

Novel Hydrogen Bonding of C(sp²) Atom in Planar Tetracoordinate Carbon Molecule

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Table S1. Comparison of the energy and interaction energy of systems at different levels of theory

| Method | $E_{\text{CAI}_4\text{Mg}^- \cdots \text{HX}}$ (a.u.) | | $E_{\text{CAI}_4\text{Mg}^-}$ (a.u.) | E_{HX} (a.u.) | IE (kJ/mol) |
|--------------------------------|--|--------------|---|---------------------------|----------------|
| (U)ωB97XD | CAI ₄ Mg ⁻ ⋯ NH ₃ | -1264.469063 | -1207.8971705 | -56.5641763 | -20.3 |
| | CAI ₄ Mg ⁻ ⋯ PH ₃ | -1551.053519 | | -343.150229 | -16.1 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ O | -1284.345518 | | -76.4359419 | -32.6 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ S | -1607.309984 | | -399.404194 | -22.6 |
| | CAI ₄ Mg ⁻ ⋯ HF | -1308.373985 | | -100.45609 | -54.4 |
| | CAI ₄ Mg ⁻ ⋯ HCl | -1668.730787 | | -460.817395 | -42.6 |
| PBE0 | CAI ₄ Mg ⁻ ⋯ NH ₃ | -1263.888497 | -1207.3671815 | -56.5130684 | -21.6 |
| | CAI ₄ Mg ⁻ ⋯ PH ₃ | -1550.390702 | | -343.015665 | -20.6 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ O | -1283.75628 | | -76.3756176 | -35.4 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ S | -1606.638615 | | -399.261404 | -26.3 |
| | CAI ₄ Mg ⁻ ⋯ HF | -1307.774626 | | -100.385354 | -58.0 |
| | CAI ₄ Mg ⁻ ⋯ HCl | -1668.050814 | | -460.664631 | -49.9 |
| CCSD(T)// (U)ωB97XD | CAI ₄ Mg ⁻ ⋯ NH ₃ | -1262.124415 | -1205.6649427 | -56.4521839 | -19.1 |
| | CAI ₄ Mg ⁻ ⋯ PH ₃ | -1548.33297 | | -342.641602 | -69.4 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ O | -1281.984781 | | -76.3075098 | -32.4 |
| | CAI ₄ Mg ⁻ ⋯ H ₂ S | -1604.569288 | | -398.887659 | -43.80 |
| | CAI ₄ Mg ⁻ ⋯ HF | -1305.993097 | | -100.307951 | -53.0 |
| | CAI ₄ Mg ⁻ ⋯ HCl | -1665.967785 | | -460.288498 | -37.7 |

Table S2. Vibrational frequencies of the monomers and their corresponding dimers, along with their corresponding intensities. The negative sign in the vibrational frequency shift indicates a redshift in the stretching frequencies upon hydrogen-bond formation.

| System | Vibrational Frequency (cm ⁻¹) | Vibrational frequency shift (cm ⁻¹) | Intensity (km/mol) |
|---|---|---|--------------------|
| PH ₃ | 2415.58 | | 32.5773 |
| CAI ₄ Mg ⁻ ⋯ PH ₃ | 2398.62 (sym. str) | -16.96 | 29.3780 |
| NH ₃ | 3522.16 (sym. str) | -22.24 | 2.2738 |
| CAI ₄ Mg ⁻ ⋯ NH ₃ | 3499.92 (sym. str) | | 0.8031 |
| H ₂ S | 2739.56(sym. str) | | 0.0067 |
| CAI ₄ Mg ⁻ ⋯ H ₂ S | 2611.63 (sym. str) | -128 | 192.37 |
| H ₂ O | 3904.8 (sym. str) | | 282.55 |
| CAI ₄ Mg ⁻ ⋯ H ₂ O | 3726.96 (sym. str) | -177.84 | 9.54 |
| HCl | 2971.98 | | 50.2769 |
| CAI ₄ Mg ⁻ ⋯ HCl | 2132.42 | -839.56 | 2097 |
| HF | 4177.37 | | 123.78 |
| CAI ₄ Mg ⁻ ⋯ HF | 3393.77 | -783.6 | 1183.1129 |

