Structural and Electronic Properties of Ag_5 Atomic Quantum Cluster Interacting with CO_2, CH_4, and H_2O Molecules

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1. Bond lengths and charge distributions of isolated systems.

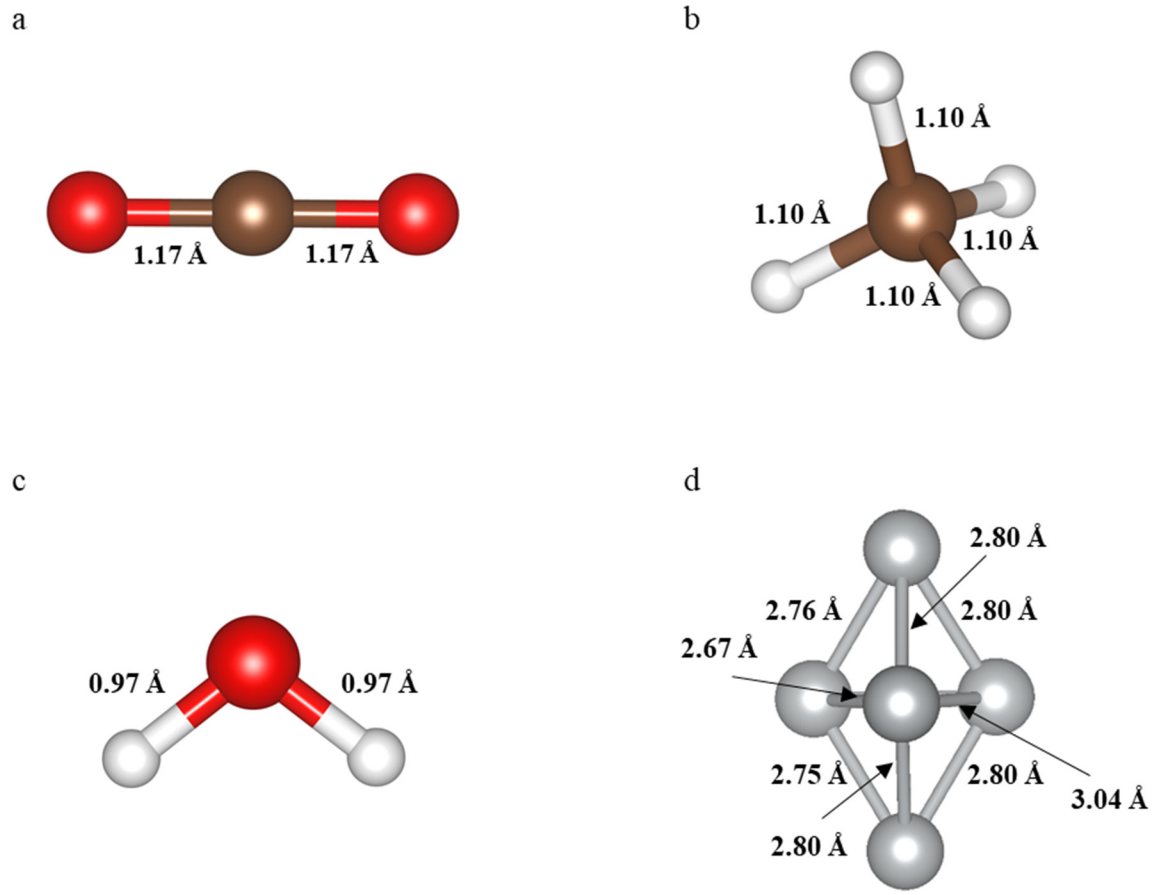

Fig. S1. Optimised structures of isolated (a) CO_2, (b) CH_4, (c) H_2O, and (d) Ag_5 systems. Note: numbers indicate bond length values.

Table S1. Charge distribution of CO_2 molecule.

Symbol	**Charge | e^- |**
C	2.02
O_1	–1.01
O_2	–1.01

Table S2. Charge distribution of CH_4 structure.

