# Computational screening analysis of iron zeolites for selectively capturing $NO_x$ and CO over $H_2O$ and $CO_2$ : Electronic Supporting Information

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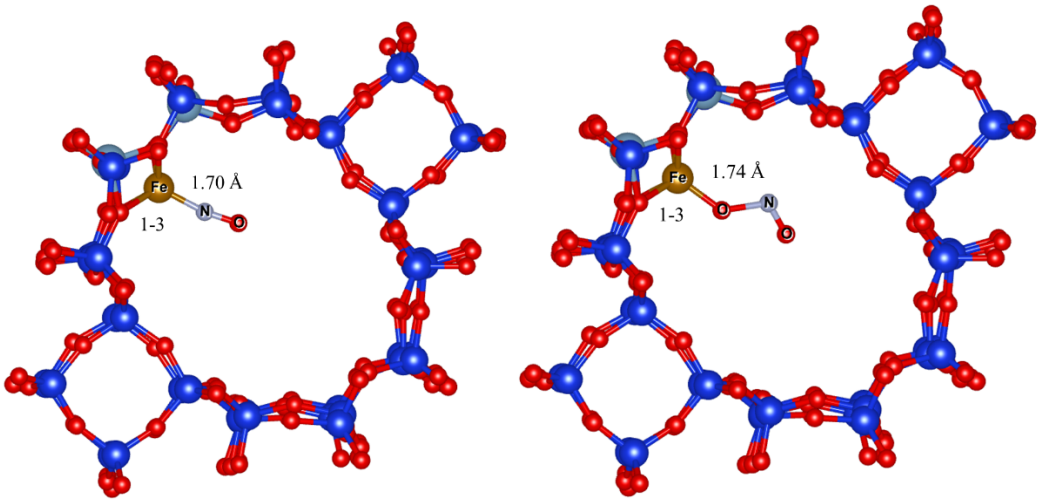
Table SI: Total interaction energies for gas adsorption on Mordenite with Si/Al ratio of 23, 11, or 5, and 1-3 or 1-4 Al distributions (Energy / kJ/mol).

| Si/Al – (configuration) | NO | $NO_2$ | CO | $H_2O$ | $CO_2$ |
|---|---|---|---|---|---|
| 23-(1-3) | -220.3 | -138.6 | -106.6 | -145.1 | -54.6 |
| 11-(1-3) | -217.7 | -140.9 | -103.5 | -104.6 | -51.6 |
| 11-(1-4) | -212.3 | -137.6 | -93.5 | -108.4 | -39.2 |
| 5-(1-3) | -216.5 | -160.1 | -98.4 | -126.7 | -45.9 |
| 5-(1-4) | -211.4 | -162.8 | -92.8 | -101.6 | -46.7 |

Table SII: Total interaction energies (kJ/mol) of the gases with the cations on site II (denoted as II), IV (denoted as IV) and areas between two of them (denoted as II-IV and IV-IV).

| Si/Al & site | NO | $NO_2$ | CO | $H_2O$ | $CO_2$ |
|---|---|---|---|---|---|
| $11_{II}$ | -194.5 | -118.9 | -83.1 | -107.3 | -40.5 |
| $5_{II}$ | -188.3 | -105.9 | -81.6 | -94.8 | -37.5 |
| $5_{IV}$ | -227.7 | -142.9 | -121.3 | -189.2 | -80.0 |
| $5_{II-IV}$ | | -163.6 | | | -69.4 |
| $3_{II}$ | -184.3 | -117.0 | -76.4 | -100.7 | -34.6 |
| $3_{IV}$ | -224.4 | -139.1 | -123.5 | -197.1 | -66.5 |
| $3_{II-IV}$ | | -145.7 | | | -73.7 |
| $3_{IV-IV}$ | | -202.4 | | | -51.0 |



