Supporting information

The Electronic Structure of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ Cluster in Mordenite Zeolite and its Effects on the Methane to Methanol Oxidation

Konstantinos D. Vogiatzis[1,*],Guanna Li[2,3], Emiel J.M. Hensen,[2,4] Laura Gagliardi[5], Evgeny A. Pidko[2,4,6*]

[1] *Department of Chemistry, University of Tennessee, Knoxville, TN 37996, United States*

[2] *Inorganic Materials Chemistry Group, Eindhoven University of Technology, PO Box 513, Eindhoven 5600 MB, The Netherlands*

[3] *Catalysis Engineering, Department of Chemical Engineering, Delft University of Technology, Van Oder Massage 9, 2629 HZ Delft, the Netherlands*

[4] *Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven 5600 MB, The Netherlands*

[5] *Department of Chemistry, and Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, United States*

[6] *Theoretical Chemistry group, ITMO University, Kronverkskiy pr., 49, St. Petersburg 197101, Russia*

***E-mail: kvogiatz@utk.edu (K. D. V.).**

***E-mail: e.a.pidko@tue.nl (E. A. P.)**

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S1. Examination of different active spaces

For the consideration of the proper active space, a formal charge of 2+ for each Cu was initially assumed, with a formal $3d^9$ electronic configuration per Cu. Based on this assumption, and in order to have a total charge of 2+ for the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core, one O^{2-} and two $O^{\bullet-}$ atoms are expected. After the examination of active spaces of various sizes, we concluded that the energetically most stable states are described by a minimal active space of size (5,5), i.e. 5 electrons in 5 orbitals. The CAS(5,5) includes bonding (σ)/antibonding (σ*) combinations of the $3d_{x2\text{-}y2}$ orbitals of two Cu atoms with the 2*p* of two neighboring O atoms, respectively, and a singly occupied $3d_{x2\text{-}y2}$ atomic orbital of the third Cu atom.

Results from the CASPT2(5,5) level of theory are of little use. Even if CASPT2(5,5) predicts correctly the doublet state (S = 1/2) as the ground state, it underestimates the energy of the quartet (S = 3/2) and sextet (S = 5/2) states. For example, the energy differences between the doublet ground state and the quartet and sextet states are 55.6 and 136.8 kJ/mol, respectively. DFT results have shown that these energy differences are considerably lower. For example, the doublet-quartet energy gap varies between 15.7 and 31.2 kJ/mol by considering different GGA and hybrid density functionals.

The (5,5) orbital space was confirmed as the minimal space that describes this system by examination of larger active spaces such as, for example, of size (11,11) (13,13), and (15,15). These active spaces augment the (5,5) minimal space with 2*p*/3*p* orbitals of the three O atoms of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core. The occupation numbers of the 2*p* orbitals vary between 1.93-1.98. Results from these active spaces are shown in supporting information (Table S1). It was found that the doubly occupied 3*d* atomic orbitals of the three Cu atoms do not participate in the bonding between the Cu and the (μ-O) atoms. Therefore, they are not further considered in this study.

All 2*p* orbitals of the three O atoms with the corresponding 3*p*-shell are needed for a balanced description of the electronic configuration of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core. The orbital space that includes all 2*p*/3*p* orbitals of the three O atoms and the $3d_{x2\text{-}y2}$ orbitals of the three Cu atoms has a size of (19,21). The current CASSCF implementations are not able to treat such large spaces. Instead of CASSCF, calculations with the RAS scheme were performed. Three individual orbital spaces are considered in the RASSCF method: RAS1, RAS2, and RAS3. The correlated orbital space of RASSCF(19,21) was organized as such: RAS2 includes the (5,5)

minimal space described above. A full CI expansion is considered within the RAS2(5,5) space, i.e. all possible configuration state functions (or Slater determinants) were constructed from the five electrons in the five orbitals of RAS2, as in the case of CAS(5,5). RAS1 includes the seven 2*p* orbitals of the three O atoms which do not participate in the bonding/antibonding combinations with the $3d_{x2-y2}$ orbitals of Cu atoms. All configurations that involve up to two electron excitations from RAS1 to RAS2 and RAS3 are considered in the CI expansion. RAS3 includes the nine unoccupied 3*p* orbitals of the three O atoms. Similarly, all configurations that involve up to two electron excitations to RAS3 from RAS1 and RAS2 are considered in the CI expansion.

The doublet state was found the most energetically favorable state for all active spaces attempted in this study. A disagreement on the electronic structure of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core between the CASSCF(11,11) and RASSCF(19,21) results indicated that the doublet CASSCF(11,11) has not converged to the most stable state. For that reason, a CASSCF(11,11) calculation was performed by using the RASSCF optimized orbitals as a starting guess. This calculation converged to a new state 59.2 kJ/mol more stable than the initial CASSCF(11,11) state (Table S1).

Table S1: CASSCF/RASSCF and CASPT2/RASPT2 energies calculated with different choices of active spaces and for different spin states.

Active Space	**Spin State**	**Dominant Configuration**[1]	**Weight**	**CASSCF/ RASSCF Energy**	**CASPT2/ RASPT2 Energy**
CAS(5,5)	Doublet	**2200u**	0.51	-9213.52694223	-9218.65212795
		0202u	0.12		
		2020u	0.11		
		0022u	0.08		
CAS(5,5)	Quartet	**u20uu**	0.73	-9213.51890924	-9218.63096689
		u02uu	0.27		
CAS(5,5)	Sextet	**uuuuu**	1.00	-9213.50696736	-9218.60001037
CAS(7,7)	Doublet	2 **2200u** 0	0.52	-9213.54536483	-9218.65480340

		2 **0202u** 0	0.20		
		2 **2020u** 0	0.16		
		2 **0022u** 0	0.07		
CAS(7,7)	Quartet	2 **u20uu** 0	0.75	-9213.53749793	-9218.63435688
		2 **u02uu** 0	0.24		
CAS(7,7)	Sextet	2 **uuuuu** 0	0.99	-9213.52236678	-9218.59942192
CAS(11,11)	Doublet	222 **2200u** 000	0.54	-9213.61524537	-9218.66002784
		222 **0202u** 000	0.22		
		222 **2020u** 000	0.11		
		222 **0022u** 000	0.04		
CAS(11,11)	Quartet	222 **u20uu** 000	0.76	-9213.60999102	-9218.63727898
		222 **u02uu** 000	0.18		
CAS(11,11)	Sextet	222 **uuuuu** 000	0.96	-9213.57952219	-9218.59340763
$CAS(11,11)^2$	**Doublet**	222 **2200u** 000	0.46	**-9213.63779207**	-9218.63302736
		222 **0202u** 000	0.25		
		222 **2020u** 000	0.15		
		222 **0022u** 000	0.08		
$CAS(11,11)^2$	Quartet	222 **u20uu** 000	0.71	-9213.63543336	-9218.62516031
		222 **u02uu** 000	0.24		
$CAS(11,11)^2$	Sextet	222 **uuuuu** 000	0.96	-9213.62917838	-9218.60329797
CAS(13,13)	Doublet	2222 **2200u** 0000	0.53	-9213.65976693	-9218.65765782
		2222 **0202u** 0000	0.20		
		2222 **2020u** 0000	0.13		
		2222 **0022u** 0000	0.05		
CAS(13,13)	Quartet	2222 **u20uu** 0000	0.76	-9213.65112376	-9218.64119261
		2222 **u02uu** 0000	0.17		
CAS(13,13)	Sextet	2222 **uuuuu** 0000	0.95	-9213.62835746	-9218.59448076
CAS(15,15)	Doublet	22222 **2200u** 00000	0.52	-9213.69928564	-
		22222 **0202u** 00000	0.23		
		22222 **2020u** 00000	0.10		

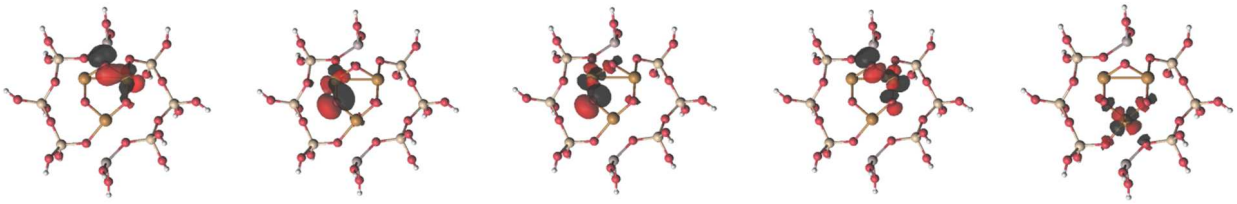
		22222 **0022u** 00000	0.05		
RAS(19,21)	Doublet	2222222 **220u0** 000000000	0.53	-9213.76508246	-9218.63494471
		2222222 **202u0** 000000000	0.18		
		2222222 **020u2** 000000000	0.14		
		2222222 **002u2** 000000000	0.05		
RAS(19,21)	Quartet	2222222 **2uuu0** 000000000	0.74	-9213.76011027	-9218.62652260
		2222222 **0uuu2** 000000000	0.18		
RAS(19,21)	Sextet	2222222 **uuuuu** 000000000	0.93	-9213.74334845	-9218.59358933

[1] 2 stands for doubly occupied MO, 0 for unoccupied MO, and u for singly occupied MO with spin 1/2. The occupation characters of the 5 core MOs are shown with bold font (see text for details).

[2] Start from RASSCF orbitals as guess orbitals.

S2. Key orbitals of the ground doublet state obtained from the CASSCF(11,11)

CASSCF(11,11)



σ (Cu(1) – O(1))	σ (Cu(3) – O(3))	σ* (Cu(3) – O(3))	σ* (Cu(1) – O(1))	$3d_{x2-y2}$ Cu(2)
1.50	1.29	0.71	0.51	1.00

Figure S1: The five most relevant MOs of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ cluster for the five most stable doublet states, as calculated from the CASSCF(11,11) level of theory. A description and their corresponding occupation numbers are given below each MO.

CASSCF(11,11) shows that Cu(2) has a pure d^9 electronic configuration, while Cu(1) and Cu(3) form bonding (σ) /antibonding (σ*) combinations with the 2*p* orbitals of O(1) and O(3), respectively. The O(1) and O(3) have a partially occupied 2*p* atomic orbital, and they have a more $O^{\bullet-}$ (oxyl) character. On the contrary, O(2) has the three 2*p* orbitals as doubly occupied (O^{2-} character). This electronic configuration is similar to the one found from RASSCF(19,21).

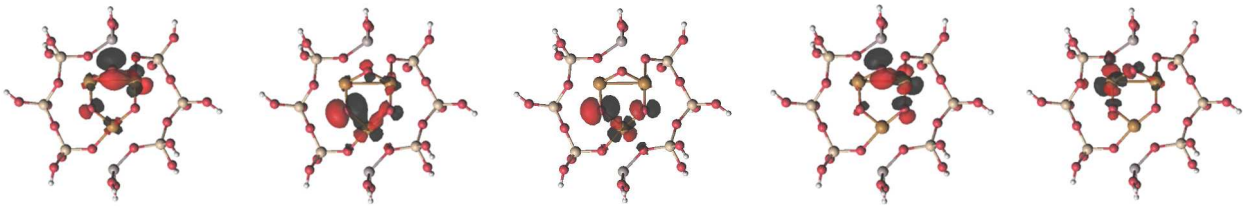
S3. Key orbitals of the 5 doublet states obtained from the SA(5)-RASSCF(19,21) level

In order to understand in depth the electronic structure of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ cluster, the low-lying states were studied by means of state-averaged (SA) RASSCF. A preliminary SA(6)-RASSCF(19,21) calculation was performed, with the six lowest doublet states optimized with equal weights. The purpose of this calculation with an arbitrary number of optimized states was to identify how many energetically low-lying degenerate or near-degenerate states exist. It was found that the first three doublet states are within an energy range of 15 kJ/mol (Figure S2). The fourth and fifth states differ by only 3.7 kJ/mol, and they are 29.0 kJ/mol higher than the ground state. On the other hand, the sixth state is 251.2 kJ/mol higher than the ground state and can be safely excluded from the rest of our analysis.

Table S2: Relative energy differences (in kJ/mol) between the six lowest doublet states, calculated at the SA(6)-RASSCF(19,21), SA(5)-RASSCF(19,21), and MS(5)-RASPT2(19,12) levels of theory.

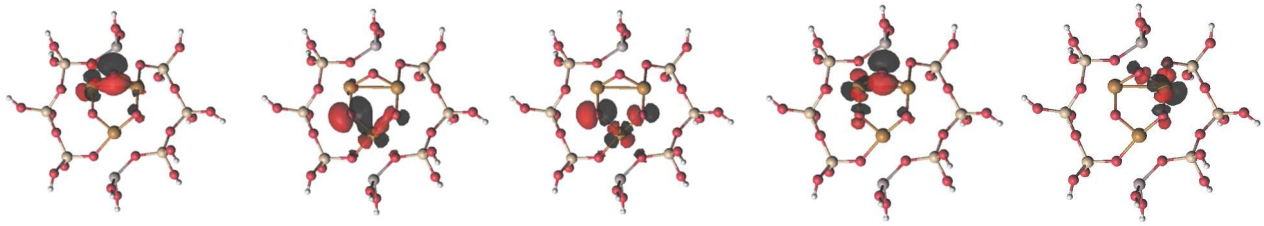
State	SA(6)-RASSCF(19,21)	SA(5)-RASSCF(19,21)	MS(5)-RASPT2(19,21)
1	0	0	0
2	8.9	9.8	17.9
3	14.7	18.9	35.1
4	29.0	31.7	60.6
5	32.7	36.3	68.7
6	251.2	-	-

State 1 (Ground state)



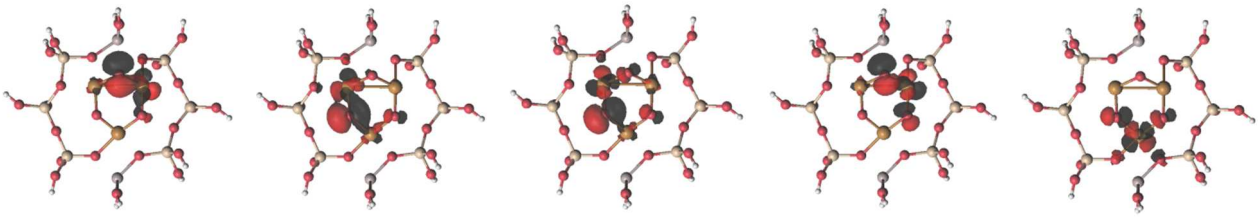
σ (Cu(1) – O(1))	σ (Cu(2) – O(3))	σ* (Cu(2) – O(3))	σ* (Cu(1) – O(1))	$3d_{x2-y2}$ Cu(3)
1.27	1.35	0.66	0.73	1.00

State 2



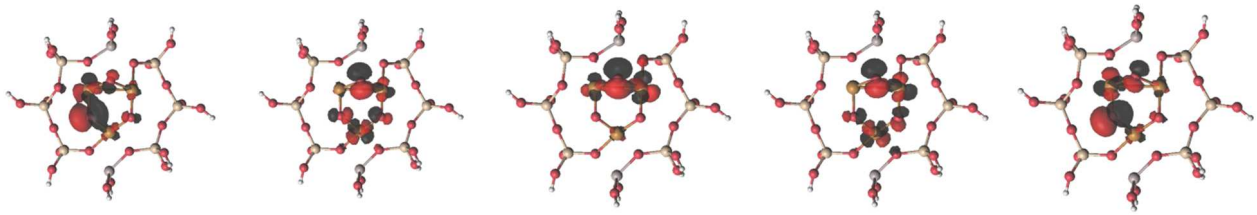
σ (Cu(3) – O(1))	σ (Cu(2) – O(3))	σ* (Cu(2) – O(3))	σ* (Cu(3) – O(1))	$3d_{x2-y2}$ Cu(1)
1.14	1.35	0.65	0.85	1.00

State 3



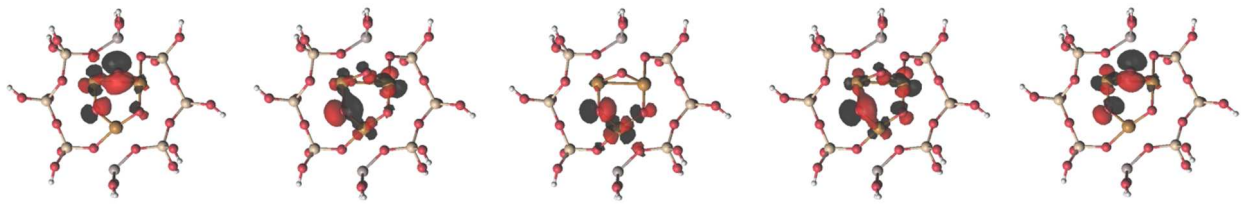
σ (Cu(1) – O(1))	σ (Cu(3) – O(3))	σ* (Cu(3) – O(3))	σ* (Cu(1) – O(1))	$3d_{x2-y2}$ Cu(2)
1.28	1.17	0.83	0.72	1.00

State 4



1.16	1.01	1.01	0.99	0.83

State 5



1.12	1.04	1.00	0.96	0.87

Figure S2: The five most relevant MOs of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ cluster for the five most stable doublet states, as calculated from the SA(5)-RASSCF(19,21) level of theory. A description and their corresponding occupation numbers are given below each MO.