Symbol	**Charge | e^- |**

C	–0.53
H_1	0.15
H_2	0.10
H_3	0.15
H_4	0.13

Table S3. Charge distribution of H_2O molecule.

Symbol	**Charge | e^- |**
H_1	0.99
H_2	0.99
O	–1.997

Table S4. Charge distribution of Ag_5 structure.

Symbol	**Charge | e^- |**
Ag_1	0.05
Ag_2	0.18
Ag_3	–0.13
Ag_4	0.047
Ag_5	–0.13

2. Density of states of isolated Systems

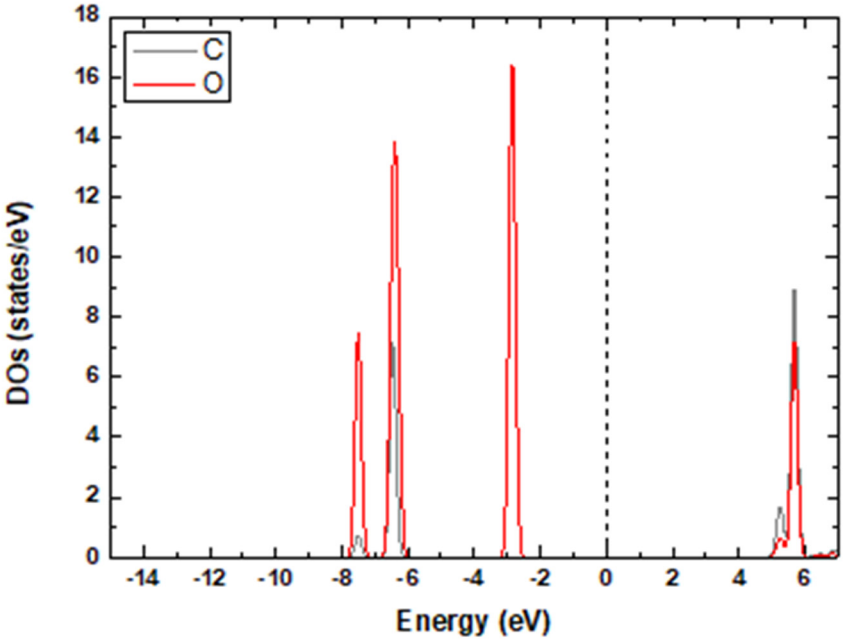

Fig. S2. Density of states of isolated CO_2 molecule.

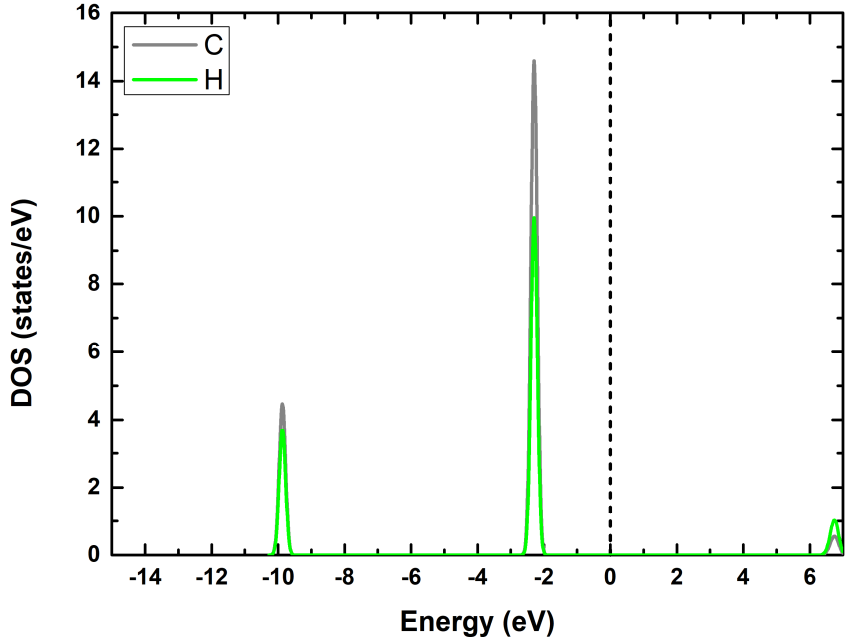

Fig. S3. Density of states of isolated CH_4 molecule.