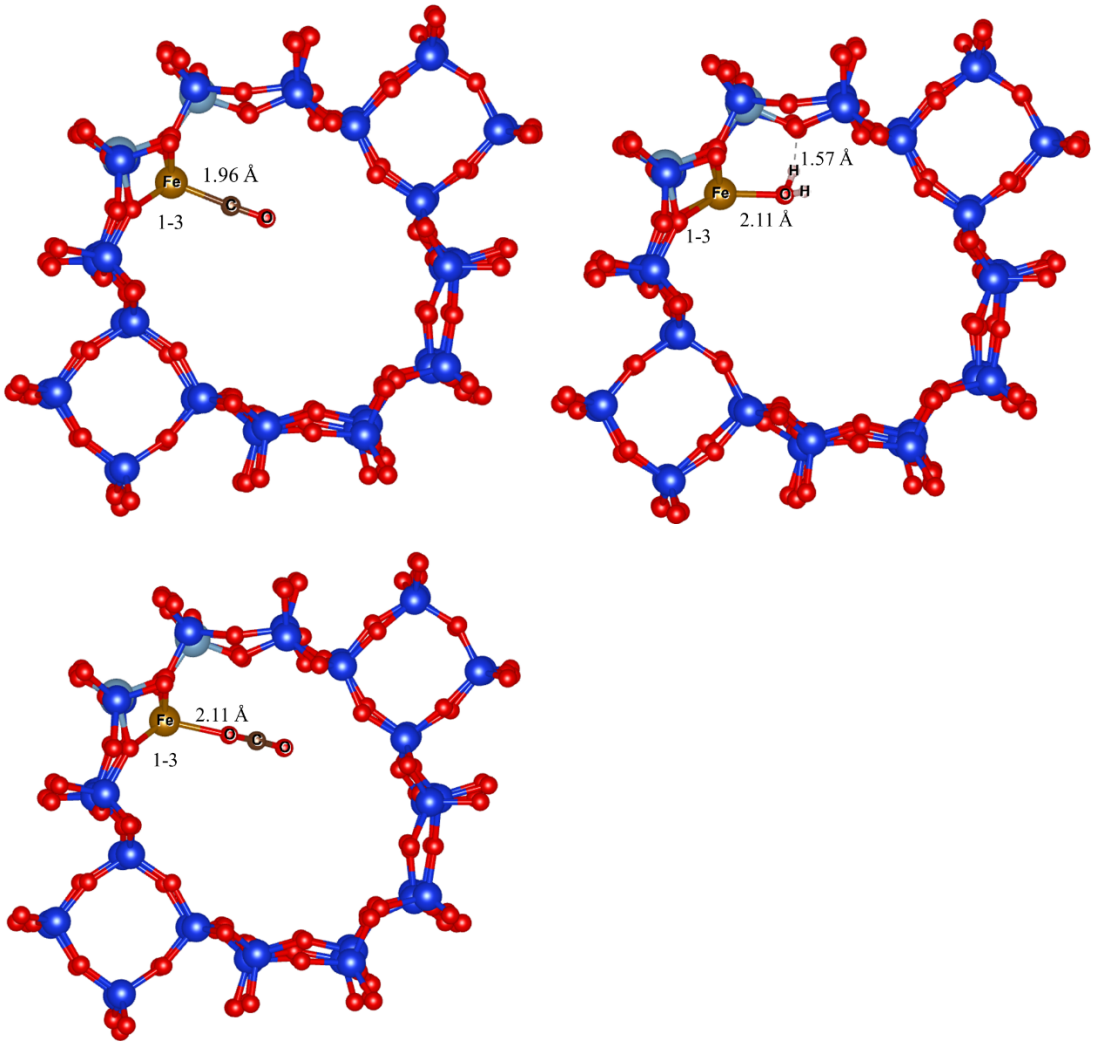
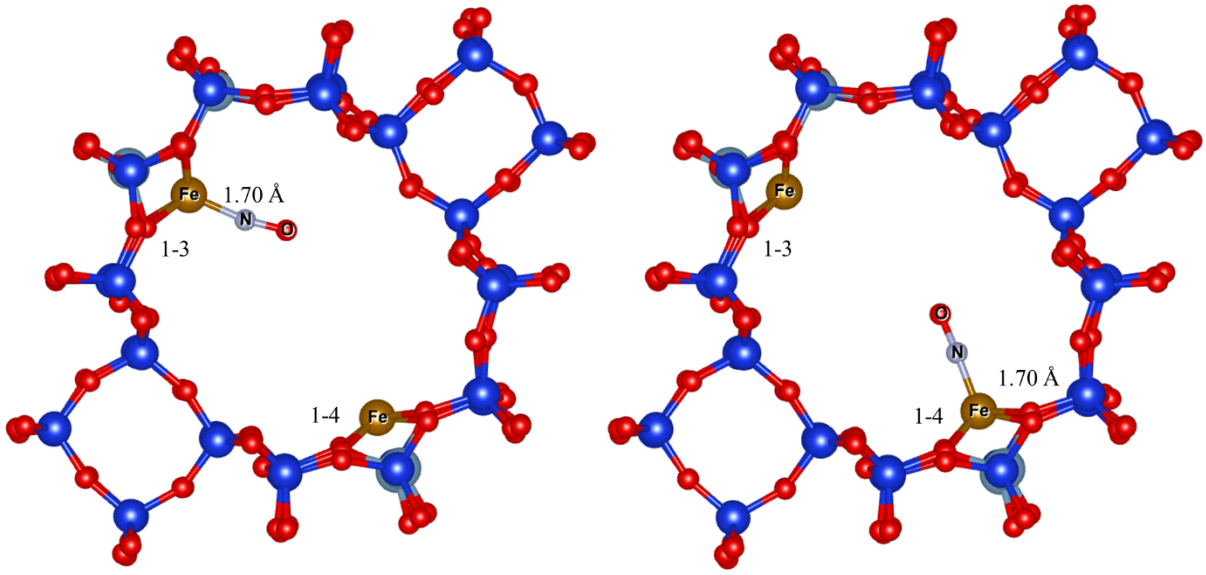
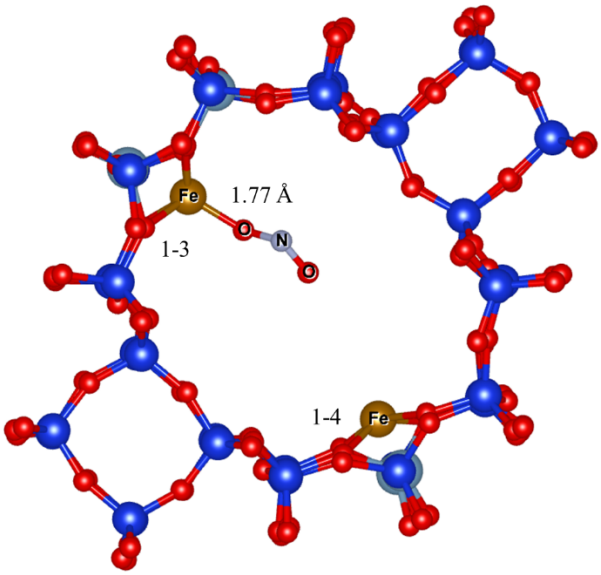