Table S3. Details of orbitals and occupancy for the CAI₄Mg⁻ ⋯ HX systems.

| System | Bond | Type | Occupancy | Atom | ED (%) | %s | %p | %d | NBO Hybrids | |
|---|---|--------|-----------|---------|--------|-------|-------|-------|---------------------------------------|--------------------------------------|
| CAI ₄ Mg ⁻ ⋯ H ₂ O | C1-AI3 | σ | 0.95124 | C | 90.01 | 8.15 | 91.73 | 0.11 | sp ^{11.25} d ^{0.01} | |
| | | | | Al | 9.99 | 34.34 | 64.65 | 1.01 | sp ^{1.88} d ^{1.01} | |
| | C1-AI4 | σ | 0.94150 | C | 88.39 | 39.89 | 59.72 | 0.39 | sp ^{1.50} d ^{0.01} | |
| | | | | Al | 11.61 | 33.84 | 65.15 | 1.01 | sp ^{1.93} d ^{0.03} | |
| | C1-AI5 | σ | 0.93911 | C | 90.77 | 51.00 | 48.52 | 0.49 | sp ^{0.95} d ^{0.01} | |
| | | | | Al | 9.23 | 10.59 | 88.72 | 0.69 | sp ^{8.38} d ^{0.07} | |
| | O7-H8 | σ | 0.99772 | O | 73.06 | 22.75 | 77.14 | 0.12 | sp ^{3.39} d ⁰ | |
| | | | | H | 26.94 | 99.82 | 0.18 | | sp ⁰ | |
| | O7-H9 | σ | 0.99804 | O | 75.55 | 27.05 | 72.83 | 0.12 | sp ^{2.69} d ⁰ | |
| | | | | H | 24.45 | 99.80 | 0.20 | | sp ⁰ | |
| | CAI ₄ Mg ⁻ ⋯ H ₂ S | C1-AI3 | σ | 0.94231 | C | 88.29 | 39.19 | 60.43 | 0.39 | sp ^{1.54} d ^{0.01} |
| | | | | | Al | 11.71 | 35.86 | 63.13 | 1.01 | sp ^{1.76} d ^{0.03} |
| C1-AI4 | | σ | 0.95216 | C | 89.80 | 8.24 | 91.65 | 0.11 | sp ^{11.12} d ^{0.01} | |
| | | | | Al | 10.20 | 35.86 | 63.13 | 1.01 | sp ^{1.76} d ^{0.03} | |
| C1- | | σ | 0.93906 | C | 90.96 | 51.58 | 47.93 | 0.49 | sp ^{0.93} d ^{0.01} | |
| | | | | Al | 9.04 | 10.40 | 88.89 | 0.71 | sp ^{8.55} d ^{0.07} | |