S4. Geometrical details of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ complex optimized with the PBE functional

Table S3 includes the key Cu-O, Cu-Si, and Ci-Al bond distances for both models (S = 3/2 and S = 1/2). The first observation is that the six Cu-O bond distances of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core are between 1.77 and 1.83 Å for both geometries. The Cu-O distances with the oxygen atoms of the MOR framework are significantly larger and they vary from 1.96 till 2.96 Å. This large variety of the Cu-O(MOR) distances leads to the conclusion that the three Cu centers of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core have different coordinative environments. Cu(2) and Cu(3) can be seen as tetra-coordinated cations, while Cu(1) as a tri-coordinated cation, due to the large Cu(1) – O(MOR-2) distance (2.628 and 2.955 Å for the S = 1/2 and S = 3/2 optimized geometries, respectively) . This shift of the Cu(1) – O(MOR-2) distance is the first structural difference between the two geometries. The second geometrical difference is between the S = 1/2 and S = 3/2 structures. The O(1) – Cu(3) bond increases from S = 1.784 Å (S = 1/2 structure) to 1.830 Å (S = 3/2 structure) and the O(2) – Cu(1)/ O(3) – Cu(3) bonds from 1.767 Å (S = 1/2 structure) to 1.781/1.801 Å (S = 3/2 structure).

Table S3: Key bond distances (in Å) for the two MOR models optimized at the doublet and quartet states. Major distortions between the two models are indicated with bold font.

Optimized model at spin:	S = 1/2	S = 3/2
O(1) – Cu(1)	1.818	1.815
O(1) – Cu(3)	**1.784**	**1.830**
O(2) – Cu(1)	1.767	1.781
O(2) – Cu(2)	1.800	1.810
O(3) – Cu(2)	1.785	1.778
O(3) – Cu(3)	1.767	1.801
Cu(1) – O(MOR-1)	1.987	1.984
Cu(1) – O(MOR-2)	**2.628**	**2.955**
Cu(1) – Si(MOR)	**2.968**	**3.105**
Cu(2) – O(MOR-1)	1.955	1.957
Cu(2) – O(MOR-2)	2.016	1.993
Cu(2) – Al(MOR)	2.746	2.745
Cu(3) – O(MOR-1)	**2.105**	**2.227**
Cu(3) – O(MOR-2)	2.044	2.080

Cu(3) – Si(MOR)	2.695	2.730

Multiconfigurational calculations were also performed for the S = 3/2 structure, and the doublet was found energetically more stable than the quartet by 23.1 (CASSCF(11,11)) and 55.5 kJ/mol (CASPT2(11,11)).

S5. Effect of the choice of the functional.

The previous discussion and analysis was based on structures obtained from periodic PBE geometries. In order to examine the effect of the density functional on the geometry and reactivity of the three (μ-O) bridging atoms, we have performed periodic DFT geometry optimizations using six popular density functionals: B3LYP, LC-wPBE, MN12-L, M06-L, M06-2X, and PBE0. The main geometrical difference between the structures optimized with different functionals is the position of ring in the MOR framework, which in some cases was closer to the middle of the MOR channel, while in other cases closer to one side of the channel. In the latter case, the ring structure was wider than in the PBE optimized structure. The wider ring was found for the geometries optimized with M06-2X and PBE0, and it is reflected on the Cu(1)-Cu(3) bond distance (Table S4).

Table S4: Cu(1)-Cu(3) bond distance (in Å) from the structures optimized with different density functionals.

Functional	**Cu(1)-Cu(3)**
PBE	2.740
B3LYP	2.747
LC-wPBE	2.712
MN12-L	2.750
M06-L	2.811
M06-2X	**2.920**
PBE0	**3.011**

Cluster models were used from the periodic structures and SA(5)-RASSCF(19,21) calculations were performed, by following the same process that was described for the periodic PBE geometry. A detailed analysis of the electronic configurations of the five lowest states will be skipped. On the contrary, we will be discuss the differences of the Mulliken charges for the three (μ-O) atoms atoms (Table S5), as they were calculated at the SA(5)-RASSCF(19,21) level. The Mulliken charges by themselves are not indicative of the electronic structure of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ core, but comparison with the charges obtained by the PBE structure can reveal which (μ-O) atoms have an oxyl radical character and which has a O^{2-} character.

Table S5: Mulliken charges of the three (μ-O) atoms calculated with SA(5)-RASSCF(19,21).

	O(1)	O(2)	O(3)
PBE	-0.5211	**-0.9860**	-0.5320
B3LYP	-0.5284	**-1.0139**	-0.5734
LC-wPBE	-0.4930	**-0.9781**	-0.5888
MN12-L	-0.5348	**-0.9548**	-0.5874
M06-L	-0.5132	**-0.9836**	-0.5718
M06-2X	**-1.0188**	-0.5377	-0.5681
PBE0	**-0.9099**	-0.5619	-0.5756

Results from B3LYP, LC-wPBE, M06-L and MN12-L agree with the conclusions extracted from the PBE structure; O(2) has an oxo character, while O(1) and O(3) have a more oxyl radical character. This was found from the electronic configurations of the five energetically lower doublet states and from the Mulliken charges. On the contrary, SA(5)-RASSCF(19,21) predicts for the two structures optimized with the M06-2X and PBE0 functionals that O(1) will have an oxo character. This result is in disagreement with previous mechanistic studies on the $[Cu_3(\mu\text{-}O)_3]^{2+}$ cluster deposited on the ZSM-5 zeolite, where O(1) is the most reactive (μ-O) atom.[1]

S6. Single point DFT energies for benchmarking the choice of the functional

The performance of a range of popular DFT methodologies was assessed by performing single-point calculations for different spin-configurations of the cluster model shown in Figure 1 using Gaussian 09.D01 program package. The (a) BLYP and PBE GGA-type functionals, (b) M06L meta-GGA, (c) MN12L and MN15L meta non-separable GGA, (d) PBE0, B3LYP, M06, M06-2X, MN15 hybrid methods, (e) LC-wPBE, CAM-B3LYP and MN12SX range-separated functionals, and (f) the B2PLYP double hybrid method were employed. The 6-311+G(d) basis set was employed for the Cu centers and its first coordination sphere, while the remaining atoms were treated with the 6-31G(d) basis set.

Single-point calculations were performed on the cluster model extracted from the fully optimized structure with periodic PBE (pPBE). Figure S**3** summarizes the DFT energy differences between the doublet-quartet and doublet-sextet states. The RASPT2(19,21) energy differences were used as benchmark values and are shown in Figure S**3** with pink and grey stars. From the functionals included in this study, the PBE, BLYP and MN12L functionals provided` energies in good agreement with RASPT2(19,21). While PBE and BLYP results are almost identical to the CASPT2 energies, MN12L overestimates the doublet-sextet difference, similarly to the RASPT2(19,21) energies. Most of the remaining functionals predict a quartet state as the ground state of the system, while, in some cases, they estimate the sextet state as more stable than the doublet.

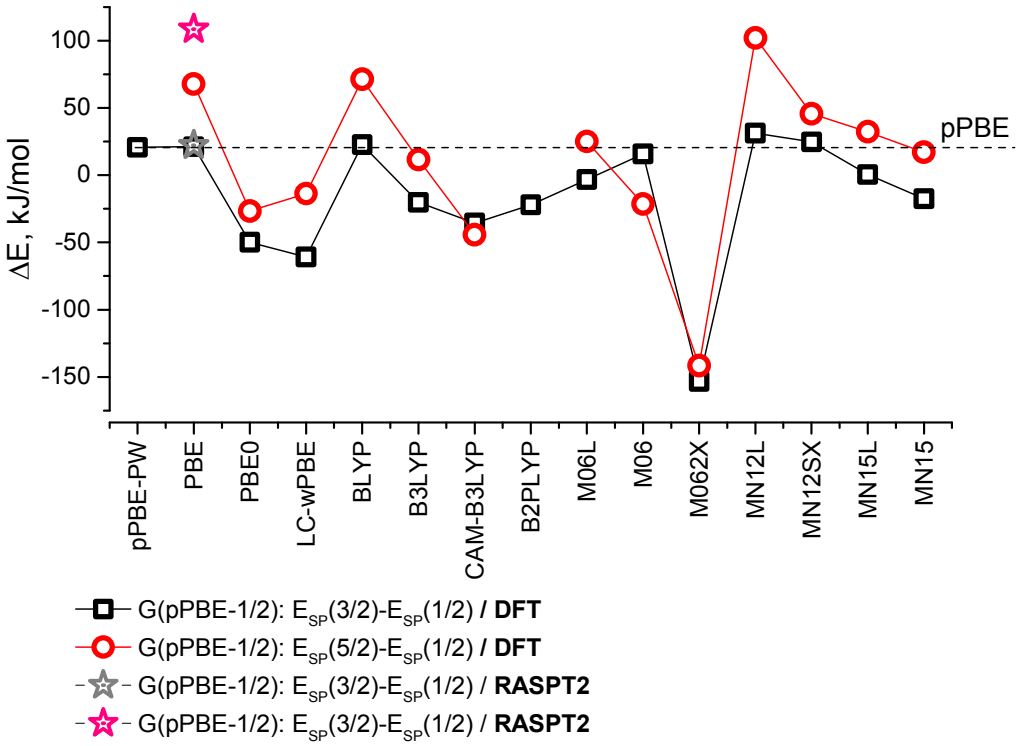


Figure S3: DFT-computed energy differences between the doublet-quartet ($E_{SP}(3/2) - E_{SP}(1/2)$, squares) and doublet-sextet ($E_{SP}(3/2) - E_{SP}(1/2)$, circles) states of the Cu_3O_3/MOR cluster model constructed from the fully optimized periodic structure in the doublet state (G(pPBE-1/2)). The respective benchmark values computed at the RASPT2(19,21) level are shown as stars.

S7. Cartesian coordinates of the $[Cu_3(\mu\text{-}O)_3]^{2+}$ cluster

Al	0.4914320	4.1305720	0.1700210
Al	-0.4058980	-3.7891180	-0.0869720
Cu	0.1535390	1.5971530	-0.8340780
Cu	1.2087780	-1.2384200	-1.1632530
Cu	-1.5134800	-0.9424020	-1.0640560
O	-0.2761380	-1.6891230	-2.1096210
O	-1.2745900	0.7541910	-1.4944310
O	1.3495280	0.4738020	-1.5746530
O	-3.3909620	-0.7649380	-0.1278780
O	-1.7585540	-2.6204640	0.0773900
O	1.1467360	-2.8746850	-0.0368580
O	3.3898140	-1.7343410	0.2157580
O	1.5780530	2.7103960	-0.0895610
O	-0.9261350	3.0113890	0.1128150
O	0.4150520	5.0999940	-1.2254090
O	0.7309260	4.9186420	1.6622140
O	2.2487960	-2.7647600	2.4096910
O	3.3550310	-4.3561980	0.6030420
O	3.4541370	0.8538610	0.4005300
O	3.6851890	2.4191850	-1.7508510
O	4.0169940	3.4143630	0.6358670
O	4.5985860	-0.5351600	2.3086420
O	5.7163840	-0.5605370	-0.0854900
O	-0.3350620	-4.8153850	1.2980200
O	-0.5668170	-4.5852330	-1.5912010
O	-2.6551090	3.4390180	2.0952040
O	-3.1479050	4.4495150	-0.3124840
O	-3.3486620	1.8573010	0.0923360
O	-3.8337930	0.3398140	2.2434080

O	-4.0565620	-2.7214270	1.5989560
O	-4.1214040	-3.1377210	-1.0476590
O	-5.6429830	0.5842880	0.2680940
H	1.1697698	5.4805353	-1.7055073
H	0.7790358	5.8911052	1.6935194
H	1.5850398	-3.3750630	2.8008807
H	3.5584040	-4.6521111	-0.3051051
H	3.2246535	1.7866995	-2.3452205
H	3.6223892	3.7351206	1.4706353
H	3.9243663	-0.9398843	2.8935953
H	6.3198062	0.2060974	-0.0426859
H	-0.2662165	-5.7815714	1.1999888
H	-0.4165428	-4.0781799	-2.4122428
H	-1.9980263	4.0473491	2.4946626
H	-2.6847109	4.7393970	-1.1251503
H	-3.6535439	1.1523578	2.7659441
H	-3.9173080	-2.1053621	2.3504593
H	-3.6324828	-3.8697479	-1.4801866
H	-5.9078585	0.6347342	-0.6702966
Si	2.5309970	-2.9917010	0.8327990
Si	3.1735530	2.3185970	-0.2185750
Si	4.3074900	-0.4800420	0.7176820
Si	-2.5170730	3.1814010	0.4947890
Si	-3.3797500	-2.4169240	0.2021180
Si	-4.0974400	0.5401190	0.6603480

S8. Structures Optimized with Periodic DFT

A. O(1) Initial geometry ([Cu_3(μ-$O)_3$]-MOR + CH4)

data_CONTCAR\9
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_cell_length_b 13.647600
_cell_length_c 15.015100
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 97.178902
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