Figure SI: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-MOR (Si/Al=23). The Al distribution of the ring and the bond length are also mentioned.

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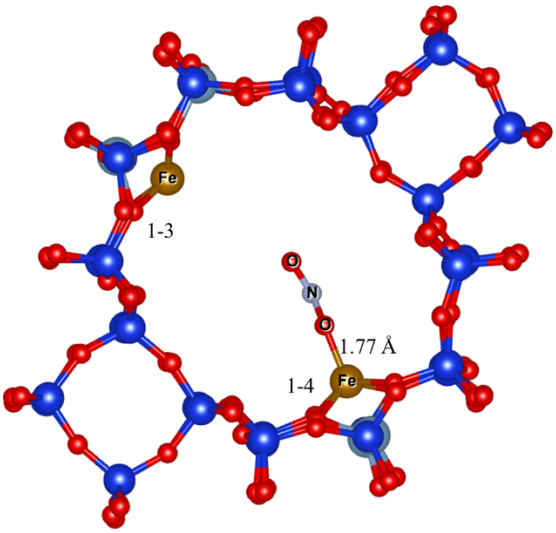
N
O
1-3
1-4
Fe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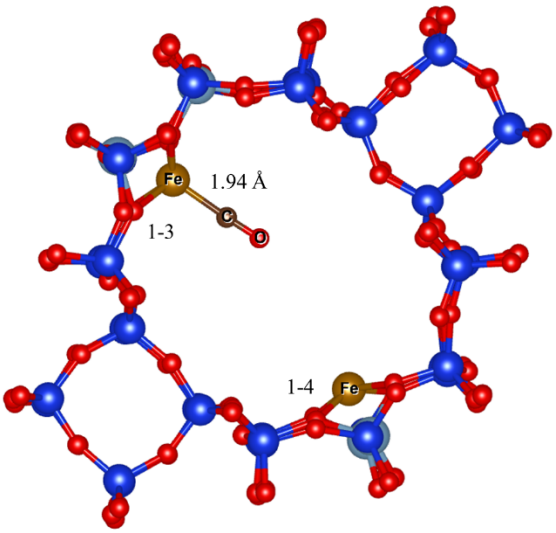
1-3
O
N
O
1.77 Å
1-4
Fe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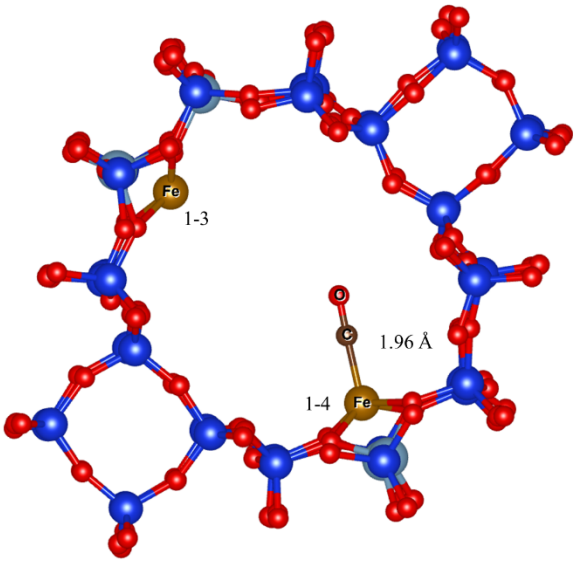
C
O
1-3
1-4
Fe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O
C
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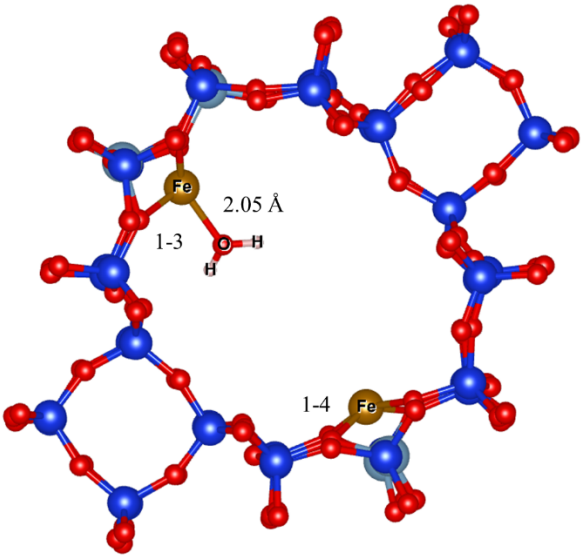
1-4
Fe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H
H
1-4
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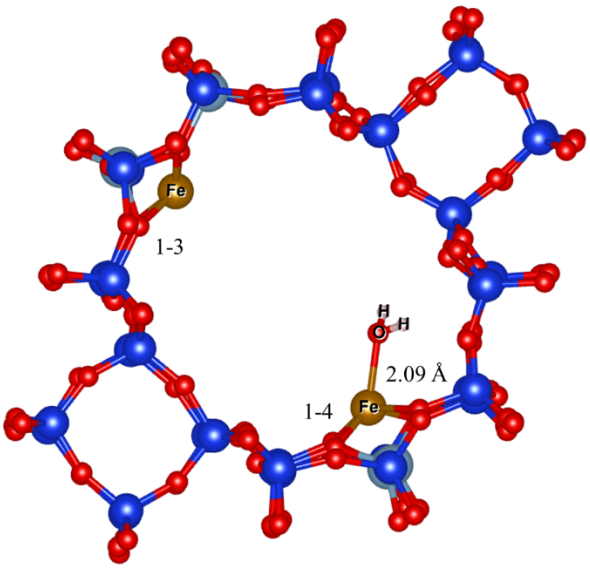
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O
H
2.09 Å
1-4
Fe