| | | | | | | | | | | |
|--|--|----------|----------|---------|---------|-------|-------|-------|----------------------|---------------------|
| | A15 | | | | | | | | | |
| | H7-S9 | σ | 0.99753 | H | 42.77 | 99.69 | 0.31 | | sp^0 | |
| | | | | S | 57.23 | 15.00 | 84.35 | 0.66 | $sp^{5.62}d^{0.04}$ | |
| | H8-S9 | σ | 0.99726 | H | 40.50 | 99.65 | 0.35 | | sp^0 | |
| | | | | S | 59.50 | 17.25 | 82.12 | 0.63 | $sp^{4.76}d^{0.04}$ | |
| | | | | | | | | | | |
| CA₄Mg⁻ ... NH₃ | C1-A13 | σ | 0.94185 | C | 88.42 | 39.46 | 60.16 | 0.38 | $sp^{1.52}d^{0.01}$ | |
| | | | | Al | 11.58 | 28.32 | 70.62 | 1.06 | $sp^{2.49}d^{0.04}$ | |
| | C1-A14 | σ | 0.95133 | C | 89.90 | 8.54 | 91.37 | 0.09 | $sp^{10.70}d^{0.01}$ | |
| | | | | Al | 10.10 | 28.92 | 70.00 | 1.07 | $sp^{2.42}d^{0.04}$ | |
| | C1-A15 | σ | 0.93862 | C | 90.78 | 51.03 | 48.48 | 0.50 | $sp^{0.95}d^{0.01}$ | |
| | | | | Al | 9.22 | 10.08 | 89.15 | 0.77 | $sp^{8.85}d^{0.08}$ | |
| | H7-N9 | σ | 0.99796 | H | 0.99796 | 99.90 | 0.10 | | sp^0 | |
| | | | | N | 67.64 | 24.97 | 74.94 | 0.09 | $sp^{3.00}d^0$ | |
| | H8-N9 | σ | 0.99793 | H | 31.23 | 99.90 | 0.10 | | sp^0 | |
| | | | | N | 68.77 | 26.29 | 73.61 | 0.10 | $sp^{2.80}d^0$ | |
| | | | | | | | | | | |
| | CA₄Mg⁻ ... PH₃ | C1-A13 | σ | 0.94075 | C | 88.77 | 40.45 | 59.16 | 0.40 | $sp^{1.46}d^{0.01}$ |
| Al | | | | | 11.23 | 28.83 | 70.09 | 1.08 | $sp^{2.43}d^{0.04}$ | |
| C1-A14 | | σ | 0.94941 | C | 90.41 | 7.78 | 92.15 | 0.07 | $sp^{1.85}d^{0.01}$ | |
| | | | | Al | 9.59 | 26.93 | 71.94 | 1.12 | $sp^{2.67}d^{0.04}$ | |
| C1-A16 | | σ | 0.94005 | C | 90.62 | 50.78 | 48.70 | 0.52 | $sp^{0.96}d^{0.01}$ | |
| | | | | Al | 9.38 | 10.45 | 88.81 | 0.74 | $sp^{8.50}d^{0.07}$ | |
| H8-P10 | | σ | 0.99540 | H | 50.51 | 99.75 | 0.25 | | sp^0 | |
| | | | | P | 49.49 | 15.17 | 84.13 | 0.69 | $sp^{5.54}d^{0.05}$ | |
| H9-P10 | | σ | 0.99504 | H | 49.14 | 99.71 | 0.29 | | sp^0 | |
| | | | | P | 50.86 | 15.92 | 83.39 | 0.69 | $sp^{5.24}d^{0.04}$ | |
| | | | | | | | | | | |
| CA₄Mg⁻ ... HF | C1-A13 | σ | 0.95162 | C | 90.30 | 8.16 | 91.67 | 0.17 | $sp^{11.23}d^{0.02}$ | |
| | | | | Al | 9.70 | 30.72 | 68.29 | 0.99 | $sp^{2.22}d^{0.03}$ | |
| | C1-A14 | σ | 0.94151 | C | 88.72 | 39.82 | 59.84 | 0.34 | $sp^{1.50}d^{0.01}$ | |
| | | | | Al | 11.28 | 28.48 | 70.48 | 1.04 | $sp^{2.48}d^{0.04}$ | |
| | C1-A15 | σ | 0.93820 | C | 91.01 | 50.95 | 48.61 | 0.45 | $sp^{0.95}d^{0.01}$ | |
| | | | | Al | 8.99 | 9.96 | 89.35 | 0.69 | $sp^{8.97}d^{0.07}$ | |

| | | | | | | | | | |
|---|--------|----------|---------|----|-------|-------|-------|------|----------------------|
| | H7-F8 | σ | 0.99822 | H | 17.91 | 99.58 | 0.42 | | sp^0 |
| | | | | F | 82.09 | 29.28 | 70.59 | 0.12 | $sp^{2.41}d^0$ |
| CA₄Mg⁻ ... HCl | C1-A13 | σ | 0.95252 | C | 90.65 | 7.79 | 92.03 | 0.18 | $sp^{11.82}d^{0.02}$ |
| | | | | Al | 9.35 | 28.50 | 70.43 | 1.07 | $sp^{2.47}d^{0.04}$ |
| | C1-A14 | σ | 0.94193 | C | 88.86 | 39.41 | 60.24 | 0.35 | $sp^{1.53}d^{0.01}$ |
| | | | | Al | 11.14 | 30.67 | 68.31 | 1.02 | $sp^{2.23}d^{0.03}$ |
| | C1-A15 | σ | 0.93878 | C | 91.21 | 51.00 | 48.53 | 0.46 | $sp^{0.95}d^{0.01}$ |
| | | | | Al | 8.79 | 8.85 | 90.36 | 0.79 | $sp^{10.21}d^{0.09}$ |
| | H7-Cl8 | σ | 0.99741 | H | 30.94 | 99.58 | 0.42 | | sp^0 |
| | | | | Cl | 69.06 | 20.42 | 79.11 | 0.47 | $sp^{3.87}d^{0.02}$ |