O	O	0.1857077719417934	0.0320997019449833	0.2249222889657061
O	O	0.2147439506817260	0.9973941573702036	0.7269526472165367
O	O	0.4254677331116584	0.7987933697149772	0.2137731815475636
O	O	0.4224720585051985	0.8076406441992540	0.7272516896732514
O	O	0.6355114239769827	0.8871088938851606	0.5111999132658953
O	O	0.6015544580629709	0.8590514659287548	0.0493652187734619
O	O	0.8015699581985456	0.0084987575537827	0.4718485786952636
O	O	0.7496110579939194	0.9773125856601766	0.9779050754595492
O	O	0.6033482216342608	0.1873056385608099	0.4766801429320838
O	O	0.5939190679899291	0.1986449968369337	0.9833485829012031
O	O	0.3661465666100006	0.1229405306369132	0.2463737784131824
O	O	0.3702093151215902	0.1331063233678381	0.7370887381526272
O	O	0.9417180583068739	0.8027691577637965	0.0476077374775259
O	O	0.9657441741642397	0.7545181817698571	0.5511924784032020
O	O	0.1816675710557806	0.5731297193955526	0.0198340733791369
O	O	0.1830552884155855	0.5756220426850122	0.5196924692132359
O	O	0.1703608840380190	0.3970801401351769	0.2289220977073672
O	O	0.1310577387911524	0.3603584940895312	0.7520378893833345
O	O	0.0309714731364289	0.2515533655205057	0.2820953228428581
O	O	0.0052325998442097	0.1990555901347736	0.7842733578072525
O	O	0.8139426474713157	0.4401610372072950	0.2874925954962200
O	O	0.8306959785189305	0.4232535742360005	0.7809987867533003
O	O	0.8515435671239863	0.6241069582956885	0.0057332906176679
O	O	0.8169454597904922	0.6259565418094474	0.4922038591216054
O	O	0.8047761515674928	0.9503571065348152	0.3030200014622060
O	O	0.7733830350699323	0.9551426339361186	0.8047500737867392

O	O	0.5424871240569810	0.1811036571535361	0.3092483194886467
O	O	0.5425028778123863	0.1947297299773200	0.8113854883800969
O	O	0.4007330673133134	0.1619309686180420	0.9944250864066883
O	O	0.3852451347709583	0.1655834037882443	0.4994330454568298
O	O	0.2434578783704025	0.0471705198346315	0.0538138643237253
O	O	0.2269880411712602	0.0436620983862487	0.5546755651138922
O	O	0.4091974655419902	0.8413002097144716	0.0368854252368837
O	O	0.4572803233089998	0.8059011488559078	0.5532915969497273
O	O	0.6324848384356258	0.8474606023695531	0.2574933201039128
O	O	0.6232849302956535	0.8440952877322760	0.7293889253788222
O	O	0.0252967613306764	0.1977286847542355	0.4548791718856762
O	O	0.0372327114129874	0.2037910777810800	0.9602973392205248
O	O	0.7841084520568767	0.4317782873916416	0.4627525481758556
O	O	0.8075425484211951	0.4396183090434858	0.9567699373983294
O	O	0.9028179597145117	0.6181183803140372	0.2446893786846529
O	O	0.8790460646646236	0.6149356591261022	0.7611102396854507
O	O	0.9949448186905300	0.7962776456791284	0.2186267691624994
O	O	0.9881852105195117	0.7882469876314565	0.7244540099399022
O	O	0.1536406528489238	0.5871625013152554	0.1974648812286054
O	O	0.1958443910207695	0.5405112580969746	0.6949543643162585
O	O	0.1038357036018264	0.3763235058017557	0.5081896602865105
O	O	0.1315695602765393	0.3836172183840501	0.9887312815491942
O	O	0.2789820294371433	0.8938603722187988	0.1534921886348763
O	O	0.2996232839286927	0.8832263670711179	0.6127174532489273
O	O	0.6925155763193943	0.0876451193869234	0.3522868171322112
O	O	0.6958882264824353	0.1086490777614050	0.8620576482964416
O	O	0.1008658509449093	0.7227127863058874	0.0890345005975214
O	O	0.1171839016934323	0.6967652587698082	0.6378206012602972
O	O	0.9026545546633279	0.3165811377198855	0.3909479311358188
O	O	0.8921598666673448	0.2910646925953460	0.8918911052515629
O	O	0.2436652051671432	0.0892247885024949	0.3861077523023663
O	O	0.2624966134230276	0.0809621314376400	0.8820064006879480
O	O	0.4891338231000707	0.8561468241542570	0.3924730305761591
O	O	0.5196933451658212	0.8727190743876323	0.8913412926911948
O	O	0.7712200367862465	0.9023667475121363	0.1350303164127259
O	O	0.7761014806198137	0.9287892381027786	0.6307222053294524
O	O	0.5165438434941351	0.1520736261990065	0.1382343928917109
O	O	0.5288796778000765	0.1668142757028570	0.6395837291582417
O	O	0.9307680997917458	0.7459042124360593	0.3797452584373347
O	O	0.9052905681406055	0.7584212604233816	0.8805825610596155
O	O	0.1365996655578428	0.5183700531401990	0.3646168917354598
O	O	0.1230570722954218	0.5139152509411050	0.8578609074337282
O	O	0.1021019481747137	0.2508684619618715	0.1203987326014635
O	O	0.0703460632738765	0.2282092662634601	0.6236915276126388
O	O	0.8632733588790052	0.4797439637268032	0.1213218557369373
O	O	0.8394832299900341	0.4973437743151431	0.6213213859019114

O	O	0.2181523650790815	0.2234509665887632	0.2610507562765297
O	O	0.1954816113229673	0.1892062706483073	0.7528144324723028
O	O	0.7583690831598551	0.7827883009772265	0.9912723908872714
O	O	0.8010884768866822	0.8141182533546544	0.4902425223191165
O	O	0.7984501400672795	0.7653340009988071	0.2523692189606093
O	O	0.7927318110899280	0.7749341107197756	0.7380545437611573
O	O	0.2296785343207645	0.2287468984270379	0.9902758142399705
O	O	0.2130007099053117	0.2285298498578968	0.5044208559070864
O	O	0.5102449904182985	0.0157960222177928	0.0090631809716951
O	O	0.4892960903306435	0.0004991796543504	0.5190941725008017
O	O	0.9944847317202468	0.5079877896070069	0.9898833501675438
O	O	0.9685071667258699	0.5247768615714127	0.4863023443326894
O	O	0.4978709837166611	0.9960780155320170	0.2461822812767105
O	O	0.5102566705195777	0.0097187204930055	0.7452828678287468
O	O	0.0002652827565030	0.4626060917593139	0.2438948778625298
O	O	0.0052170689773380	0.4898479531858361	0.7141557371503938
O	O	0.0963861383855966	0.9161646486789038	0.1027783397273096
O	O	0.1065781919102723	0.8888630398126137	0.6085633451277599
O	O	0.2913609706932191	0.7030037447871038	0.1178990432335172
O	O	0.3097783017997628	0.6889375315666642	0.6220105581783222
O	O	0.8877167032611040	0.1259942948202591	0.3438830412048710
O	O	0.8855781466080513	0.0939759048251505	0.8931110027722952
O	O	0.7115350796234038	0.2848742229018741	0.3525088440912391
O	O	0.7005029087273388	0.3040321681964219	0.8630712197836993
O	O	0.3234544801251211	0.5579635678701277	0.3044560688122189
O	O	0.5176480137405155	0.6721931450043181	0.3223248420161380
O	O	0.3814604019255214	0.6052506379005073	0.4668734842046252
Si	Si	0.5036571280559903	0.1304144834082386	0.0334477611994208
Si	Si	0.7207662759509906	0.8792694287366487	0.0387803047328031
Si	Si	0.7539756759714155	0.9101776169871915	0.5242721995858812
Si	Si	0.2544232930771922	0.1169593995849719	0.2815832229001229
Si	Si	0.2589368982761870	0.1002542401442566	0.7754051524744265
Si	Si	0.8948720888090850	0.5014786721800997	0.2242572420760934
Si	Si	0.8895655598532756	0.5071702385274514	0.7186866340899338
Si	Si	0.1295543039291117	0.2796208001435878	0.2232027456118397
Si	Si	0.1011247969928895	0.2445582506772847	0.7266828239777183
Si	Si	0.1072374532682463	0.4933746185031718	0.9637005521970673
Si	Si	0.8789646001787658	0.7348525159700603	0.4773234405779982
Si	Si	0.8641219650652224	0.7403592744877784	0.9815883269785900
Si	Si	0.5192486619067340	0.8958014871681304	0.4934536100347253
Si	Si	0.5107604003565779	0.8978950790786147	0.9944794209121528
Si	Si	0.2695985365802506	0.1323776790851733	0.4862174366309968
Si	Si	0.2835178402406995	0.1294505616048416	0.9805839154071889
Si	Si	0.4817214178280866	0.1094659301679451	0.2365388644411331
Si	Si	0.4855473985407653	0.1200482984447280	0.7395868856789929
Si	Si	0.7476334929497467	0.8664224794360013	0.2376694348729680

Si	Si	0.7485037637293014	0.8783130734366316	0.7258114896012439
Si	Si	0.1179717288411148	0.4919622213726559	0.2584529677311610
Si	Si	0.1129370489571528	0.4751253865540102	0.7553372915290185
Si	Si	0.9056993833560609	0.7323780595398615	0.2741634007199236
Si	Si	0.8925905477536625	0.7329840884156378	0.7760477880224583
Si	Si	0.8806024355501219	0.5134919597531115	0.0187474514017865
Si	Si	0.8544806376563964	0.5189512423575435	0.5149886969463529
Si	Si	0.1254040660912120	0.2678602054956459	0.0154135549926028
Si	Si	0.2020820191765282	0.9735063692000542	0.1332534462658611
Si	Si	0.2130555561957452	0.9541093790151930	0.6249827007650308
Si	Si	0.3520746792657150	0.8132613393925795	0.1290622827921092
Si	Si	0.3703571691653544	0.7980862470566608	0.6316150650610068
Si	Si	0.7965462523162059	0.0436520171799983	0.3674427584618740
Si	Si	0.7761882025086659	0.0347441777947360	0.8860337474931093
Si	Si	0.6336378654295777	0.2004656103044757	0.8820144997775927
Si	Si	0.0334627405745536	0.8087564810195977	0.1160506388224330
Si	Si	0.0451175713014253	0.7821386676242095	0.6294447087263130
Si	Si	0.1802421581051580	0.6456948868277855	0.1053752402744271
Si	Si	0.2021067199380151	0.6258774687186749	0.6187727495346576
Si	Si	0.9620948414251668	0.2234369014470879	0.3684400034520885
Si	Si	0.9554092889541190	0.1982427639680093	0.8820337213686986
Si	Si	0.8025686547099984	0.3678084991270545	0.3737433107489549
Si	Si	0.8092574186928139	0.3644363822584533	0.8735902054933173
Si	Si	0.1038965949748750	0.2603853607368081	0.5222105942766102
Si	Si	0.6378551636708725	0.1854669633825545	0.3743196787715192
Al	Al	0.0836478325994184	0.4910530415062066	0.4735900919533523
Al	Al	0.5168742099622691	0.8789811455299570	0.2760831819313641
Al	Al	0.5088491543440053	0.8893671334001325	0.7801228625198766
Al	Al	0.4966922129460076	0.1273407570890102	0.5222917696869382
Cu	Cu	0.2667570656375304	0.5683612691512326	0.4119605972622810
Cu	Cu	0.4594299111131321	0.7097492245019609	0.4241176739770145
Cu	Cu	0.3989362097798785	0.6639200637696727	0.2621351025257107
C	C	0.5854752741128871	0.4759854814974018	0.3265210683386371
H	H	0.5843498544126623	0.2193388595983485	0.6411136505117142
H	H	0.6010899484959642	0.7831976177358427	0.6968667112194900
H	H	0.5387685053807821	0.4091227978040014	0.3048636978369921
H	H	0.6452920580905530	0.4959070357730564	0.2787230217896556
H	H	0.5409280404795428	0.5380354376865588	0.3303993258929893
H	H	0.6162042981215614	0.4654945227254899	0.3927933951294534

B. O(1) Transition state ([Cu_3(μ-O)$_3$]-MOR•••CH4)

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_cell_length_a    13.647600
_cell_length_b    13.647600
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_cell_length_c 15.015100
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_cell_angle_beta 90.000000
_cell_angle_gamma 97.178902
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

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O	O	0.2139342570446203	0.9962458832906478	0.7273385172487039
O	O	0.4272490678569412	0.7948478637966403	0.2154515867957372
O	O	0.4217092840033985	0.8074673996752679	0.7277678405587622
O	O	0.6358407161601036	0.8892689598550376	0.5121025996606292
O	O	0.6029609162431342	0.8615009525951933	0.0497058200948501
O	O	0.8036696815575581	0.0078129262555677	0.4721547247176048
O	O	0.7508354517608353	0.9788547427592462	0.9782395976939213
O	O	0.6034432116723494	0.1869649784703853	0.4766568747652329
O	O	0.5929871822015045	0.1987517655049231	0.9825744109820462
O	O	0.3686071055166380	0.1219668654695667	0.2462928118198278
O	O	0.3697764702053803	0.1318533849157504	0.7379359541770327
O	O	0.9433754540521946	0.8034437946405930	0.0465721463617896
O	O	0.9649720505553319	0.7553677669056640	0.5511554546344541
O	O	0.1828290572782905	0.5726644629376736	0.0200074079529671
O	O	0.1846230525654988	0.5740219469993733	0.5193415286803997
O	O	0.1710919741383776	0.3959635544616091	0.2275038070769497
O	O	0.1334438738702417	0.3600233675427376	0.7511916661364282
O	O	0.0340034117785990	0.2498921443112820	0.2827910151132471
O	O	0.0049043366415091	0.2010113572471894	0.7843112126239546
O	O	0.8129817816284159	0.4389039290674148	0.2871221363945580
O	O	0.8304723242565899	0.4228914559997392	0.7803874934811219
O	O	0.8515921003929137	0.6245784083262151	0.0073107311390928
O	O	0.8181630575586638	0.6252748030280486	0.4912606772980297
O	O	0.8057076651708215	0.9490118625170254	0.3036232538014332
O	O	0.7716393097358534	0.9548911558197517	0.8048077786660528
O	O	0.5451779892897832	0.1806360515000591	0.3076775923820065
O	O	0.5428158870416979	0.1952694038832661	0.8104537089827133
O	O	0.4000783022497600	0.1630855938214069	0.9947727276182761
O	O	0.3866126019442433	0.1673867319013240	0.5015243855002396
O	O	0.2445462980123736	0.0470164737058596	0.0554665207890466
O	O	0.2278477883912942	0.0442442102336997	0.5553948788537539
O	O	0.4112975562765868	0.8401425473589299	0.0386003530888743