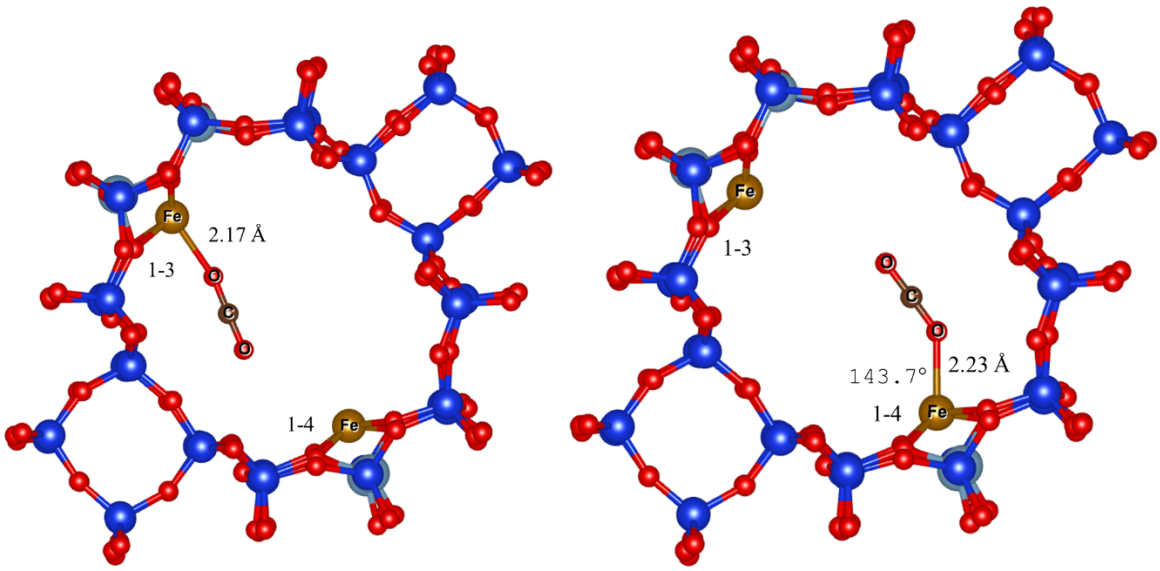
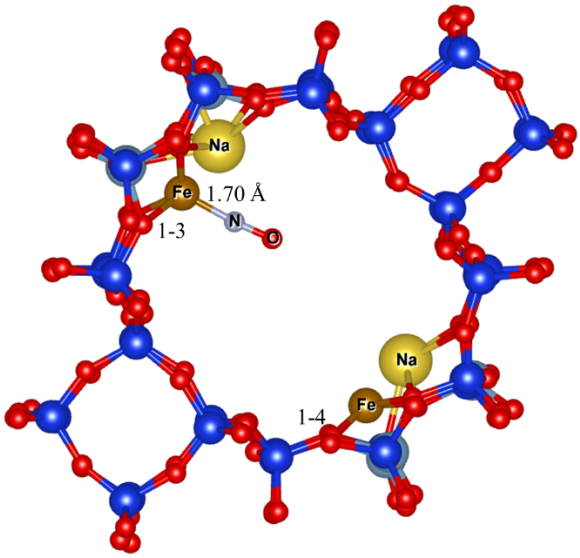