Table S4. Details of donor-acceptor orbitals and their interaction energies.

| System | Front Donation | | Back Donation | |
|--|---|----------------------------|---|----------------------------|
| | Interaction | ΔE^2 (kcal/mol) | Interaction | ΔE^2 (kcal/mol) |
| CA₄Mg⁻ ... NH₃ | $\sigma(C1-A16) \rightarrow \sigma^*(H8-N9)$ | 0.03 | $\sigma(H8-N9) \rightarrow \sigma^*(C1-A16)$ | 0.11 |
| | LP(C1) $\rightarrow \sigma^*(H8-N9)$ | 0.41 | $\sigma(H8-N9) \rightarrow \sigma^*(C1-A13)$ | 0.12 |
| | | | $\sigma(H8-N9) \rightarrow \sigma^*(C1-A14)$ | 0.09 |
| | Total | 0.44 | Total | 0.32 |
| CA₄Mg⁻ ... PH₃ | LP(C1) $\rightarrow \sigma^*(H9-P10)$ | 0.16 | $\sigma(H9-P10) \rightarrow \sigma^*(C1-A13)$ | 0.08 |
| | $\sigma(C1-A16) \rightarrow \sigma^*(H9-P10)$ | 0.15 | $\sigma(H9-P10) \rightarrow \sigma^*(C1-A14)$ | 0.06 |
| | | | $\sigma(H9-P10) \rightarrow \sigma^*(C1-A16)$ | 0.06 |
| | Total | 0.21 | Total | 0.20 |
| CA₄Mg⁻ ... H₂O | LP(C1) $\rightarrow \sigma^*(O7-H9)$ | 2.87 | $\sigma(O7-H9) \rightarrow \sigma^*(C1-A13)$ | 0.21 |
| | $\sigma(C1-A13) \rightarrow \sigma^*(O7-H9)$ | 0.03 | $\sigma(O7-H9) \rightarrow \sigma^*(C1-A14)$ | 0.18 |
| | | | $\sigma(O7-H9) \rightarrow \sigma^*(C1-A15)$ | 0.19 |
| | Total | 2.90 | Total | 0.58 |
| | LP(C1) $\rightarrow \sigma^*(H8-S9)$ | 2.18 | $\sigma(H8-S9) \rightarrow RY^*6(C1)$ | 0.18 |