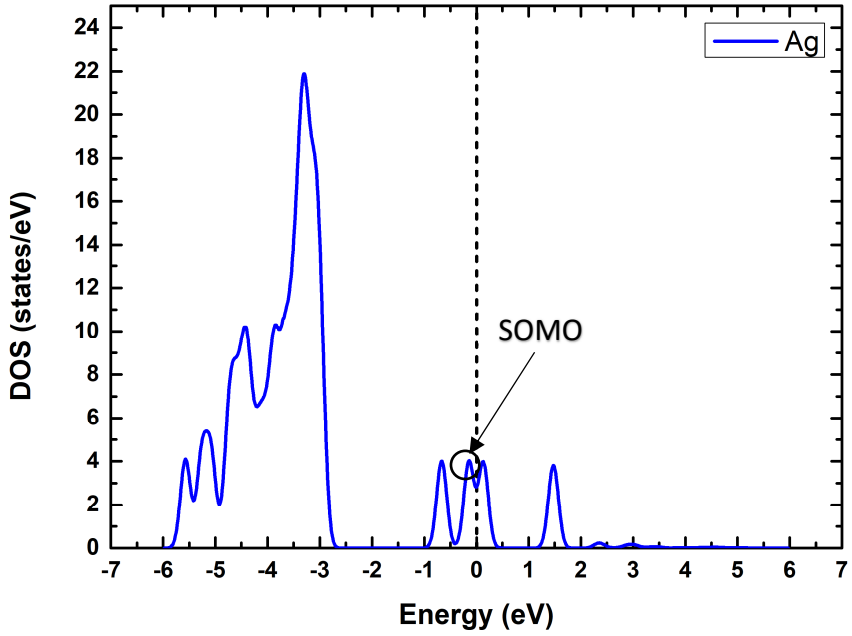

Fig. S4 Density of states of bare Ag_5 cluster. SOMO: singly occupied molecular orbital.

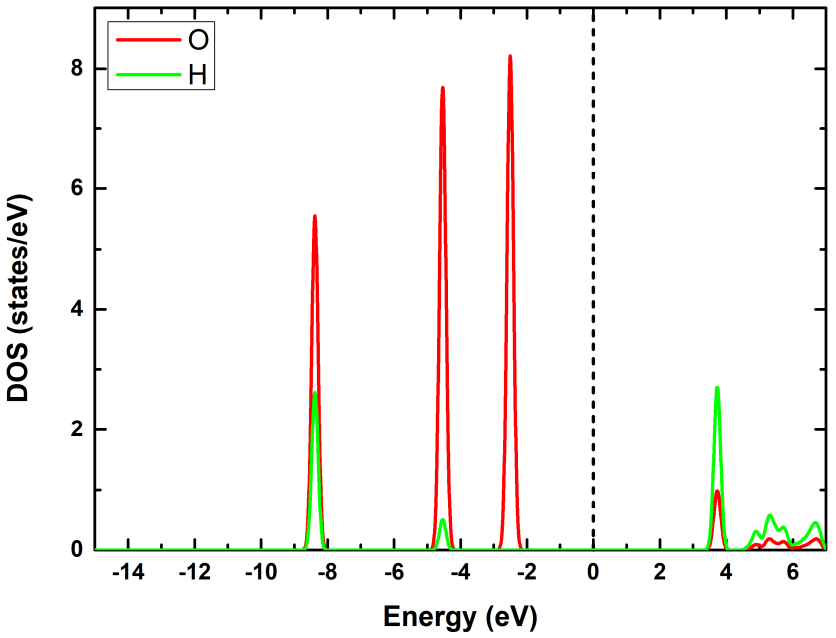

Fig. S5 Density of states of isolated H_2O molecule.