O	O	0.4581164268684859	0.8065697324270360	0.5545144509685542
O	O	0.6337037391120717	0.8459905919055117	0.2569056231801810
O	O	0.6231625087941879	0.8438108949550980	0.7282336633927216
O	O	0.0260626079127491	0.1963218639988398	0.4553440998265756
O	O	0.0361052251099707	0.2040682146633941	0.9608012298049502
O	O	0.7859504043827528	0.4319749955291883	0.4623191029324119
O	O	0.8083300609631365	0.4406913509942143	0.9563851354751733
O	O	0.9029116711716938	0.6164380555563653	0.2460602656117388
O	O	0.8793202953044670	0.6144881454533646	0.7602201258786536
O	O	0.9954172218145771	0.7943309678131740	0.2177821060111569
O	O	0.9887526088596985	0.7878177755039033	0.7241585147652074
O	O	0.1538453876270438	0.5864010285344037	0.1972400620495733
O	O	0.1962460817003304	0.5410791916806517	0.6952447309269232
O	O	0.1036426679318296	0.3748046978800517	0.5086412466851726
O	O	0.1307285226090542	0.3831124054301611	0.9907025324492906
O	O	0.2819384842847867	0.8934473095084883	0.1549995248749667
O	O	0.2998965878619160	0.8835700102294624	0.6127675407601458
O	O	0.6942857215640146	0.0873664299491708	0.3532268734008142
O	O	0.6969078477402775	0.1103140167288004	0.8620566381227306
O	O	0.1020937674561466	0.7222494307631919	0.0883891249057385
O	O	0.1164658369962055	0.6958062483448728	0.6360383863774075
O	O	0.9041242698979985	0.3156611289605635	0.3898212677943178
O	O	0.8907943244297201	0.2905446843182276	0.8923634953190103
O	O	0.2468070331347576	0.0898187509863462	0.3870189756211388
O	O	0.2626138555893149	0.0784250060715408	0.8830975594585766
O	O	0.4923165808823313	0.8487709632414138	0.3920188666298401
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O	O	0.7728511903722648	0.9026996583830424	0.1353527998201187
O	O	0.7773982688908774	0.9280370893649064	0.6307314121666678
O	O	0.5178241863987623	0.1487331895971238	0.1369733691969799
O	O	0.5292362829943329	0.1642769139476030	0.6394492188374130
O	O	0.9311148078619667	0.7463539549505072	0.3795651193113017
O	O	0.9057676089266806	0.7570002175482173	0.8804391479346165
O	O	0.1389952227759181	0.5164379900228937	0.3638683676767656
O	O	0.1247082798154366	0.5124394654073825	0.8585207185096593
O	O	0.1039502307287279	0.2479498934889719	0.1209531595045874
O	O	0.0713845036404805	0.2266375689536275	0.6241494583619556
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O	O	0.8426288329213421	0.4970959233001651	0.6202826332769646
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Si	Si	0.7980756605654378	0.0426205216525375	0.3677465846349506
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Si	Si	0.1814953203170049	0.6454113903256413	0.1055189926382525
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Si	Si	0.9638005960833240	0.2221610321666461	0.3683140603402535
Si	Si	0.9549372266933531	0.1985043878917310	0.8819295224755095
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Si	Si	0.8091430325155500	0.3649342557321162	0.8734587575088284
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Al	Al	0.5178107091380468	0.8764980481120119	0.2765609884557776
Al	Al	0.5090564955545389	0.8885056114478900	0.7802207179466691
Al	Al	0.4971144628175068	0.1260595872118273	0.5220476322716436
Cu	Cu	0.2707718822850837	0.5645548058743133	0.4119554996013596
Cu	Cu	0.4603911027500625	0.7028889632914472	0.4226441105689531
Cu	Cu	0.3982092940335658	0.6576446398702416	0.2613473888202327
C	C	0.5681700845185261	0.4825990765712377	0.3287797914538584
H	H	0.5845675416452399	0.2169630829156980	0.6409479269393148
H	H	0.6000442544635073	0.7861965831228394	0.6915790399169420
H	H	0.5022772528959459	0.4325075578308845	0.3110916310905694
H	H	0.6266256597936130	0.4915242826912357	0.2784437116844901
H	H	0.5407609887280022	0.5723192211134731	0.3271481124687001
H	H	0.5941367507508062	0.4763352359127870	0.3972080344466012

C. O(1) Final geometry ([Cu_3(μ-OH)(μ-$O)_2$]-MOR + CH3)

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_cell_length_b 13.647600
_cell_length_c 15.015100
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 97.178902
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z

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_atom_site_label
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_atom_site_fract_y
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  O    O  0.2135503104329167  0.9961169610792153  0.7273868898540096
  O    O  0.4269900682247448  0.7954159144211658  0.2157287022017597
  O    O  0.4227012590961450  0.8072062664215777  0.7268888872873411
  O    O  0.6356665626404925  0.8898832071943853  0.5124050505822898
  O    O  0.6029488322911750  0.8608112920709234  0.0492937633055391
  O    O  0.8042686540763352  0.0072036620792731  0.4722065965888969
  O    O  0.7507808853058907  0.9784769327971057  0.9781452916343496
  O    O  0.6037661084060967  0.1862113188065440  0.4767200740168290
  O    O  0.5931081702671772  0.1987290826453316  0.9826554960757289
  O    O  0.3688557368940943  0.1214906826156191  0.2467745507047359
  O    O  0.3696591636431142  0.1313842510153844  0.7380230347721630
  O    O  0.9439578410780601  0.8028711410929633  0.0462847197384941
  O    O  0.9646975449353508  0.7555544570819268  0.5508525549068845
  O    O  0.1834591316129519  0.5718566561799144  0.0202345866275753
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  O    O  0.1713685747125412  0.3955616136018055  0.2268609070012949
  O    O  0.1337945649357274  0.3600477567736571  0.7508068543613233
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  O    O  0.0051115053445564  0.2011930368333691  0.7847136369804729
  O    O  0.8145480368327074  0.4359511336626524  0.2867710192363931
  O    O  0.8300942283098743  0.4228138263126418  0.7802675146488283
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  O    O  0.8186443217385251  0.6245874310827206  0.4905551976998371
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Si	Si	0.7981638491244676	0.0416677259171863	0.3677545759975455
Si	Si	0.7762985228948692	0.0351123910404093	0.8857118699301317

Si	Si	0.6336354472100014	0.2011960164525653	0.8816175327832231
Si	Si	0.0350921696588152	0.8072521286421106	0.1151718688835900
Si	Si	0.0453417053115687	0.7818291902460001	0.6282938720049442
Si	Si	0.1821106989097089	0.6448902929998024	0.1054987970301166
Si	Si	0.2022215437184285	0.6250757451784535	0.6178752951801154
Si	Si	0.9652928894414382	0.2201741528206219	0.3687943415791308
Si	Si	0.9549641929373303	0.1986549590814087	0.8822311716729700
Si	Si	0.8058930830828176	0.3647934041414916	0.3741182973136896
Si	Si	0.8091628186759872	0.3649175321826628	0.8734636894644361
Si	Si	0.1047696156167337	0.2583955257190436	0.5232036397581519
Si	Si	0.6395511943504416	0.1835730425549835	0.3748073591516887
Al	Al	0.0867865485433557	0.4888948413651015	0.4722096056501947
Al	Al	0.5180094402034114	0.8770439891633753	0.2763716516117986
Al	Al	0.5091700143722850	0.8885078302211714	0.7801539160369609
Al	Al	0.4969893820942945	0.1266633371753642	0.5222898199167422
Cu	Cu	0.2717722530395123	0.5642114867898360	0.4117004584099177
Cu	Cu	0.4585027588936385	0.7085727119525671	0.4255495032095605
Cu	Cu	0.3961149280582941	0.6588509503790992	0.2614639726136603
C	C	0.5800897080687617	0.4620765063856010	0.3241479541671556
H	H	0.5844555130581822	0.2174211155445377	0.6414993471467662
H	H	0.6007204295570121	0.7837228012088753	0.6948550639326929
H	H	0.5175653938671326	0.4083818612540389	0.3059285718542409
H	H	0.6309172274595307	0.4934122281116871	0.2727196141329974
H	H	0.5297621394351941	0.5881640876158931	0.3319643727185475
H	H	0.6031839914340895	0.4685635055940754	0.3935904766209659

D. O(2) Initial geometry ([Cu_3(μ-$O)_3$]-MOR + CH4)

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_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
  O     O    0.1835948223647478    0.0321732451754341    0.2258736960450980
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O	O	0.4248923699460340	0.7941133340605282	0.2167950007954609
O	O	0.4202350509279242	0.8074968187938825	0.7278268885494811
O	O	0.6351244557181434	0.8873837384017924	0.5119940823872537
O	O	0.6008330217862949	0.8606575392820996	0.0512716191026578
O	O	0.8001508858356021	0.0096766237886007	0.4729233405836167
O	O	0.7486706029028726	0.9779691692632640	0.9782193537945473
O	O	0.5998412675972463	0.1881609651276915	0.4774476736211892
O	O	0.5934521535730596	0.1974222797288677	0.9837499852547552
O	O	0.3642628586248063	0.1215020169316011	0.2445849364581277
O	O	0.3684033715851481	0.1327713664680976	0.7394190163725406
O	O	0.9410459146615351	0.8043334700438709	0.0475788466649587
O	O	0.9648244831135069	0.7545722289808315	0.5516904175893023
O	O	0.1810569086859773	0.5727966202097872	0.0197907722420628
O	O	0.1798766738051539	0.5759894606197287	0.5197531177960782
O	O	0.1653133134561103	0.3967035999909220	0.2295374552051123
O	O	0.1313253416569349	0.3602961151088621	0.7513502233365111
O	O	0.0291325343779143	0.2504002987976239	0.2823677193716986
O	O	0.0033987058945474	0.2007391529715183	0.7843048431137518
O	O	0.8067601923492930	0.4428973312508838	0.2880882680513545
O	O	0.8299959094161199	0.4228338748581855	0.7812258899503363
O	O	0.8518602280757837	0.6251635191260020	0.0062980412079622
O	O	0.8160773195136040	0.6265056370959255	0.4922578195152396
O	O	0.8012518721047506	0.9510394694040958	0.3045839195090502
O	O	0.7720834619188103	0.9542097500888258	0.8052460998853712
O	O	0.5390756047839055	0.1791266444696226	0.3093830669835035
O	O	0.5416397150684377	0.1950669872763034	0.8120782815482124
O	O	0.3999742543618087	0.1625570110851206	0.9938273139730178
O	O	0.3829959889397615	0.1657722670808384	0.5026918029680374
O	O	0.2454895147983687	0.0459001031201618	0.0558130472739250
O	O	0.2240853172575656	0.0439772702437831	0.5552992108503625
O	O	0.4084543447422457	0.8404701695129407	0.0410743643490919
O	O	0.4571816017802946	0.8061132334678145	0.5544912800996429
O	O	0.6312067879589377	0.8449566491118122	0.2570760615304136
O	O	0.6212232420919505	0.8442325313266327	0.7302536984195623
O	O	0.0208963851003203	0.1993626288215920	0.4556796906142770
O	O	0.0359934505284793	0.2038184872362146	0.9606083556226940
O	O	0.7808619692744535	0.4324532357821894	0.4634127014645859
O	O	0.8068377253443910	0.4410979074026264	0.9566380639929964
O	O	0.9005006785126289	0.6190572085517585	0.2444150584619368
O	O	0.8792092950251729	0.6147128334822241	0.7615773749734983
O	O	0.9948803907681812	0.7963444744280860	0.2185782341644472
O	O	0.9862127772428558	0.7893337765837899	0.7247929109414989
O	O	0.1477360291589323	0.5857691650107701	0.1966348807081395
O	O	0.1949942883549413	0.5408701123848149	0.6951384773832849
O	O	0.1027731301054703	0.3760728860518275	0.5091735967804283

O	O	0.1311080639479549	0.3829500999222561	0.9896657605784415
O	O	0.2786133116921058	0.8926467021241641	0.1578757183834727
O	O	0.2994576047285568	0.8845616230068707	0.6121208597153787
O	O	0.6908494446041642	0.0898747557905035	0.3537794755739455
O	O	0.6956902559087695	0.1090333746935333	0.8616548294431727
O	O	0.0992901417054639	0.7222942569667531	0.0879274239172594
O	O	0.1148845873696902	0.6963470600360486	0.6394773737297105
O	O	0.8977742341034991	0.3168224699240613	0.3881358341619912
O	O	0.8904166484657825	0.2909211143363766	0.8933144826411997
O	O	0.2448470582396794	0.0880642520409185	0.3865356077103111
O	O	0.2603454894884395	0.0783829151386094	0.8835619097813384
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O	O	0.5163326183073453	0.8686541558152969	0.8936630409447932
O	O	0.7704676086005060	0.9044249627376656	0.1361636390923757
O	O	0.7752811337112574	0.9274502227009649	0.6312624533119442
O	O	0.5157389087123556	0.1493719197724233	0.1377972210029138
O	O	0.5273906098766514	0.1637526280791633	0.6411877753871619
O	O	0.9310536961926764	0.7458388112718979	0.3799456314146252
O	O	0.9033803075738563	0.7589372219219146	0.8807256534141206
O	O	0.1329194358357786	0.5183670823288715	0.3643586084383957
O	O	0.1214685034695873	0.5127598073561852	0.8582189531764843
O	O	0.1020345500525054	0.2491666410381212	0.1211765823787490
O	O	0.0700343972486084	0.2270303919758951	0.6240641985928029
O	O	0.8603713933039879	0.4802702487322695	0.1216263301611732
O	O	0.8383423601532660	0.4977786157788539	0.6215965690343673
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O	O	0.1931141484313410	0.1874585059968775	0.7548806879062191
O	O	0.7573870833893024	0.7836048992127942	0.9929516118560037
O	O	0.8011752350821526	0.8150045414952740	0.4892904340551512
O	O	0.7986293901193480	0.7670755794438489	0.2529982135319050
O	O	0.7904352403670248	0.7735234608179575	0.7385485541634620
O	O	0.2282995065500585	0.2270840242223270	0.9907556389877633
O	O	0.2101158151448004	0.2276600839039752	0.5025077701323891
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O	O	0.9941731329503530	0.4616360416708832	0.2462090250634873
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O	O	0.2889874158826575	0.7018460949119104	0.1199352652880158
O	O	0.3073226124311653	0.6900653604015540	0.6213540896476875
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O	O	0.8851048040958117	0.0937358618608273	0.8926067012391843
O	O	0.7050349031171868	0.2877198118891048	0.3527953446776610
O	O	0.6992754281293666	0.3045952294731780	0.8641779133296877
O	O	0.3186065728454303	0.5589836465365714	0.3040572850068359
O	O	0.5207804603668166	0.6590096030416948	0.3272505980325406
O	O	0.3760784476328118	0.6091655892347289	0.4669665111864627
Si	Si	0.5022414781828498	0.1295496931056223	0.0327262306800666
Si	Si	0.7199523460942077	0.8805834134291186	0.0400344209748484
Si	Si	0.7537433087667640	0.9103268769519184	0.5245311837385234
Si	Si	0.2534757304169824	0.1165622174395137	0.2820631361787057
Si	Si	0.2569723579402344	0.0986084781968085	0.7770808548541366
Si	Si	0.8895711390339835	0.5022070252270661	0.2251029712385020
Si	Si	0.8888854429371719	0.5068052744735323	0.7188113275059285
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Si	Si	0.2679733391434939	0.1319676652555317	0.4868295937926604
Si	Si	0.2828078602178347	0.1282154693309832	0.9815022854544070
Si	Si	0.4799034530932855	0.1073302357234769	0.2358496309930531
Si	Si	0.4836481993391923	0.1191706334206468	0.7418841009940782
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Si	Si	0.7466932124998591	0.8772362561777004	0.7263459212115745
Si	Si	0.1120992961097290	0.4912930780256714	0.2583960002895216
Si	Si	0.1123260720428846	0.4749474456156663	0.7553539839281973
Si	Si	0.9054184763315989	0.7332265996040551	0.2743910959128845
Si	Si	0.8911659911145869	0.7327854047123201	0.7762624691898291
Si	Si	0.8799567403655060	0.5142183402988852	0.0192655293319440
Si	Si	0.8526164399069633	0.5190660760716670	0.5150627491583588
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Si	Si	0.2120749697704535	0.9542055190143375	0.6252065709489333
Si	Si	0.3508430340460114	0.8111503525290110	0.1327562007473265
Si	Si	0.3692008529455566	0.7986574291011148	0.6316402869639262
Si	Si	0.7942873139239225	0.0447470829852598	0.3684823747116965
Si	Si	0.7756004946652547	0.0346636156095546	0.8859697977398826
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Si	Si	0.0438203353494433	0.7824369161211543	0.6302487722598347
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Si	Si	0.9590785448928600	0.2242024035752285	0.3680813721604534
Si	Si	0.9541876947205458	0.1986522659354383	0.8822625718320378