| | | | | |
|--|---|--------------|---|-------------|
| CA₄Mg⁻ ... H₂S | | | $\sigma(\text{H8-S9}) \rightarrow \sigma^*(\text{C1-A13})$ | 0.11 |
| | | | $\sigma(\text{H8-S9}) \rightarrow \sigma^*(\text{C1-A14})$ | 0.10 |
| | | | $\sigma(\text{H8-S9}) \rightarrow \sigma^*(\text{C1-A16})$ | 0.13 |
| | Total | 2.18 | Total | 0.55 |
| CA₄Mg⁻ ... HF | $\sigma(\text{C1-A13}) \rightarrow \sigma^*(\text{H7-F8})$ | 0.27 | $\sigma(\text{H7-F8}) \rightarrow \sigma^*(\text{C1-A13})$ | 0.24 |
| | $\sigma(\text{C1-A14}) \rightarrow \sigma^*(\text{H7-F8})$ | 0.49 | $\sigma(\text{H7-F8}) \rightarrow \sigma^*(\text{C1-A14})$ | 0.25 |
| | $\sigma(\text{C1-A15}) \rightarrow \sigma^*(\text{H7-F8})$ | 0.33 | $\sigma(\text{H7-F8}) \rightarrow \sigma^*(\text{C1-A15})$ | 0.18 |
| | $\text{LP}(\text{C1}) \rightarrow \sigma^*(\text{H7-F8})$ | 10.96 | $\sigma(\text{H7-F8}) \rightarrow \text{RY}^*5(\text{C1})$ | 0.13 |
| | Total | 12.05 | Total | 0.80 |
| CA₄Mg⁻ ... HCl | $\sigma(\text{C1-A13}) \rightarrow \sigma^*(\text{H7-Cl8})$ | 0.33 | $\sigma(\text{H7-Cl8}) \rightarrow \sigma^*(\text{C1-A13})$ | 0.24 |
| | $\sigma(\text{C1-A14}) \rightarrow \sigma^*(\text{H7-Cl8})$ | 0.70 | $\sigma(\text{H7-Cl8}) \rightarrow \sigma^*(\text{C1-A14})$ | 0.24 |
| | $\sigma(\text{C1-A15}) \rightarrow \sigma^*(\text{H7-Cl8})$ | 0.56 | $\sigma(\text{H7-Cl8}) \rightarrow \sigma^*(\text{C1-A15})$ | 0.17 |
| | $\text{LP}(\text{C1}) \rightarrow \sigma^*(\text{H7-Cl8})$ | 15.62 | | |
| | Total | 71.94 | Total | 0.65 |

Table S5. Details of charge distribution of atoms before and after interactions of CA₄Mg⁻ ... HX systems.

| Systems | q _H (Interacting hydrogen of complex) | q _C (Interacting carbon of complex) | q _H (Non-interacting hydrogen of complex) | HX (Isolated molecule) | |
|--|---|---|---|------------------------------------|--|
| | | | | q _H (Hydrogen in HX) | q _X (P-block atom in HX) |
| CA ₄ Mg ⁻ ... NH ₃ | 0.372 | -2.760 | 0.353, 0.351 | 0.352 | -1.057 |
| CA ₄ Mg ⁻ ... PH ₃ | 0.016 | -2.769 | -0.011, -0.010 | -0.014 | 0.041 |
| CA ₄ Mg ⁻ ... H ₂ O | 0.499 | -2.782 | 0.457 | 0.460 | -0.921 |
| CA ₄ Mg ⁻ ... H ₂ S | 0.180 | -2.779 | 0.142 | 0.136 | -0.272 |
| CA ₄ Mg ⁻ ... HF | 0.599 | -2.803 | N.A. | 0.550 | -0.550 |
| CA ₄ Mg ⁻ ... HCl | 0.319 | -2.800 | N.A. | 0.258 | -0.258 |

Table S6. Critical point properties of the $\text{CaI}_4\text{Mg}^- \cdots \text{HX}$ systems

| Systems | Atoms | $\rho(r)$ Electron density (au) | $\text{Sign}(\lambda_2)$ ρ (au) | $\nabla^2\rho(r)$ Laplacian of electron density (au) | $V(r)$ Potential energy density (au) | $G(r)$ Lagrangian kinetic energy density (au) |
|--|----------|--|--|--|--|--|
| CaI_4Mg^- $\cdots \text{NH}_3$ | C1 - H8 | 0.007571 | -0.0076 | 0.016651 | -0.0031 | 0.0037 |
| CaI_4Mg^- $\cdots \text{PH}_3$ | Al3 - H7 | 0.004005 | -0.0040 | 0.007861 | -0.0012 | 0.0016 |
| | Al4 - H8 | 0.003714 | -0.0037 | 0.007577 | -0.0011 | 0.0015 |
| | C1 - H9 | 0.005162 | -0.0052 | 0.010596 | -0.0018 | 0.0022 |
| CaI_4Mg^- $\cdots \text{H}_2\text{O}$ | C1 - H9 | 0.015807 | -0.0158 | 0.038264 | -0.0078 | 0.0087 |
| CaI_4Mg^- $\cdots \text{H}_2\text{S}$ | C1 - H8 | 0.010645 | -0.0106 | 0.023211 | -0.0042 | 0.0050 |
| CaI_4Mg^- $\cdots \text{HF}$ | C1 - H7 | 0.033343 | -0.0333 | 0.052160 | -0.0209 | 0.0170 |
| CaI_4Mg^- $\cdots \text{HCl}$ | C1 - H7 | 0.032602 | -0.0326 | 0.051732 | -0.0183 | 0.0156 |