3. Charge distributions of CO_2@Ag_5, H_2O@Ag_5, and CH_4@Ag_5 systems

Table S5. Charge distribution of CO_2@Ag_5 structure.

Symbol	**Charge | e^- |**
Ag_1	0.0417
Ag_2	–0.0034
Ag_3	–0.1306
Ag_4	0.2442
Ag_5	–0.1479
C	2.1541
O_1	–1.046
O_2	–1.116

Table S6. Charge distribution of CH_4@Ag_5 structure.

Symbol	**Charge | e^- |**
Ag_1	0.0083
Ag_2	–0.0716
Ag_3	0.1107
Ag_4	–0.0684
Ag_5	0.0402
C	–0.378
H_1	0.0749
H_2	0.1596
H_3	0.043
H_4	0.081

Table S7. Charge distribution of H_2O@Ag_5 structure.

Symbol	**Charge | e^- |**
Ag_1	–0.0202
Ag_2	0.2524
Ag_3	–0.1524
Ag_4	0.0130
Ag_5	–0.1631
O	–1.9245

H_1	0.997
H_2	0.977

4. CO_2@Ag_5, CH4@Ag_5, and H_2O@Ag_5

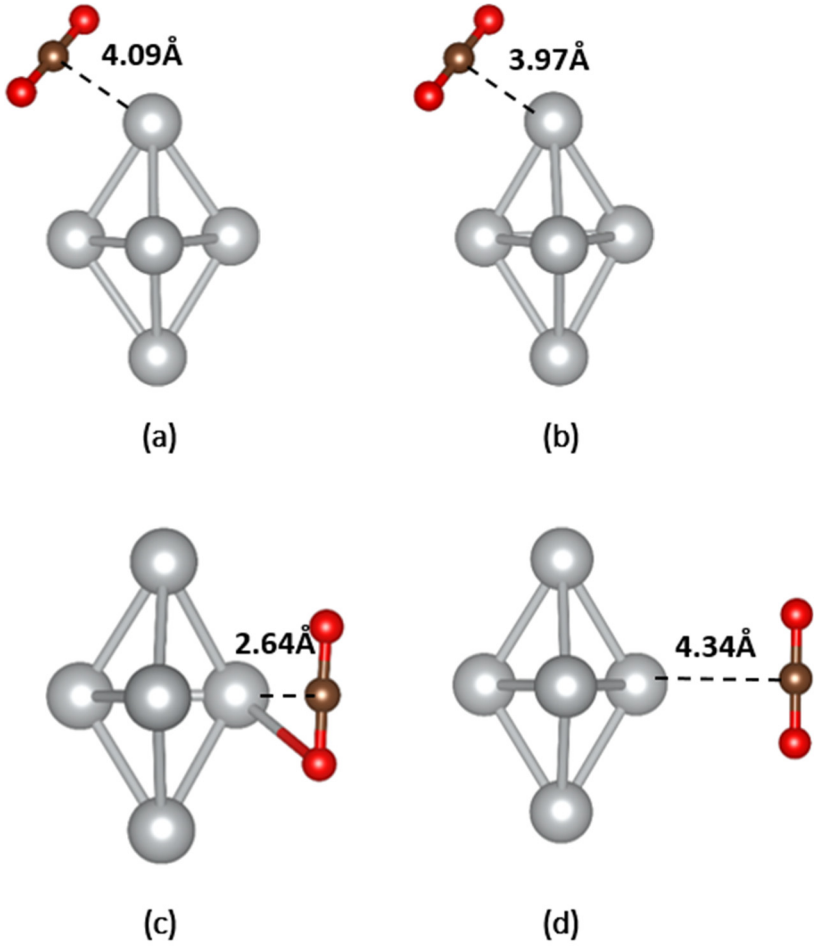

Fig. S6 Different adsorption sites of CO_2@Ag_5.

Table S8. Total energy of the structures presented in Fig. S6 and Fig. 1.