Si	Si	0.7976059678318541	0.3691362558447675	0.3737272021776852
Si	Si	0.8081829072387484	0.3648448121834485	0.8743230381394164
Si	Si	0.1016626103124135	0.2598411263358897	0.5223293419245347
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Al	Al	0.0815667497281051	0.4898566451531857	0.4734211213113918
Al	Al	0.5162855446855280	0.8771989649666090	0.2766656976250403
Al	Al	0.5062627661703505	0.8879911808176736	0.7827619205827089
Al	Al	0.4943439168945732	0.1265021368268566	0.5235765330429087
Cu	Cu	0.2626116057350201	0.5699670819878038	0.4116140025701360
Cu	Cu	0.4606263225356111	0.7083649681787134	0.4234740463623345
Cu	Cu	0.4062158854298738	0.6573356818828827	0.2639589557874757
C	C	0.4022451137570576	0.4059744672883770	0.1548411053012955
H	H	0.5819526150824363	0.2172584898516133	0.6425979760336912
H	H	0.5982296934769332	0.7846238087220234	0.6961466010205001
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H	H	0.3696431159659989	0.4483295637327140	0.2067973447035415
H	H	0.4525147696154225	0.3594324455546754	0.1860172485942388

E. O(2) Transition state ([Cu_3(μ-$O)_3$]-MOR•••CH4)

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+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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O	O	0.4234736484300115	0.8071688795941014	0.7255250943306919
O	O	0.6340829267943136	0.8861425319718350	0.5142229940100620
O	O	0.6001905645309265	0.8620320207682184	0.0520051170926052
O	O	0.7984368356302056	0.0090545850307322	0.4726826685381766
O	O	0.7477044088544460	0.9783360976599695	0.9778516215193420

O	O	0.5996002295267715	0.1867622217295661	0.4768637887146667
O	O	0.5934014119816311	0.1966316315837418	0.9833485506420345
O	O	0.3651914291739899	0.1197341987725480	0.2441006502367244
O	O	0.3683771202912212	0.1321134145204752	0.7379073715187019
O	O	0.9405298012224748	0.8023149810493493	0.0476463933370042
O	O	0.9650792820256555	0.7550276704858803	0.5513078561773597
O	O	0.1800880709577939	0.5720772074427813	0.0196124833496540
O	O	0.1805720844960774	0.5778926241408797	0.5196963947843969
O	O	0.1640955055686888	0.3935786044073737	0.2220424965195633
O	O	0.1329623100735091	0.3600860224108331	0.7520476834608232
O	O	0.0296468869606699	0.2489857186767992	0.2819859394023183
O	O	0.0035415424703729	0.2005929633780283	0.7831193011396067
O	O	0.8071085815296399	0.4427625587158133	0.2878906082959887
O	O	0.8292784133989883	0.4227989552505420	0.7804379711098264
O	O	0.8490970808647162	0.6242043646988051	0.0057556771546174
O	O	0.8181721018826735	0.6258243398387080	0.4912070944507576
O	O	0.8018274959592588	0.9503999243857209	0.3046091981300165
O	O	0.7716417216898250	0.9534577889876701	0.8049959285752166
O	O	0.5395343130403489	0.1778526415933044	0.3080971842073907
O	O	0.5408230515088661	0.1948511423370647	0.8119464150685829
O	O	0.3998627489052922	0.1638324734050300	0.9951306582383239
O	O	0.3833253648246000	0.1652260140004813	0.5012630996476162
O	O	0.2439524604242180	0.0473314531853504	0.0548453134343916
O	O	0.2249306188408653	0.0437619408618204	0.5552580620459011
O	O	0.4071657969824827	0.8387585099736441	0.0375032186399338
O	O	0.4534574681682457	0.8025521101995992	0.5502436832988238
O	O	0.6323787707655342	0.8446171948617547	0.2561238951128217
O	O	0.6218895897092835	0.8438927275530688	0.7291931899845281
O	O	0.0218952443679470	0.2001784507183757	0.4555817303457488
O	O	0.0363509529850887	0.2023190294234496	0.9588693550127800
O	O	0.7827737496736091	0.4321744548437252	0.4633610415310159
O	O	0.8060506389143853	0.4395477558670535	0.9565011062535334
O	O	0.9022094537104692	0.6187865508864547	0.2441710452826484
O	O	0.8800666175030756	0.6142285620292327	0.7608840111851336
O	O	0.9961231236644750	0.7963888329589253	0.2184365023347610
O	O	0.9853496430026851	0.7901770687309764	0.7245102463331747
O	O	0.1485235985548599	0.5847661788724423	0.1963083775300163
O	O	0.1952745530662412	0.5416042764695490	0.6960279196046386
O	O	0.1045720135756909	0.3776195149312755	0.5072896750137019
O	O	0.1287340429006179	0.3822703503616154	0.9919244920988177
O	O	0.2764990418997826	0.8919037120562550	0.1534876833629042
O	O	0.2997518050257071	0.8842427307923515	0.6129209035341248
O	O	0.6920508906367289	0.0908726405635534	0.3527211015507774
O	O	0.6954055984509040	0.1089355449864584	0.8606612996936889
O	O	0.1006735489608701	0.7234072094611079	0.0878483390135401
O	O	0.1150317147923872	0.6971929014137075	0.6414063269662833

O	O	0.8970013927009575	0.3150633599908375	0.3865014894037913
O	O	0.8903374877591901	0.2901489544918121	0.8922693887422142
O	O	0.2446343206340558	0.0876660528393600	0.3859638311292173
O	O	0.2618179504875400	0.0792314280931876	0.8829910155871445
O	O	0.4893108660874290	0.8538643673397104	0.3939145583064843
O	O	0.5185422452508774	0.8665235399264120	0.8930164775700149
O	O	0.7713386016455388	0.9053272735083766	0.1357606267692120
O	O	0.7764598942282106	0.9268257238358331	0.6309633707783320
O	O	0.5165315042303860	0.1453400077809874	0.1373893647910478
O	O	0.5277535922483594	0.1634005586116984	0.6409917726687553
O	O	0.9311994407987072	0.7467102513979498	0.3794260461639283
O	O	0.9025788363318412	0.7580346052124298	0.8806830349189099
O	O	0.1415652750588379	0.5123614922444872	0.3607680383606890
O	O	0.1211812379228903	0.5113021642940367	0.8588733664483641
O	O	0.1005653010761094	0.2429489201253574	0.1196942583418377
O	O	0.0712760759760229	0.2290554171826713	0.6232323163641453
O	O	0.8596532448908931	0.4799583729658394	0.1218341954220818
O	O	0.8429069780786520	0.4978020139939687	0.6197019319149391
O	O	0.2179381698982894	0.2222059980586053	0.2609878393208476
O	O	0.1932232845026931	0.1871196963739337	0.7542182712002585
O	O	0.7566709607807383	0.7841818149006201	0.9930613848502290
O	O	0.8004015562288487	0.8142356048174690	0.4888489184786522
O	O	0.7998726120118533	0.7667085952226742	0.2510871649890873
O	O	0.7900080444396380	0.7725094188051216	0.7385142004580274
O	O	0.2287148845281024	0.2286009513466922	0.9894167569466461
O	O	0.2108854965253286	0.2277827888205266	0.5017319426665807
O	O	0.5044499706784364	0.0141820785009799	0.0041722084432365
O	O	0.4871410162466248	0.9989224201166991	0.5203229818652062
O	O	0.9923957138720212	0.5075018701476210	0.9914050652392064
O	O	0.9691625027077038	0.5226587180147533	0.4803031991390228
O	O	0.4957959749534027	0.9901847392730616	0.2482906899401200
O	O	0.5077246460724609	0.0083576796386069	0.7500353600596199
O	O	0.9949514693103296	0.4609141832461532	0.2459219054413495
O	O	0.0049253598564221	0.4871655680837819	0.7149266024864644
O	O	0.0952637757050212	0.9165986331156546	0.1012746323184359
O	O	0.1058290187576389	0.8887253482903574	0.6085894107359309
O	O	0.2894061724051227	0.7000707843750504	0.1199773935072628
O	O	0.3070777409868271	0.6891915163985374	0.6217483742974252
O	O	0.8872794136202558	0.1242608044381583	0.3442438826818091
O	O	0.8847659699942767	0.0930336523577395	0.8915287633463436
O	O	0.7036516263571784	0.2887704669996793	0.3530439612079590
O	O	0.6989346251997404	0.3043218056195656	0.8634587242226814
O	O	0.3367243095831676	0.5361648899998005	0.2887659057649531
O	O	0.5156722749684955	0.6670972352192974	0.3186318849675635
O	O	0.3874615972231175	0.5968368375061681	0.4651974343967906
Si	Si	0.5021333242156842	0.1285149362781155	0.0320273872618131

Si	Si	0.7194587565903134	0.8813167657194754	0.0403594134061862
Si	Si	0.7532099342222409	0.9095984547742262	0.5244660180235385
Si	Si	0.2542419504746931	0.1149369634789679	0.2813441510597841
Si	Si	0.2571685151344596	0.0985777351726398	0.7763905556511830
Si	Si	0.8903405008017558	0.5017602134302805	0.2251881448748918
Si	Si	0.8898937118845893	0.5061613488877512	0.7181939445612571
Si	Si	0.1272468395149176	0.2751677752305284	0.2219619946219566
Si	Si	0.1008423518435890	0.2447551063039910	0.7265114943411248
Si	Si	0.1048139965635357	0.4918303184263948	0.9645238349987508
Si	Si	0.8789411216860472	0.7351139948227825	0.4768849755066995
Si	Si	0.8618927491971817	0.7407168014562018	0.9818599015915481
Si	Si	0.5185257963685572	0.8950316225867638	0.4943560544915115
Si	Si	0.5084531539527433	0.8961864491090950	0.9951266348981989
Si	Si	0.2680097972748641	0.1316445246970233	0.4863767083551096
Si	Si	0.2828633477375107	0.1292420158320198	0.9809099410827358
Si	Si	0.4808038551853997	0.1036234507974285	0.2357811493814239
Si	Si	0.4835445595258818	0.1186112801637123	0.7415076803024405
Si	Si	0.7474006798586714	0.8667903197715034	0.2378037558678443
Si	Si	0.7471957458382903	0.8765861941606587	0.7258907751968664
Si	Si	0.1134972987505094	0.4882768829083517	0.2563039978485051
Si	Si	0.1133162490580446	0.4746168105903124	0.7555069970954449
Si	Si	0.9063829575871054	0.7330428036853434	0.2738908877347654
Si	Si	0.8910718549241210	0.7322458032276415	0.7760054077080838
Si	Si	0.8779943940821795	0.5135331437059349	0.0192808216448981
Si	Si	0.8567404178272255	0.5189788961785808	0.5129272254763748
Si	Si	0.1235301029378419	0.2656949848243855	0.0152935779973902
Si	Si	0.2008068525330131	0.9728405520622161	0.1331497974471745
Si	Si	0.2121021002117871	0.9539082244963524	0.6252706962142796
Si	Si	0.3497872341189350	0.8114548735111171	0.1296756840707758
Si	Si	0.3686442723005072	0.7973022548424140	0.6312618492017137
Si	Si	0.7944533872449071	0.0443760619019216	0.3681849149160072
Si	Si	0.7749881066336002	0.0342716708369082	0.8852820830387174
Si	Si	0.6327638016837369	0.2003112228895958	0.8816871578199965
Si	Si	0.0328398123837133	0.8090054238935735	0.1154790290940682
Si	Si	0.0437814653352859	0.7824994612199561	0.6303053557279839
Si	Si	0.1774246320653958	0.6442924639438772	0.1052674848812387
Si	Si	0.1988863621953740	0.6258098787654021	0.6181754074580894
Si	Si	0.9595456871973127	0.2232956852145449	0.3680142277968770
Si	Si	0.9542138210982287	0.1977336405031878	0.8811545613427114
Si	Si	0.7977059639002277	0.3688777939036498	0.3735440539304662
Si	Si	0.8081207709526907	0.3642747547432421	0.8734034148995633
Si	Si	0.1029673379309912	0.2619130058475321	0.5213869408534819
Si	Si	0.6341194622726221	0.1865622753121201	0.3745312096109856
Al	Al	0.0873014649855790	0.4929931191496664	0.4707208693939506
Al	Al	0.5156515316117236	0.8712747326200585	0.2768835871358561
Al	Al	0.5078432502477312	0.8873486984951739	0.7825297398974698

Al	Al	0.4942540999063780	0.1260221453092782	0.5236604112269561
Cu	Cu	0.2764449824745184	0.5570306059251534	0.4043115214945632
Cu	Cu	0.4597359284837614	0.7036255914366532	0.4213294987428318
Cu	Cu	0.4013330353187967	0.6565583430084471	0.2512396144095604
C	C	0.4014317707642346	0.4211995694692819	0.1757911390359785
H	H	0.5828846053450523	0.2162822568613492	0.6425394428197770
H	H	0.5979419543458020	0.7860507526219870	0.6930857185870142
H	H	0.3331410744049262	0.3814374027350596	0.1497881149132213
H	H	0.4402615849275487	0.4759413087003515	0.1309432865305226
H	H	0.3635767176744307	0.4755050931587856	0.2467647916677810
H	H	0.4482006599232594	0.3782249533876033	0.2152587190430086

F. O(2) Final geometry ([Cu_3(μ-OH)(μ-$O)_2$]-MOR + CH3)

data_POSCAR
_cell_length_a 13.647600
_cell_length_b 13.647600
_cell_length_c 15.015100
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000
_cell_angle_gamma 97.178902
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