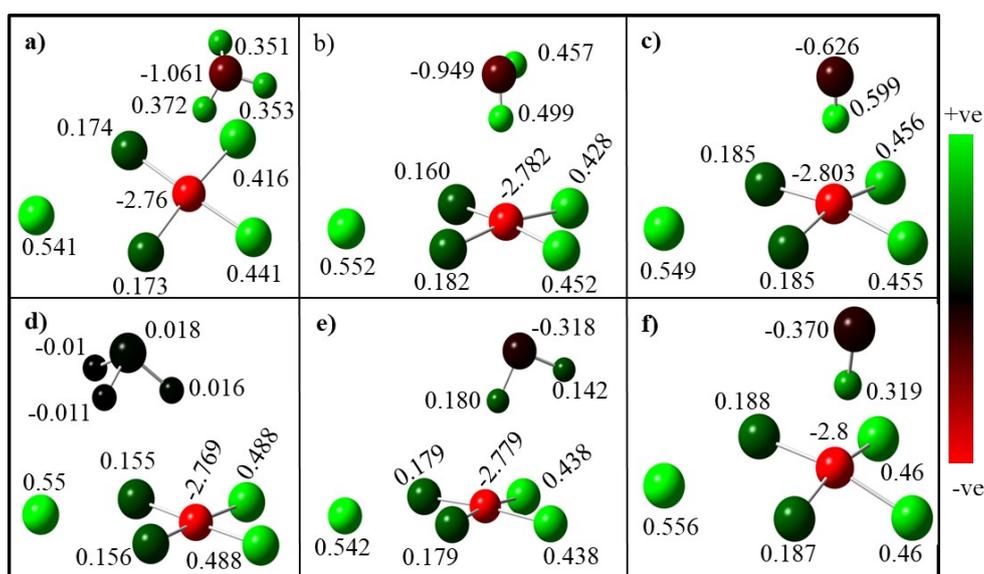


Fig. S1. The NBO charges of each atoms in a) $\text{CaI}_4\text{Mg}^- \cdots \text{NH}_3$ b) $\text{CaI}_4\text{Mg}^- \cdots \text{H}_2\text{O}$ c) $\text{CaI}_4\text{Mg}^- \cdots \text{HF}$ d) $\text{CaI}_4\text{Mg}^- \cdots \text{PH}_3$ e) $\text{CaI}_4\text{Mg}^- \cdots \text{H}_2\text{S}$ and f) $\text{CaI}_4\text{Mg}^- \cdots \text{HCl}$ dimers.

Coordinates of the optimized structures at ω B97XD /6-311++G (2d, 2p) level.

1) $\text{CAI}_4\text{Mg}^- \cdots \text{NH}_3$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | -0.264777 | 0.367670 | -0.328875 | -0.943797 |
| Mg | 3.417603 | -0.479264 | 0.307863 | -0.037445 |
| Al | 0.846455 | -1.073852 | -0.935440 | 0.078359 |
| Al | 1.105051 | 1.252857 | 0.680329 | 0.021139 |
| Al | -1.734778 | -0.389090 | -1.424620 | -0.090632 |
| Al | -1.481905 | 1.856671 | 0.142217 | -0.031685 |
| H | -2.338516 | -2.538482 | 1.211043 | 0.173098 |
| H | -1.491388 | -1.255516 | 1.699569 | 0.187395 |
| N | -2.292136 | -1.832709 | 1.937107 | -0.535661 |
| H | -3.100417 | -1.237514 | 1.796224 | 0.179258 |