Figure SII: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-MOR (Si/Al=11). The Al distribution of the rings and the bond length are also mentioned.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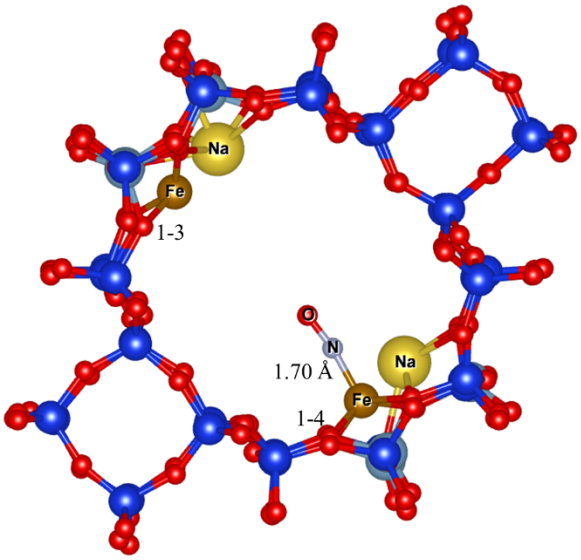
N
O
1-3
Na
Fe
1-4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Fe
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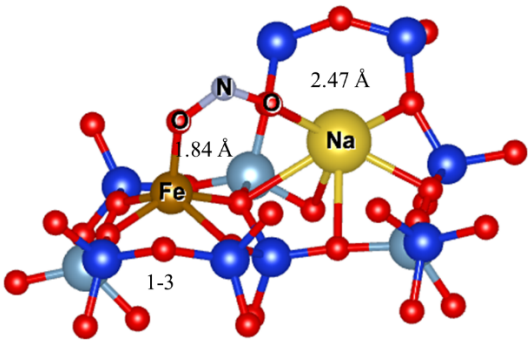
O
N
1.70 Å
Na
Fe
1-4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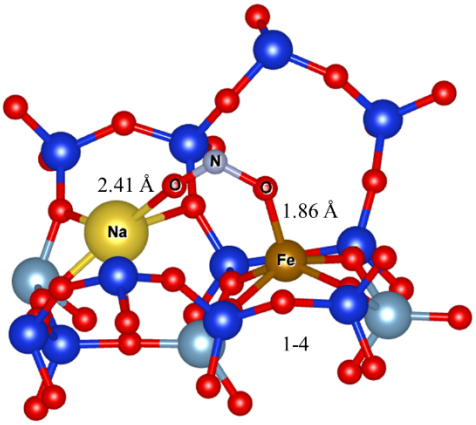
O
1.84 Å
Na
Fe
1-3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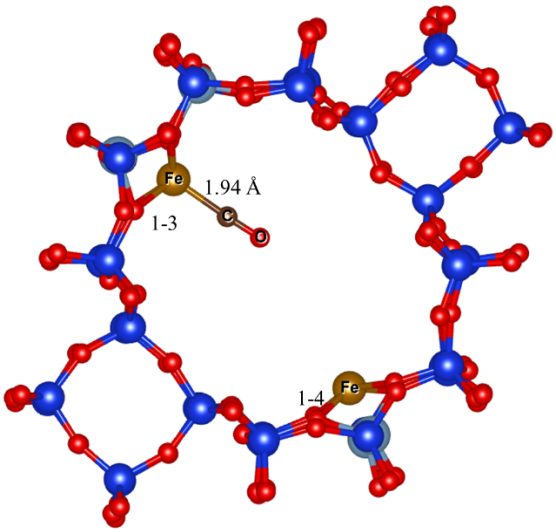
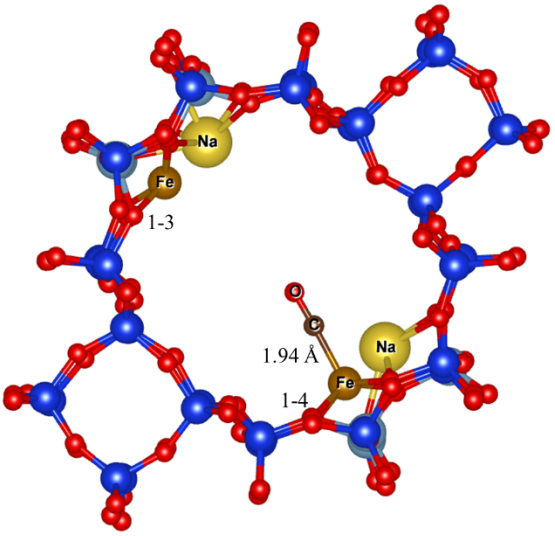
O
O
1.86 Å
Na
Fe
1-4


Fe
1.94 Å
C
O
1-3
1-4
Fe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Fe
1-3
O
C
1.94 Å
Na
Fe
1-4