O	O	0.1844586317926865	0.0303692357813476	0.2247052211496731
O	O	0.2130038241754736	0.9968437374771453	0.7270956320261144
O	O	0.4247782224630292	0.7976679721402986	0.2119498693267245
O	O	0.4246426173154884	0.8073332012169006	0.7246382630822216
O	O	0.6338187560060632	0.8855827374317340	0.5153479634146459
O	O	0.5996805386681083	0.8606342279001270	0.0499215908065747
O	O	0.7975094576786065	0.0086706777405424	0.4721855859999929
O	O	0.7477352761341318	0.9776096003987560	0.9773160542530828
O	O	0.6001637732893806	0.1862663590042329	0.4762990535001962
O	O	0.5936104278545604	0.1952290694904364	0.9834747685198819
O	O	0.3652859551443139	0.1193421033066016	0.2440877292421198
O	O	0.3692161389621364	0.1315070192310335	0.7373749453904191
O	O	0.9407289173042853	0.8009375072194894	0.0484137322443614
O	O	0.9640331026920794	0.7551633217442726	0.5521086498801968
O	O	0.1818660310787535	0.5729446022806588	0.0195329653773730

O	O	0.1803397983055418	0.5780304700443532	0.5196619409871700
O	O	0.1651590314008072	0.3944558152170593	0.2262500582067234
O	O	0.1311585361336018	0.3600411858835464	0.7531864472325690
O	O	0.0298137325757050	0.2483148148393602	0.2817991119658088
O	O	0.0043167695686026	0.1988112453920158	0.7834735051497409
O	O	0.8073961801787339	0.4431947774299523	0.2883952738474400
O	O	0.8284830338351122	0.4232266392370063	0.7809393813240931
O	O	0.8492600933288407	0.6237234264508005	0.0045280933861780
O	O	0.8170929543686040	0.6256724724811866	0.4915828716293200
O	O	0.8020316196232141	0.9504203374025670	0.3039192739472739
O	O	0.7725819238738727	0.9538803731468065	0.8043293356037796
O	O	0.5396730704290240	0.1791013607629464	0.3078219457569136
O	O	0.5413844834053452	0.1945710991054715	0.8118994245198353
O	O	0.3998443728499487	0.1631367360148197	0.9947307381533828
O	O	0.3836260896721719	0.1651062460583603	0.4997918263786524
O	O	0.2429370549880538	0.0479005218622669	0.0540433966021515
O	O	0.2254824613788164	0.0436418794731698	0.5546157533913396
O	O	0.4065291193293951	0.8367455021369348	0.0349078981129007
O	O	0.4524988765464428	0.8026807164733283	0.5492412866276086
O	O	0.6326894994391355	0.8433383279244939	0.2568222555687756
O	O	0.6231482957947988	0.8436211740170296	0.7283154061586529
O	O	0.0222544335040502	0.2007440287035101	0.4557005758074705
O	O	0.0360413045698845	0.2032999698614100	0.9595087102457559
O	O	0.7820060505507913	0.4314992719766270	0.4638104134679931
O	O	0.8070370695925918	0.4389129923107542	0.9568242838263203
O	O	0.9032808552952576	0.6183520581452444	0.2448337281924660
O	O	0.8802830198192294	0.6147053992881447	0.7618425196471577
O	O	0.9976828910239175	0.7953410898715882	0.2186195660512933
O	O	0.9864323971093548	0.7902651995151995	0.7251201032503877
O	O	0.1474719788431686	0.5848813139131901	0.1961865501407558
O	O	0.1940405356474448	0.5407521313698178	0.6956777318254310
O	O	0.1054912560639885	0.3780350079948750	0.5079792808581310
O	O	0.1295842775921947	0.3831920636274848	0.9909957407698876
O	O	0.2768645620402573	0.8922301895025256	0.1510788272072935
O	O	0.2995629246814137	0.8841480382604694	0.6132813076024072
O	O	0.6921301024557591	0.0907952906943840	0.3515443073495692
O	O	0.6957526430997368	0.1084940246620488	0.8602849748535351
O	O	0.1032618093954143	0.7245332970526550	0.0871831119946096
O	O	0.1143353015129755	0.6967126804458905	0.6406366758666577
O	O	0.8975470819854539	0.3154104129457170	0.3866677587137148
O	O	0.8907233291166887	0.2902199757582819	0.8910709591546554
O	O	0.2440602177551191	0.0872764090076090	0.3855517961659720
O	O	0.2618826195567971	0.0799373869354857	0.8822508762102711
O	O	0.4906495540953910	0.8544596647950656	0.3934958306984788
O	O	0.5186358643664485	0.8687709285475356	0.8907368963481521
O	O	0.7701323109877923	0.9045855601301540	0.1353507472705608

O	O	0.7777085836221950	0.9271588333245968	0.6304055415851445
O	O	0.5168022581109822	0.1455248924398840	0.1372803581786384
O	O	0.5277370732128418	0.1657633630855005	0.6401194566844045
O	O	0.9316215751710426	0.7461548512941203	0.3799162437685003
O	O	0.9034991545086094	0.7590147702326615	0.8809810478787162
O	O	0.1338370161815688	0.5162519957784650	0.3620828815129550
O	O	0.1204080096817183	0.5127360796521374	0.8588860269265846
O	O	0.1018633515606067	0.2457825642017203	0.1198613455092232
O	O	0.0712837178877977	0.2292740357577033	0.6233809681544257
O	O	0.8579137481175655	0.4806566775012148	0.1216728038761233
O	O	0.8390823973118533	0.4980205451813597	0.6214001209659993
O	O	0.2181061797663949	0.2219414209831631	0.2609729830148149
O	O	0.1946586048909623	0.1885625884249369	0.7532955972312467
O	O	0.7570516523368737	0.7835462412176610	0.9928252843193097
O	O	0.8000778585342326	0.8139843000389333	0.4882477704038092
O	O	0.8012438558151327	0.7668392641324767	0.2508689225494125
O	O	0.7910614085183484	0.7729537564992547	0.7382876615370931
O	O	0.2286132996388757	0.2289594811400492	0.9886380059937779
O	O	0.2111638179337759	0.2277580999241312	0.5017961859609062
O	O	0.5035287860337242	0.0132158055009043	0.0051807992226962
O	O	0.4874474646477943	0.9990965286242379	0.5207726615189028
O	O	0.9935135692067983	0.5083298321174441	0.9930138336003724
O	O	0.9674775144774409	0.5223861668791042	0.4853180786771583
O	O	0.4972994370136012	0.9916126662666750	0.2487504546001912
O	O	0.5102755616670260	0.0093589075305957	0.7466575712991831
O	O	0.9943428245394648	0.4590352837281279	0.2427789462219915
O	O	0.0037918167782480	0.4873642973795034	0.7147221184856966
O	O	0.0948138576099820	0.9167544163489723	0.1011493827780942
O	O	0.1059613093817860	0.8886498113961389	0.6082244814087355
O	O	0.2909577861676976	0.6995502791395706	0.1230561524489766
O	O	0.3065293919362178	0.6892370739765823	0.6231100509480562
O	O	0.8874172613510110	0.1241851345543243	0.3448714140116601
O	O	0.8849495583274606	0.0930657265372419	0.8922948333999851
O	O	0.7042785029154863	0.2886528057652827	0.3527430929156202
O	O	0.6989992773086978	0.3038076727297945	0.8642935498869586
O	O	0.3224126728970960	0.5398082745923278	0.2892310598613552
O	O	0.4945477124959473	0.6665057492442416	0.3279474885828723
O	O	0.3875652074710527	0.6007880610130096	0.4655231475443389
Si	Si	0.5018680864888272	0.1279535449509037	0.0321701742651323
Si	Si	0.7191491793078698	0.8805444946909203	0.0396039308239869
Si	Si	0.7530157802468885	0.9092235820426152	0.5242592143791427
Si	Si	0.2542495881745108	0.1147342603892121	0.2810006981735391
Si	Si	0.2576929586857040	0.0993425884731495	0.7756517977489295
Si	Si	0.8901856694266819	0.5014880243669136	0.2246855001235400
Si	Si	0.8888514282891025	0.5067111935255869	0.7188087884149307
Si	Si	0.1280557638523069	0.2763181127314456	0.2226460082156260

Si	Si	0.1008444913569518	0.2446182634695274	0.7266829522220232
Si	Si	0.1056978352078100	0.4930021958242951	0.9648112410839159
Si	Si	0.8786289392912285	0.7346844555444000	0.4770810463642370
Si	Si	0.8623366036939617	0.7403295536448189	0.9818751847982142
Si	Si	0.5187253768585464	0.8953487760557188	0.4941575681854239
Si	Si	0.5079192118217797	0.8955627595923216	0.9934499155572679
Si	Si	0.2681481579672528	0.1316609584171177	0.4856044849302500
Si	Si	0.2827463553574303	0.1297127874898672	0.9803584052058071
Si	Si	0.4811129663493249	0.1045350154891197	0.2356724161767667
Si	Si	0.4847442883427884	0.1193775210116835	0.7403618221891549
Si	Si	0.7475161555557276	0.8661956693919644	0.2376013031626746
Si	Si	0.7483128605700567	0.8770241352750339	0.7252271538504030
Si	Si	0.1122119133538746	0.4890359347537764	0.2573013278863977
Si	Si	0.1119163699771745	0.4746648520939859	0.7559564564116442
Si	Si	0.9074974660626486	0.7327249433736268	0.2741808646687491
Si	Si	0.8918428804915922	0.7327270117670873	0.7764886888103135
Si	Si	0.8784974163811237	0.5134627330541996	0.0192835888093141
Si	Si	0.8541930835894270	0.5184333610731108	0.5147923630535944
Si	Si	0.1240080220372146	0.2667296202542723	0.0150740745436887
Si	Si	0.2006600672006011	0.9731341553858114	0.1322657996274962
Si	Si	0.2121269959765289	0.9541993302854467	0.6249871492453714
Si	Si	0.3508318766052356	0.8122328396136457	0.1283495004886393
Si	Si	0.3686111843938914	0.7973059113202945	0.6311447381036377
Si	Si	0.7943659684396078	0.0441317742019737	0.3677649642457628
Si	Si	0.7754070913912601	0.0340569520796912	0.8851058494794084
Si	Si	0.6330306197146567	0.1995342711856549	0.8820277720203930
Si	Si	0.0337143652262016	0.8084652865558405	0.1153876454305498
Si	Si	0.0436480142456852	0.7826984993498665	0.6303337101190191
Si	Si	0.1787212522836637	0.6443573832053522	0.1057378759008396
Si	Si	0.1987009790238048	0.6257989147714472	0.6188104057082231
Si	Si	0.9598593746468251	0.2233102247473436	0.3679702174918051
Si	Si	0.9543885215223868	0.1976653769924312	0.8812495047266035
Si	Si	0.7979900944521786	0.3688842393943333	0.3736469069153635
Si	Si	0.8080251945505201	0.3640904828389788	0.8735312235306880
Si	Si	0.1033576154660097	0.2620870477453893	0.5216143239698476
Si	Si	0.6345299010361986	0.1865587766167866	0.3738674806064900
Al	Al	0.0844836591775683	0.4924644077175456	0.4718123922749426
Al	Al	0.5167858516597088	0.8729820979271349	0.2768042539442933
Al	Al	0.5094943774993268	0.8885992501285337	0.7797420875674117
Al	Al	0.4945391263569502	0.1262453235155117	0.5232342733443992
Cu	Cu	0.2712991077484496	0.5648433076525038	0.4087700272417908
Cu	Cu	0.4513001087590216	0.7130685150345941	0.4291736663070178
Cu	Cu	0.3901948456963860	0.6590129598225530	0.2488506874967022
C	C	0.4132272188612200	0.3837865266481851	0.1362713564751885
H	H	0.5828892784146581	0.2186322673816392	0.6412920868770857
H	H	0.6006976634296581	0.7820029044106701	0.6969710049008295

H	H	0.3357667529726495	0.3553891411442996	0.1282749437454284
H	H	0.4474206139317024	0.4395653040427200	0.0903898919517197
H	H	0.3695129437767901	0.4915008437299087	0.2943171617734073
H	H	0.4579643205289970	0.3506301096405900	0.1850751076882923

G. O(3) Initial geometry ([Cu_3(μ-O)$_3$]-MOR + CH4)

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_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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O	O	0.1832791687147079	0.0326819572708668	0.2246351180998296
O	O	0.2151452783848418	0.9971614026035822	0.7268520462498296
O	O	0.4243326991481461	0.7940164753429400	0.2169729651102900
O	O	0.4242741411075877	0.8086033089397540	0.7256355529856824
O	O	0.6350644995049886	0.8871872627752762	0.5119029514754928
O	O	0.6014867810030954	0.8572707144063243	0.0480031235263865
O	O	0.7999545484847413	0.0089563688668338	0.4713862382775632
O	O	0.7505485368708411	0.9761988939819765	0.9777502878220917
O	O	0.6014250462523697	0.1872082741128533	0.4776272759529761
O	O	0.5942704030162222	0.1978997643847895	0.9831788829747637
O	O	0.3643286228122556	0.1205780034523987	0.2441319495985478
O	O	0.3698980083183034	0.1339378245542403	0.7400251375488121
O	O	0.9411992081495757	0.8036372064739343	0.0472558857114590
O	O	0.9654282467164652	0.7546308171136703	0.5511177492483282
O	O	0.1814084751158453	0.5723991660240176	0.0198434564331197
O	O	0.1822681606165348	0.5748258099022776	0.5189121266212681
O	O	0.1676149430887354	0.3968257586539810	0.2279045040772483
O	O	0.1306819134166807	0.3603022724364640	0.7510181106790398
O	O	0.0302327733413824	0.2513237504021431	0.2823502790149697
O	O	0.0052594018735884	0.1984569629543287	0.7839937029434564
O	O	0.8085111103566192	0.4423335249727917	0.2882754869192999
O	O	0.8308036333558055	0.4234469009165665	0.7811385965015317