Structure	**Total energy (Ry)**
Fig. (b)	–442.847
Fig. (d)	–442.845
Fig. 1b (in the main manuscript)	–442.85

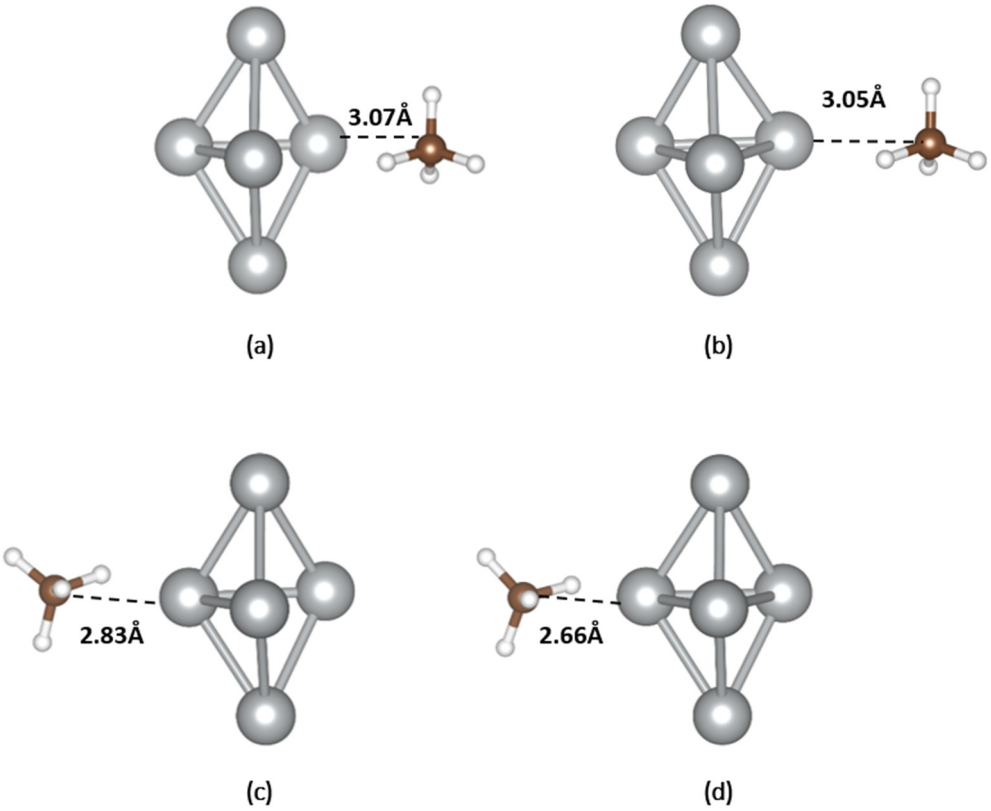

Fig. S7 Different adsorption sites of CH_4@Ag_5.

Table S9. Total energy of the structures presented in Fig. S7 and Fig. 3.

Structure	**Total energy (Ry)**
Fig. (b)	–383.83
Fig. (d)	–383.84
Fig. 3b (in the main manuscript)	–383.86

