480415	-60.692086
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H	23.733833	-30.689470	-58.083455
H	25.016557	-29.486518	-58.026367
H	20.060629	-33.767794	-61.265101
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H	19.562071	-30.836945	-58.350418
H	21.583666	-29.705168	-58.207637
H	22.953500	-28.066447	-59.097821
H	21.396673	-27.692361	-61.153222
C	26.060951	-27.439178	-63.994971
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O	27.365462	-28.589075	-65.638122
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C	26.459665	-28.225660	-62.736302
C	24.291075	-30.873302	-66.772989
C	24.349246	-31.441513	-65.381443
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H	31.685472	-38.444720	-62.198048
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O	28.008426	-33.648539	-63.373733
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H	29.166749	-32.260232	-65.700799
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O	28.184327	-31.623788	-55.991977
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O	27.240522	-40.930273	-60.762660
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H	26.508870	-34.334753	-55.235436
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H	26.138193	-39.088784	-63.512251
H	26.273571	-38.143034	-62.249062
H	29.104710	-27.882352	-65.475856
H	30.205933	-27.995458	-64.425076
H	28.208143	-40.885197	-60.884380
H	26.864014	-40.359672	-61.483088
H	27.834077	-36.124610	-53.939542
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H	25.001742	-38.196439	-54.837950
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H	26.229596	-29.084389	-56.113779
H	25.516742	-30.284762	-55.285416
H	29.593180	-31.633989	-58.782306
H	29.781756	-30.257052	-58.109288
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H	27.114241	-36.386280	-56.054110

Mn^{IV}O•

PDB ID code: 6JLP

B3LYP-D3(BJ)/BS1: -9420.70497388 a.u.

Grimme-D3(BJ): -0.8628763524 a.u.

IEFPCM-B3LYP(_wHF15%)/BS2: -9419.72349425 a.u.

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O	26.361612	-36.474855	-61.436883
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O	28.387758	-32.560746	-58.974726
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C	29.965771	-42.320885	-54.799756
C	29.921726	-40.023495	-54.113323
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C	23.489169	-40.464841	-59.526908
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