O	O	0.8535810308371123	0.6239526031671145	0.0050698839831755
O	O	0.8166516200052754	0.6261893529526060	0.4919655087878944
O	O	0.8008139575070291	0.9501271137887524	0.3031516064609359
O	O	0.7767113478002770	0.9553379565721618	0.8044621115709247
O	O	0.5384169736654545	0.1783219313989738	0.3105320789104895
O	O	0.5440499891515945	0.1966153274557715	0.8110319549710083
O	O	0.4010280726210554	0.1594403528648431	0.9927765113227085
O	O	0.3836740661533491	0.1654606543727019	0.4999236078818765
O	O	0.2456178413287017	0.0444727042082333	0.0546954738069928
O	O	0.2260805063736925	0.0433536524259336	0.5544646596655840
O	O	0.4089572839568248	0.8412285474899931	0.0411748450451405
O	O	0.4560995908783457	0.8051267811256301	0.5512161885519186
O	O	0.6309009767993378	0.8442856532425985	0.2554502972575409
O	O	0.6237546700845029	0.8452877517976061	0.7321046711591613
O	O	0.0214635830180388	0.1981402221939071	0.4548400016583177
O	O	0.0388414671809909	0.2024187625200084	0.9599198536802392
O	O	0.7818570374066331	0.4320316169802465	0.4634671820581657
O	O	0.8074761780292874	0.4396386423778916	0.9567666194518479
O	O	0.9029233349635726	0.6179953448661529	0.2448432733832371
O	O	0.8791740586493964	0.6151275057955993	0.7610662812367101
O	O	0.9946440073409720	0.7961800693122452	0.2181941959706758
O	O	0.9886205303831312	0.7882132107813622	0.7242404125519402
O	O	0.1484186175823524	0.5861764427791597	0.1966137770556249
O	O	0.1954083136514978	0.5406659851037260	0.6948636851337608
O	O	0.1029428627454041	0.3755734097953033	0.5073389745871276
O	O	0.1329414237485718	0.3823258068651947	0.9889137004758176
O	O	0.2783081951542575	0.8923608644076377	0.1578463219302179
O	O	0.2997615439574131	0.8832734983005991	0.6124913039881418
O	O	0.6919490016356876	0.0906551889020254	0.3521525993195115
O	O	0.6942142625514969	0.1056729938583976	0.8619176682366688
O	O	0.0995977687596863	0.7222487646005203	0.0876728779141289
O	O	0.1168802754392923	0.6963529993149397	0.6367999477838876
O	O	0.8972995919516304	0.3149287725132163	0.3880899371629973
O	O	0.8960813915713499	0.2934326378559975	0.8923205841430067
O	O	0.2439337960683554	0.0877517132077251	0.3855017718441046
O	O	0.2594801683013879	0.0793814194188519	0.8828091213397772
O	O	0.4912870772995435	0.8552789653495665	0.3916835985513032
O	O	0.5139810994991590	0.8730712999533400	0.8924077887940233
O	O	0.7707116670164849	0.9016530474135760	0.1349184068374304
O	O	0.7756354561620937	0.9288124954637942	0.6306130796037487
O	O	0.5161907414530447	0.1533018398901159	0.1383497354867169
O	O	0.5269877436876181	0.1676244466436138	0.6397891945286345
O	O	0.9309669660963182	0.7460419714350401	0.3796986498581706
O	O	0.9053911213230624	0.7588498283641626	0.8802186065328651
O	O	0.1332379516337017	0.5174342700438211	0.3634524627350027
O	O	0.1216388890371127	0.5126641107800204	0.8581882535806732

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O	O	0.0700835946577421	0.2275851140854286	0.6230967016722063
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O	O	0.1950941402132169	0.1888269377112198	0.7526083536001382
O	O	0.7582304414413084	0.7816533942954873	0.9912007586481479
O	O	0.8011580039527143	0.8145902749324869	0.4898039560721833
O	O	0.7983971897106743	0.7652088136948906	0.2527383800720852
O	O	0.7928979774246542	0.7748184025412460	0.7374430213849854
O	O	0.2305384474825826	0.2270751913446103	0.9924909786916507
O	O	0.2105735965732532	0.2272376900320764	0.5020909950331319
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O	O	0.4879762430673492	0.0000054771600480	0.5182482239579352
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O	O	0.3093718573773723	0.6889202660375254	0.6218112089665806
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Si	Si	0.7206540485634039	0.8783752169944293	0.0385591044276278
Si	Si	0.7536853320968787	0.9102801289599062	0.5241451603590894
Si	Si	0.2534959166911330	0.1165152082669455	0.2811215586853383
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Si	Si	0.1072520270901711	0.4918483451628606	0.9642537717803326
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Si	Si	0.2682931359722639	0.1316322114435236	0.4855748215413412

Si	Si	0.2832871571341877	0.1273247167227586	0.9812141157180519
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Si	Si	0.4854193113499670	0.1217750544062741	0.7404652750702673
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Si	Si	0.1134611199944407	0.4906801797782910	0.2573226247963434
Si	Si	0.1124092186796198	0.4751343151543840	0.7552170832253861
Si	Si	0.9056959198355026	0.7323366243188332	0.2741374763120870
Si	Si	0.8928410214743968	0.7331566024603373	0.7757388617195785
Si	Si	0.8805524223484184	0.5127858029665984	0.0192141661667846
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Si	Si	0.1260167667906931	0.2665625992979677	0.0161362428611462
Si	Si	0.2022523632081799	0.9723044168221315	0.1345975238428853
Si	Si	0.2131057689430611	0.9539602738821426	0.6248994466656952
Si	Si	0.3508748460509756	0.8112057405503321	0.1325420852990348
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Si	Si	0.1785513455505937	0.6451115806366763	0.1053318110934209
Si	Si	0.2017986063801409	0.6255119820645066	0.6180473662864826
Si	Si	0.9595263150508039	0.2231801184937298	0.3673456887163234
Si	Si	0.9564884826481957	0.1984724033079776	0.8822283301307710
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Al	Al	0.5162880929589926	0.8779401751552188	0.2752761882079347
Al	Al	0.5079818268356646	0.8912531585151031	0.7809462255831062
Al	Al	0.4948907000203653	0.1267797283032286	0.5230001646575526
Cu	Cu	0.2636097476811626	0.5680478881649602	0.4092498543131262
Cu	Cu	0.4609954786767832	0.7098536791074446	0.4241974819080183
Cu	Cu	0.4067128310729998	0.6570637930691970	0.2648136466437158
C	C	0.4776942512332318	0.4940387295112829	0.6414632685023561
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H	H	0.6011248294533936	0.7824427720256608	0.7027770390070792
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H	H	0.5154750534542177	0.5545842706421406	0.6816276872786814
H	H	0.5289537388254871	0.4400157123316232	0.6277597047906464

H. O(3) Transition state ([Cu_3(μ-$O)_3$]-MOR•••CH4)

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_cell_length_c    15.015110
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_cell_angle_beta     90.000000
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+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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  O    O  0.2140144450280062  0.9974433053878684  0.7272313066786040
  O    O  0.4238176202743915  0.7927477002847851  0.2183083771161236
  O    O  0.4243247012595717  0.8079051783077986  0.7259648267773429
  O    O  0.6339517270551767  0.8863439388559087  0.5131249106306015
  O    O  0.6009068110388540  0.8588915140743865  0.0491244038536109
  O    O  0.7988681184397848  0.0085304206891692  0.4718754534028378
  O    O  0.7488666803829744  0.9768390340067938  0.9775116257921823
  O    O  0.6010875911586595  0.1859484374809384  0.4775544272797134
  O    O  0.5936683901823301  0.1968486158063882  0.9832623978981800
  O    O  0.3649145818003703  0.1190900603373564  0.2446215300804440
  O    O  0.3699767159091039  0.1321860624611659  0.7388627038837825
  O    O  0.9413182038170689  0.8035272930414692  0.0478118645776533
  O    O  0.9641179186990811  0.7560305163480194  0.5521115943462505
  O    O  0.1821062008437977  0.5720383756867022  0.0204248522030497
  O    O  0.1852658504149005  0.5733852031757962  0.5220006915600734
  O    O  0.1679645139814667  0.3970308766985298  0.2291698532398172
  O    O  0.1314740191186772  0.3604955498842202  0.7522006416425810
  O    O  0.0318622908862025  0.2506978550622279  0.2842634059516982
  O    O  0.0059573824142092  0.1985119810487461  0.7854050781875230
  O    O  0.8088754528220932  0.4419500386697379  0.2882565639779529
  O    O  0.8297862039571484  0.4233931736992673  0.7808265311051272
  O    O  0.8520423472329242  0.6244563961221772  0.0058926534444055
  O    O  0.8178578246795922  0.6259432437682051  0.4916029880050559
  O    O  0.8012630091002890  0.9501794493195490  0.3035933079267252
  O    O  0.7750873858954392  0.9555827715164611  0.8044137937004905
  O    O  0.5390004198115648  0.1777644320902141  0.3098827571744280
  O    O  0.5432520515135764  0.1956874361749854  0.8109372955464949
  O    O  0.4004830289552999  0.1625472546330968  0.9937177902302778
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O	O	0.3836016345094961	0.1654936219897536	0.5002622586564272
O	O	0.2456799648580628	0.0455956161018349	0.0548678043282251
O	O	0.2257794756062168	0.0433141449916477	0.5545179028375884
O	O	0.4090494193474612	0.8396576979092529	0.0414256903258163
O	O	0.4553656938427650	0.8026281147211591	0.5516263606183998
O	O	0.6314481531849339	0.8433141715621844	0.2571160270125148
O	O	0.6237055750539895	0.8445313714709854	0.7314892661125327
O	O	0.0215715436572523	0.1991262842251231	0.4570822583760332
O	O	0.0367497074093919	0.2035265451539345	0.9616935075554096
O	O	0.7840482408708311	0.4323828072450624	0.4638448464384339
O	O	0.8079212964151949	0.4402053434743252	0.9569207799820205
O	O	0.9026538214564397	0.6183400931054237	0.2455236255033668
O	O	0.8791004103585252	0.6148819975244564	0.7618617034121939
O	O	0.9963070722229475	0.7958972831858162	0.2183274787848006
O	O	0.9882163037060181	0.7883750017773608	0.7253606758667388
O	O	0.1502172521478471	0.5862325912580104	0.1976717967266310
O	O	0.1960152891435172	0.5417163123989468	0.6975949554861671
O	O	0.1040751877610404	0.3764395805191398	0.5095630887940175
O	O	0.1315654166925171	0.3826813960104047	0.9901844729975053
O	O	0.2793621782198130	0.8928879857902174	0.1572378658428448
O	O	0.2999806407372105	0.8841635587182779	0.6131944985388174
O	O	0.6935958263340183	0.0918967036108569	0.3519414880241953
O	O	0.6955284069531373	0.1079762050486863	0.8612711089950125
O	O	0.0998121900788931	0.7213419165310384	0.0875039628888885
O	O	0.1152906472404496	0.6959554286085279	0.6373889477094536
O	O	0.8968001209770549	0.3138358345289802	0.3879950253208264
O	O	0.8932116092496543	0.2920396341995755	0.8915800577756414
O	O	0.2437315337653487	0.0880653855695925	0.3856676099446332
O	O	0.2610891732660221	0.0795542262137516	0.8830460265051556
O	O	0.4897380347779574	0.8519752057925558	0.3930374917729367
O	O	0.5151005038650851	0.8708346688422282	0.8926061291601073
O	O	0.7699107992349354	0.9028688910294917	0.1354039873319692
O	O	0.7757453023015159	0.9279705625285715	0.6304969389431605
O	O	0.5161817881400808	0.1496644643151797	0.1379686809304275
O	O	0.5270638827653400	0.1664005556702719	0.6396665389404532
O	O	0.9315601404945539	0.7469250923636963	0.3799091578424409
O	O	0.9045032333494092	0.7590026295536774	0.8808573219993576
O	O	0.1372368605620125	0.5177462492262705	0.3651364539022737
O	O	0.1214382757874688	0.5126297717445141	0.8592880677135639
O	O	0.1021509800680107	0.2491585725280672	0.1220328319813859
O	O	0.0706608746649238	0.2276433051841735	0.6248118950860331
O	O	0.8615967396261368	0.4801316096472519	0.1223082580461963
O	O	0.8402446872679619	0.4984638276324205	0.6212522445385815
O	O	0.2194900424247592	0.2239361819138779	0.2619850541141062
O	O	0.1961569924688007	0.1895273142072824	0.7538357508702873
O	O	0.7577729538533688	0.7825832019887642	0.9919718707233471

O	O	0.7996803747757113	0.8137603934312239	0.4891650324431325
O	O	0.7998798581384321	0.7660987815137972	0.2520446684198632
O	O	0.7924838977257522	0.7745452562816411	0.7379292674279654
O	O	0.2290765362878489	0.2274795800093727	0.9914853558871997
O	O	0.2109064346592575	0.2274512899114285	0.5033062273168056
O	O	0.5073696786436557	0.0145648600151773	0.0086313915701055
O	O	0.4866353920057236	0.9986039634348742	0.5188315228986724
O	O	0.9944445027871467	0.5071191634562169	0.9923098237060586
O	O	0.9699698826376206	0.5245719008802396	0.4864902500750929
O	O	0.4977813793434009	0.9925992350715802	0.2460503318983811
O	O	0.5110921103179464	0.0100234805445467	0.7462605593496434
O	O	0.9970277589923668	0.4616430377882850	0.2467123672091418
O	O	0.0050157317870330	0.4895300424574103	0.7147363921273566
O	O	0.0978083876663476	0.9150788487979256	0.1020062348382282
O	O	0.1065554156387023	0.8884861425213586	0.6090537127984206
O	O	0.2895908774268818	0.7019496419936644	0.1189559499171011
O	O	0.3084757974688301	0.6894387420221406	0.6229572749700694
O	O	0.8891172927633022	0.1233559737851380	0.3438405761072332
O	O	0.8851042161122535	0.0946237487981421	0.8940592514565822
O	O	0.7032968365647818	0.2894466236153974	0.3539429826765002
O	O	0.7011857933274825	0.3036549188576672	0.8643830355719118
O	O	0.3259158973277124	0.5554890587550525	0.3022355289540913
O	O	0.5249292273885531	0.6604305568721378	0.3343596465241099
O	O	0.3951969490460839	0.5843206309979533	0.4720489999788683
Si	Si	0.5025538239794543	0.1293587586968883	0.0329282753452205
Si	Si	0.7199868226282433	0.8792971494384290	0.0390785450200113
Si	Si	0.7528153396012698	0.9096119953678254	0.5241216731969658
Si	Si	0.2540567086520085	0.1163478974990255	0.2811162329914865
Si	Si	0.2583033716599274	0.0996385024465596	0.7766766112809620
Si	Si	0.8920997976824836	0.5014168025573298	0.2257490932012942
Si	Si	0.8894739464292343	0.5073280571513195	0.7188798880854392
Si	Si	0.1298271648626752	0.2792501417419189	0.2247003121057105
Si	Si	0.1014376360311573	0.2444234295320342	0.7276715176985817
Si	Si	0.1069041840029570	0.4924164524287207	0.9653180628775786
Si	Si	0.8787250541000304	0.7352466930195760	0.4769963388655682
Si	Si	0.8637646323622263	0.7407397177069655	0.9819575116786012
Si	Si	0.5181385694794045	0.8945784930094476	0.4925644853444879
Si	Si	0.5083871217316513	0.8965094355491274	0.9960555173256864
Si	Si	0.2681650783163647	0.1316811000476932	0.4856468155937037
Si	Si	0.2831605015286272	0.1285293803891889	0.9813760470960204
Si	Si	0.4807259666283983	0.1058993556663168	0.2356784624008981
Si	Si	0.4854923753264728	0.1200640032851013	0.7403117263996108
Si	Si	0.7465575878763602	0.8655027426884558	0.2378306868252480
Si	Si	0.7488740196533854	0.8783650272119914	0.7259698136564765
Si	Si	0.1153420369163598	0.4917235441934480	0.2599230440382740
Si	Si	0.1123938352377465	0.4750807430799000	0.7565553388059101