2) $\text{CAI}_4\text{Mg}^- \cdots \text{PH}_3$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | 1.178399 | 0.163193 | 0.000693 | -0.843751 |
| Mg | -2.040025 | 2.234486 | 0.003630 | -0.067602 |
| Al | 0.115608 | 0.890545 | 1.423708 | -0.047809 |
| Al | 0.118246 | 0.899340 | -1.419773 | -0.044594 |
| Al | 2.354923 | -0.639639 | 1.373105 | -0.006339 |
| Al | 2.357862 | -0.630421 | -1.374498 | -0.006641 |
| H | -2.767499 | -1.055267 | 1.021622 | -0.090894 |
| H | -2.833180 | -1.086057 | -1.043375 | -0.091483 |
| H | -1.258038 | -1.964410 | -0.045575 | -0.121788 |
| P | -2.669179 | -2.029666 | -0.000896 | 0.320885 |

3) $\text{CAI}_4\text{Mg}^- \cdots \text{H}_2\text{O}$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | 0.511955 | -0.255357 | -0.213127 | -1.291291 |
| Mg | -3.317905 | -0.051333 | -0.118799 | -0.026626 |
| Al | -0.741540 | 0.943402 | -1.048700 | 0.099207 |
| Al | -0.823259 | -1.389328 | 0.581207 | 0.103110 |
| Al | 1.952568 | 0.650954 | -1.233707 | -0.019501 |
| Al | 1.872137 | -1.586703 | 0.353144 | 0.046375 |
| O | 0.709615 | 2.026302 | 2.138584 | -0.554360 |
| H | 1.025872 | 2.680050 | 1.513786 | 0.220651 |
| H | 0.661569 | 1.219460 | 1.606619 | 0.422398 |

4) $\text{CAI}_4\text{Mg}^- \cdots \text{H}_2\text{S}$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | -0.127710 | -0.743500 | 0.000031 | -1.099981 |
| Mg | -3.372225 | 1.298414 | -0.000025 | -0.060639 |
| Al | -1.232971 | -0.081093 | -1.424021 | 0.086591 |

| | | | | |
|----|-----------|-----------|-----------|-----------|
| Al | -1.232887 | -0.080875 | 1.424048 | 0.086609 |
| Al | 0.969160 | -1.660872 | -1.376360 | 0.005148 |
| Al | 0.969235 | -1.660669 | 1.376498 | 0.005105 |
| H | 3.437002 | 0.886249 | 0.000181 | 0.059419 |
| H | 1.551821 | 1.285545 | -0.000153 | 0.028217 |
| S | 2.693823 | 1.999616 | -0.000129 | -0.110305 |

5) $\text{CaI}_4\text{Mg}^- \cdots \text{HF}$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | -0.522305 | 0.000206 | -0.192845 | -1.427025 |
| Mg | 3.319445 | -0.000226 | -0.171627 | -0.040257 |
| Al | 0.775449 | -1.426326 | -0.266840 | 0.128669 |
| Al | 0.775661 | 1.426802 | -0.264660 | 0.128791 |
| Al | -1.911977 | -1.370210 | -0.608150 | 0.034909 |
| Al | -1.911117 | 1.371356 | -0.606938 | 0.034664 |
| H | -0.680289 | -0.001204 | 1.736837 | 0.542834 |
| F | -0.720382 | -0.002046 | 2.687265 | -0.402563 |

6) $\text{CaI}_4\text{Mg}^- \cdots \text{HCl}$

| | | | | |
|----|-----------|-----------|-----------|-----------|
| C | 0.338449 | -0.602324 | 0.000288 | -1.524184 |
| Mg | -3.410767 | 0.236778 | 0.000380 | -0.044047 |
| Al | -0.948798 | -0.412937 | -1.426427 | 0.132663 |
| Al | -0.948079 | -0.407961 | 1.426879 | 0.132781 |
| Al | 1.606341 | -1.310687 | -1.368313 | 0.043588 |
| Al | 1.606659 | -1.304932 | 1.371532 | 0.043455 |
| H | 0.898109 | 1.300345 | -0.001966 | 0.516089 |
| Cl | 1.228870 | 2.596880 | -0.003061 | -0.300414 |