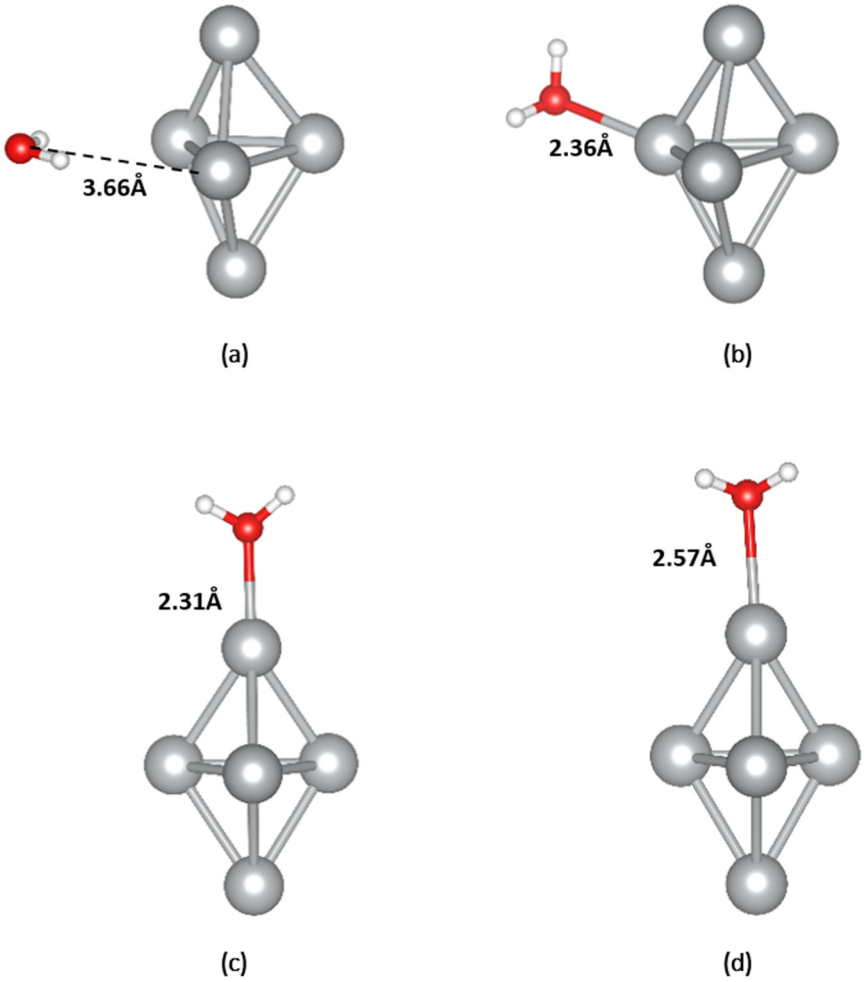

Fig. S8 Different adsorption sites of $H_2O@Ag_5$.

Table S10. Total energy of the structures presented in Fig. S8 and Fig. 5.

Structure	**Total energy (Ry)**
Fig. (b)	–401.97
Fig. (d)	–401.95
Fig. 5b (in the main manuscript)	–401.97