Si	Si	0.9068398575984489	0.7328715175547131	0.2741503983724201
Si	Si	0.8923522674148643	0.7329487264190604	0.7764993554342396
Si	Si	0.8803700054684285	0.5137260132869699	0.0198104579086262
Si	Si	0.8561613285547196	0.5193736265767228	0.5147289128874348
Si	Si	0.1251787277611953	0.2670458992930307	0.0171800751362881
Si	Si	0.2028051713151129	0.9723941395244609	0.1344282785575786
Si	Si	0.2125325846865564	0.9544105112865040	0.6252600628776577
Si	Si	0.3513161794231010	0.8105661502475101	0.1333588717092695
Si	Si	0.3697256777409663	0.7983047008546649	0.6315902862564400
Si	Si	0.7953892614437663	0.0442048280908693	0.3673998474163369
Si	Si	0.7761733949956593	0.0346908721312289	0.8860535712097146
Si	Si	0.6339416500034929	0.2000651360853425	0.8821218580333934
Si	Si	0.0339063048853774	0.8081248809187045	0.1153665597657252
Si	Si	0.0442625152822274	0.7823415211820333	0.6299512705934660
Si	Si	0.1793212942630120	0.6446660804358473	0.1059181327990544
Si	Si	0.2008015299799979	0.6256316732788321	0.6198291098890465
Si	Si	0.9603784130744941	0.2228366415584375	0.3687665542196967
Si	Si	0.9556053097766295	0.1984002490981851	0.8828992328624281
Si	Si	0.7981092117573354	0.3685112732702507	0.3739415524857890
Si	Si	0.8097168625218600	0.3649760213450719	0.8738850624247050
Si	Si	0.1025023011367239	0.2603099216618574	0.5231051376444569
Si	Si	0.6345945727104407	0.1864979900848525	0.3747608042198323
Al	Al	0.0855655095038728	0.4913445037864079	0.4731258648846861
Al	Al	0.5160474711200891	0.8750509674325215	0.2773193335815662
Al	Al	0.5086494926618457	0.8897358065760059	0.7814502783584771
Al	Al	0.4944712013743953	0.1258552881851003	0.5227869710170125
Cu	Cu	0.2727969464474511	0.5604009261151582	0.4137598172585161
Cu	Cu	0.4699558126242559	0.7043449982660331	0.4370548055272525
Cu	Cu	0.4121900476863207	0.6570666845026873	0.2714290195968322
C	C	0.4627753368812995	0.5079081514601007	0.6138099594539922
H	H	0.5848117741731969	0.2163832192618358	0.6401054167493214
H	H	0.6014161057297258	0.7827215620838288	0.7005110206070668
H	H	0.3962125452081465	0.4696694532614616	0.6447054309819447
H	H	0.4156787410516604	0.5500498956981524	0.5343268636290316
H	H	0.4977462949805552	0.5729723295421461	0.6491107737692110
H	H	0.5120073801453550	0.4625868966258306	0.5802245049944890

I. O(3) Final geometry ([Cu_3(μ-OH)(μ-$O)_2$]-MOR + CH3)

data_MORwithtwoAlinSPand2Alfa
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_cell_length_b 13.647634
_cell_length_c 15.015110
_cell_angle_alpha 90.000000
_cell_angle_beta 90.000000

_cell_angle_gamma 97.178906
loop_
_symmetry_equiv_pos_as_xyz
+x,+y,+z
loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

O	O	0.1831024965803094	0.0318886490755527	0.2244965686789506
O	O	0.2125591661959324	0.9982055155386940	0.7279034606055330
O	O	0.4272779563290361	0.7998240682264639	0.2095557519641009
O	O	0.4261955616570300	0.8084617541168857	0.7240582881775114
O	O	0.6325829095431450	0.8871886050543045	0.5123137588361528
O	O	0.5958478855550710	0.8581168574951589	0.0477755054414945
O	O	0.7979165536791447	0.0080772758562163	0.4694179767225018
O	O	0.7433365658643025	0.9747926588704664	0.9742823033643134
O	O	0.6011490396600625	0.1836050425108411	0.4766832002969669
O	O	0.5942353826282737	0.1927031758648492	0.9830952059180909
O	O	0.3656145979310480	0.1128964985388427	0.2456127796352353
O	O	0.3701136105793318	0.1306502135441867	0.7382876537174782
O	O	0.9408204290591565	0.8014083457162002	0.0490102652812317
O	O	0.9626776536163036	0.7577849441127142	0.5528019101850549
O	O	0.1841711747403116	0.5727261293523416	0.0213813648975558
O	O	0.1844166977617077	0.5768392492491539	0.5208053115347403
O	O	0.1700163647077582	0.3978476372501895	0.2301494946737708
O	O	0.1317829482069267	0.3616047641017581	0.7547577250217913
O	O	0.0374117208449300	0.2514407534626628	0.2886872062976165
O	O	0.0082109343244673	0.1984666814176612	0.7898304785811936
O	O	0.8081282131646842	0.4428826043261596	0.2894057680797300
O	O	0.8294126910092050	0.4234610291829218	0.7817274784782452
O	O	0.8505041898469122	0.6242279548741936	0.0057314507002326
O	O	0.8190478057338167	0.6258855432554427	0.4909865074417556
O	O	0.8043586698223810	0.9518925842604106	0.3008053364383152
O	O	0.7764576172388902	0.9565771912940978	0.8017966062787524
O	O	0.5394431700039829	0.1783164411199301	0.3088795404664302
O	O	0.5424833360807280	0.1963153515367533	0.8116731592301694
O	O	0.4001418638490372	0.1655849341338266	0.9948888472439452
O	O	0.3836801812770224	0.1660303409492151	0.4987873261689805
O	O	0.2444664752973643	0.0483197841541287	0.0548309207581111
O	O	0.2269941330931871	0.0434121089130810	0.5551672882601574
O	O	0.4026868624069158	0.8354691460755186	0.0326634618580996
O	O	0.4518003809108414	0.8034604697291561	0.5487910565965998
O	O	0.6341318067566287	0.8418207521644419	0.2619542045659204
O	O	0.6249153160795990	0.8445919057726661	0.7296203802153015

O	O	0.0193680747890998	0.2007688877118264	0.4610549959308883
O	O	0.0335437299002059	0.2041347050591985	0.9668651627386732
O	O	0.7846930716384160	0.4320265731845714	0.4651734805664424
O	O	0.8093305275911148	0.4398090161600577	0.9579996349894029
O	O	0.9041449875064649	0.6179064356152973	0.2471025320653809
O	O	0.8794528621945864	0.6153153732789595	0.7638784659243135
O	O	0.0001041386957260	0.7938773423185317	0.2183819544422526
O	O	0.9884723044371960	0.7890223495463822	0.7263082969825893
O	O	0.1446870764554836	0.5859486731191629	0.1970609867777607
O	O	0.1948333288749912	0.5426518537670320	0.6973846324378299
O	O	0.1061361760843516	0.3773709024158134	0.5115587559711317
O	O	0.1297860316025055	0.3835653848561137	0.9927986422219047
O	O	0.2767739850802135	0.8926449971266542	0.1523138663440451
O	O	0.2984761988365663	0.8835809874812830	0.6150570327645846
O	O	0.6959568060704556	0.0941373232402313	0.3490401609255718
O	O	0.6970397174386193	0.1095482986508738	0.8582802359849323
O	O	0.1053333846646202	0.7254486907215538	0.0857278024979240
O	O	0.1152134712848052	0.6977452812603069	0.6378946102736188
O	O	0.8966232021458065	0.3138228069415889	0.3869790197472867
O	O	0.8910286554098555	0.2903601428070300	0.8922594207253197
O	O	0.2427500738255115	0.0868463676641113	0.3860376217532683
O	O	0.2625661220449766	0.0801328354202689	0.8835034047578839
O	O	0.4863360670928908	0.8585937666043743	0.3928982687836443
O	O	0.5158103857769505	0.8720919770048913	0.8891968570825670
O	O	0.7647005201001977	0.9046701392366141	0.1343641689674058
O	O	0.7763265914846369	0.9276368615079296	0.6280788415262197
O	O	0.5160155806650337	0.1482598940526193	0.1375774053042465
O	O	0.5268956966420985	0.1693724671857260	0.6397842809650466
O	O	0.9319193087731577	0.7483675787849677	0.3797841390035894
O	O	0.9023579126834039	0.7604797639922404	0.8815884223935873
O	O	0.1356690099633391	0.5181213920653535	0.3646058144944759
O	O	0.1223535043568256	0.5137236970984841	0.8607353639576653
O	O	0.1047908882925599	0.2491246685549570	0.1245425545238667
O	O	0.0718018112169446	0.2289201876315743	0.6276237240422466
O	O	0.8607904065774210	0.4809481893511145	0.1232334748529137
O	O	0.8411083843373874	0.5001158270102473	0.6223018325663671
O	O	0.2242126545498869	0.2237269835152719	0.2620742656510494
O	O	0.1978368745020114	0.1910643943504538	0.7555578533945309
O	O	0.7558475083743202	0.7821243948309271	0.9937183062569486
O	O	0.7977846058262682	0.8130113533608729	0.4869937345037118
O	O	0.8036096562436227	0.7679281669992490	0.2482609928277425
O	O	0.7930677252199247	0.7747305480935516	0.7367369729698454
O	O	0.2276049915943140	0.2289920471646792	0.9899737605593687
O	O	0.2100518875185478	0.2265928891539598	0.5035318137600876
O	O	0.4999546818474083	0.0126415390017884	0.0079608296660686
O	O	0.4856071583875123	0.9995316311211366	0.5241065190510760

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O	O	0.9706079434394647	0.5232935739340996	0.4873682953486429
O	O	0.5036877561172217	0.9922273767253587	0.2457874560236762
O	O	0.5139492237463228	0.0118993286682331	0.7444941652483199
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O	O	0.0048389412051637	0.4898701108851942	0.7170802040601468
O	O	0.0954067655538690	0.9169746392276579	0.1008190278385041
O	O	0.1055067694792330	0.8899412881838726	0.6092124652133026
O	O	0.2914334382639568	0.6992992967567643	0.1280432720675846
O	O	0.3083043017422862	0.6890917088424785	0.6221930746253425
O	O	0.8919124941507300	0.1236423131819141	0.3438229121239778
O	O	0.8846071090336587	0.0930689010539335	0.8961511621401661
O	O	0.7022477392297433	0.2909694024927517	0.3550001078197857
O	O	0.6997021301594939	0.3048421824114486	0.8663355055230054
O	O	0.3268083369421650	0.5553959084825976	0.2980943157390347
O	O	0.4923068719291293	0.6698460146018068	0.3235479745987377
O	O	0.3991825039748162	0.5848861799621713	0.4672203005586792
Si	Si	0.5012271618142711	0.1284036863726790	0.0327119175338707
Si	Si	0.7152646299597034	0.8788739648087354	0.0382336291173068
Si	Si	0.7518435992922675	0.9094352464121240	0.5217978513429532
Si	Si	0.2548784267585421	0.1142215862480460	0.2814439559922488
Si	Si	0.2586464000267393	0.0998952339076163	0.7770774616813206
Si	Si	0.8917978553417585	0.5010958333306285	0.2266258150007151
Si	Si	0.8895279755927015	0.5079318183546435	0.7203166743831638
Si	Si	0.1338347573128422	0.2794427593544525	0.2268851923233176
Si	Si	0.1023241444050850	0.2454056367783565	0.7307269011294651
Si	Si	0.1070043610668004	0.4934645913232353	0.9665542926083937
Si	Si	0.8784581817388568	0.7358577016530290	0.4766226291532626
Si	Si	0.8619684367719969	0.7406862885873912	0.9827856832384705
Si	Si	0.5169203615575416	0.8970276407883219	0.4935150004585273
Si	Si	0.5044281737399791	0.8955410404737537	0.9923644903418493
Si	Si	0.2681107002255361	0.1315140781362777	0.4857068438319713
Si	Si	0.2830782990394448	0.1308158475803185	0.9812869473644097
Si	Si	0.4825462733031757	0.1040432212472356	0.2355991563562687
Si	Si	0.4860722464680651	0.1212313314212258	0.7400155256366808
Si	Si	0.7475364013326893	0.8662042617910123	0.2373107842635256
Si	Si	0.7499472555271390	0.8786198069419315	0.7238241033346333
Si	Si	0.1138081549814521	0.4906666512685048	0.2598989126621254
Si	Si	0.1127893056016194	0.4762401378977746	0.7577512318638283
Si	Si	0.9088206796675917	0.7330238196427249	0.2739197874178400
Si	Si	0.8924291658713516	0.7335588205548904	0.7770602957182097
Si	Si	0.8804638116110518	0.5142961010193126	0.0208663939893739
Si	Si	0.8569151866252579	0.5194370054299542	0.5154954493342709
Si	Si	0.1244692847940147	0.2678071493211525	0.0192310578284980
Si	Si	0.2008325458937718	0.9737257069328032	0.1327483014934417
Si	Si	0.2120376946447237	0.9547539342238375	0.6260338292019477

Si	Si	0.3505481395353358	0.8130146729365046	0.1280562038523608
Si	Si	0.3688944909296982	0.7979318973768963	0.6312183007992591
Si	Si	0.7967742055873400	0.0450903165659587	0.3651573927677541
Si	Si	0.7753725105128969	0.0341867941939598	0.8843472575928299
Si	Si	0.6339959127534670	0.1999333247933964	0.8818079379710426
Si	Si	0.0348086415274997	0.8083790159354829	0.1148967217275783
Si	Si	0.0436524006532936	0.7835434126369125	0.6302706237438430
Si	Si	0.1792527721641447	0.6443913877340084	0.1070755416638900
Si	Si	0.1999173779236478	0.6263771752933941	0.6193068315865276
Si	Si	0.9616916533449564	0.2235122667143866	0.3703972758166041
Si	Si	0.9545991634461691	0.1975189294937526	0.8861540124994490
Si	Si	0.7980740946896270	0.3688083294049692	0.3747247228476345
Si	Si	0.8089864148284078	0.3647953701476653	0.8746659303738624
Si	Si	0.1028163813214819	0.2610628856842174	0.5253464138156834
Si	Si	0.6349410398743355	0.1867506061009804	0.3739362907199644
Al	Al	0.0872933082449630	0.4918492796420112	0.4743677905241597
Al	Al	0.5177777587859890	0.8732154538238535	0.2771479832694497
Al	Al	0.5106820233942309	0.8913787382305625	0.7778774098509948
Al	Al	0.4941889889389202	0.1266108798223904	0.5235842529480002
Cu	Cu	0.2721251385494629	0.5656079368000659	0.4095369038717430
Cu	Cu	0.4521828001477454	0.7147911741348202	0.4314898905080160
Cu	Cu	0.3877676715653148	0.6641925703849965	0.2508436755151895
C	C	0.4805071335985845	0.4848513113442809	0.6604011916502971
H	H	0.5841919452308051	0.2198514358898224	0.6405680383711270
H	H	0.6032601252752914	0.7804629479682500	0.7022856652448131
H	H	0.4026771112001952	0.4578396788187445	0.6688242720682546
H	H	0.4365281297870805	0.5472327553379396	0.4260382816410014
H	H	0.5118774083591701	0.5516049341039874	0.6948313079853423
H	H	0.5259937471466588	0.4482467061741673	0.6146855874953544

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