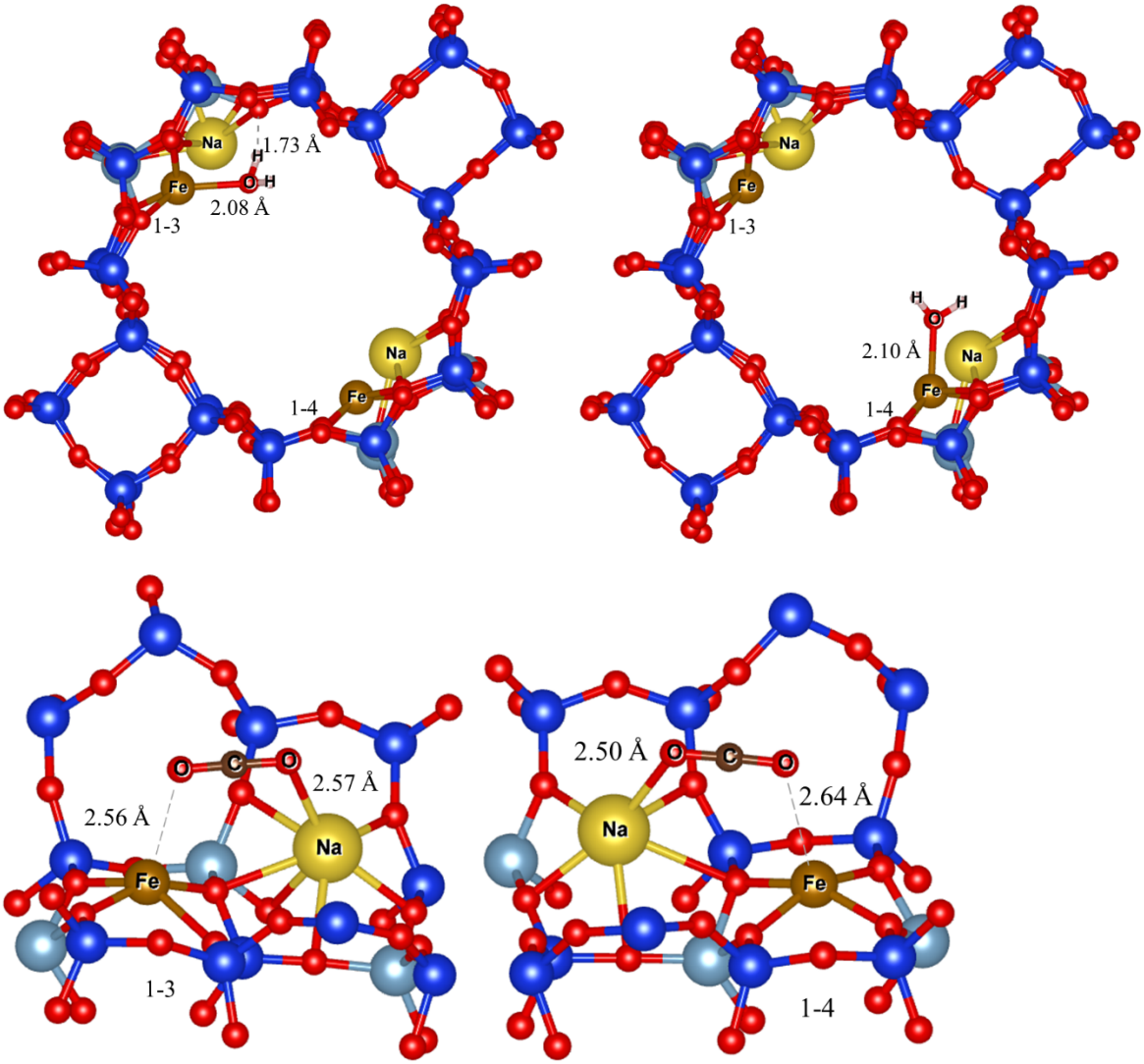


Figure SIII: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-MOR (Si/Al=5). $CO_2$ and $NO_2$ were adsorbed by two cations at the same time, thus an alternative perspective is provided for them. The Al distribution of the rings and the bond length are also mentioned.

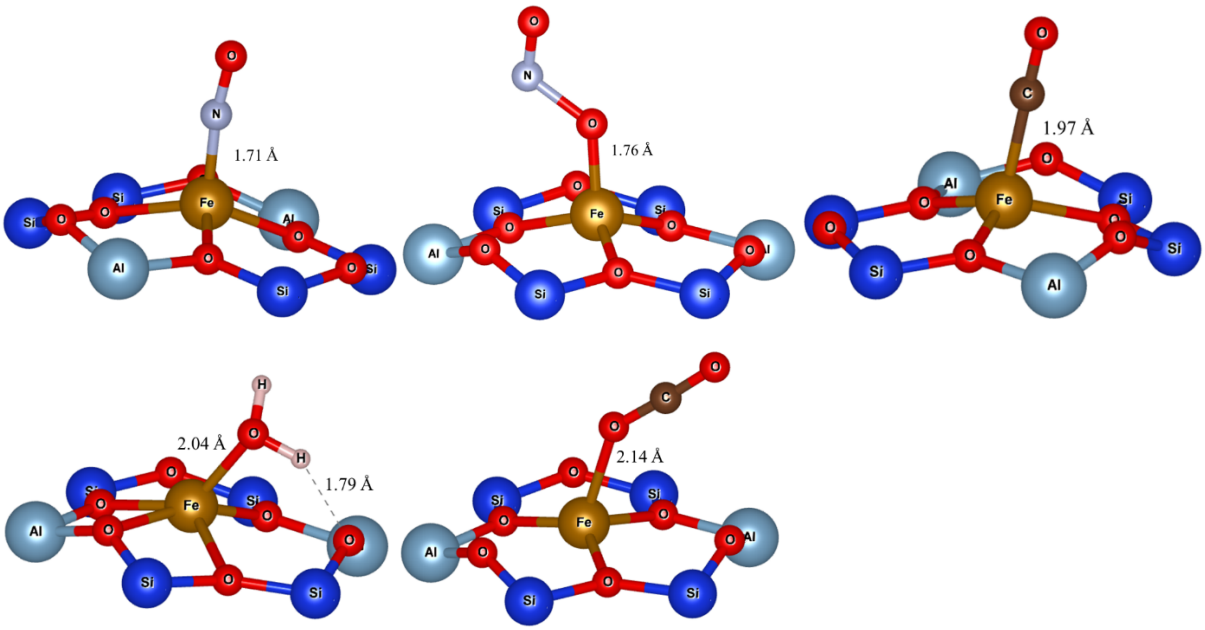


Figure SIV: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-CHA (Si/Al=11) on the 6MR. The bond length is also mentioned.