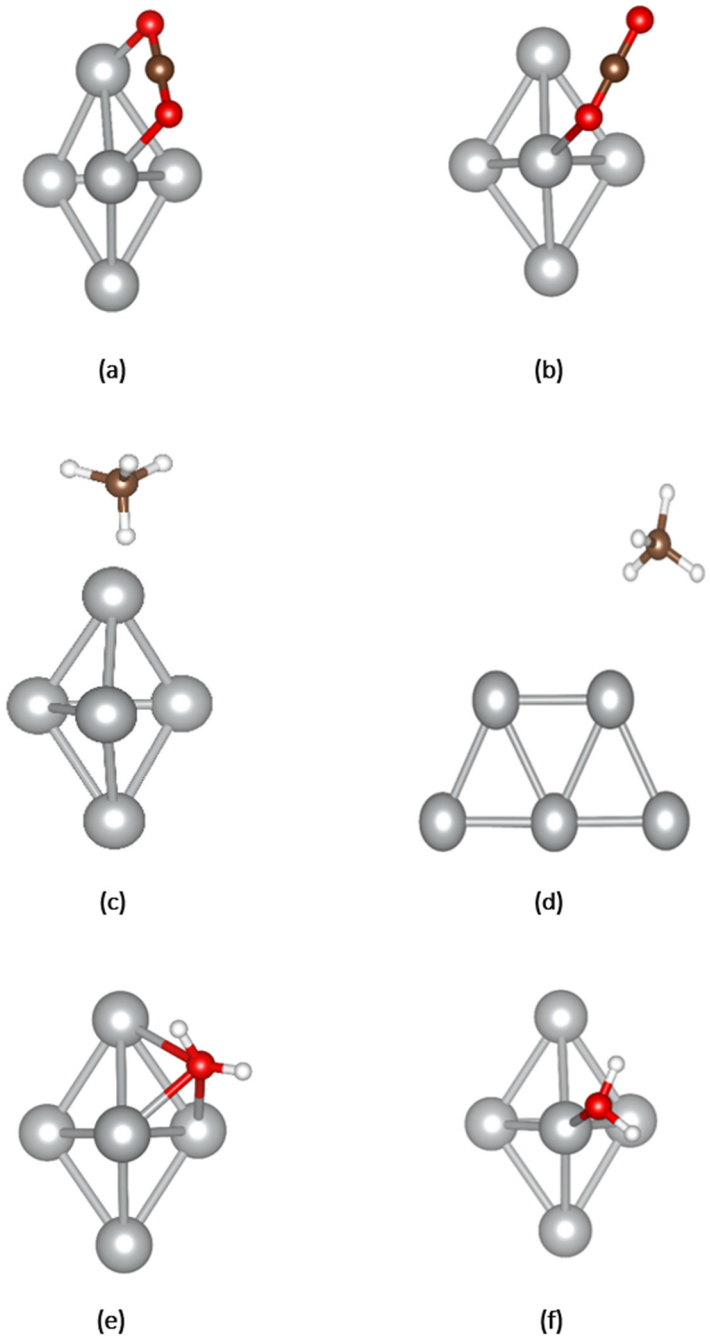

Fig. S9 Initial (a), (c), and (e) and optimised (b), (d), and (f) structures of CO_2@Ag_5, CH_4@Ag_5, and H_2O@Ag_5, respectively using a cut-off energy value of 50 Ry.

5. Coordinates for structures appeared in the main manuscript (i.e. most stable configurations)

4.1 CO_2

C	6.190970003	5.007840246	5.000000000
O	5.019143545	5.015333639	5.000000000
O	7.362808452	4.999711115	5.000000000

4.2 CH_4

C	5.802491596	5.813692074	5.794837750
H	6.299387533	5.156933492	6.518220475
H	6.469649758	5.990568297	4.943277625
H	4.879524577	5.338058317	5.443318636
H	5.561130537	6.769328819	6.274534514

4.3 H_2O

O	5.711105283	5.071112939	5.522269943
H	4.875344723	5.209916216	5.041195636
H	5.691178994	5.734104844	6.235838421

4.4 Ag_5

Ag	14.9398786494	15.1589231789	10.2601349678
Ag	13.7898089800	17.5695921120	10.3584394046
Ag	15.1094581004	16.8618035090	8.0413882405
Ag	16.4541157247	17.8012599369	10.3117668660
Ag	15.2025185485	16.7230812631	12.5730605220

4.5 $CO_2@Ag_5$

Ag	6.611341632	4.682388766	6.658463874
Ag	4.507929647	6.783250783	7.167060581
Ag	6.137569213	6.835171078	4.885220170

Ag	7.193440756	7.174856844	7.422062672
Ag	5.876375881	5.495312606	9.250320223
C	7.368147269	9.098659050	10.042701401
O	6.847236473	9.140026890	11.085669433
O	7.908287129	9.073307983	8.995476646

4.6 $CH_4@Ag_5$

Ag	5.626397269	5.156450229	7.023635238
Ag	4.176794751	5.822571492	4.819498174
Ag	6.317047542	7.341193871	5.469859884
Ag	8.471872477	8.827740067	6.142919080
Ag	7.817992273	6.701337028	7.706950766
C	8.012733686	6.782678557	11.247270388
H	8.733252916	7.564848022	10.977937575
H	7.011402477	7.069474840	10.902016927
H	8.000014388	6.657478997	12.337492538
H	8.303465222	5.833600897	10.778214430

4.7 $H_2O@Ag_5$

Ag	9.324361659	4.961668275	6.427752826
Ag	7.367543392	6.725200727	7.124589535
Ag	8.166178632	6.568329727	4.452494653
Ag	9.659301642	7.921653786	6.415879475
Ag	9.626557176	6.430647613	8.786407035
O	5.249911599	6.401403325	8.111018921
H	4.765323763	5.685702419	7.658773906
H	5.400919136	6.086222127	9.021768649