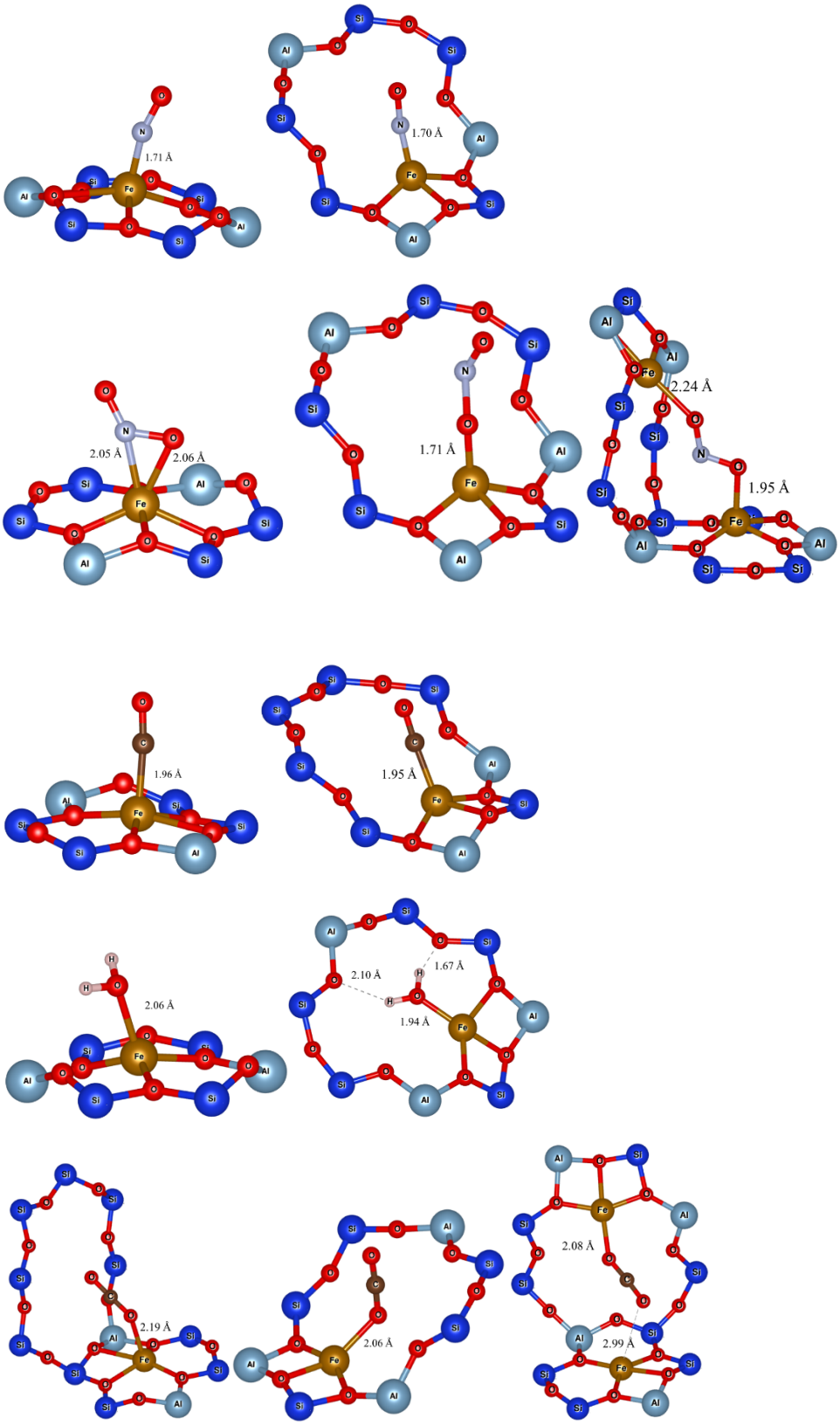


Figure SV: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-CHA (Si/Al=5) on the 6MR and 8MR. Cross adsorptions are feasible for the dioxides. The bond length is also mentioned.

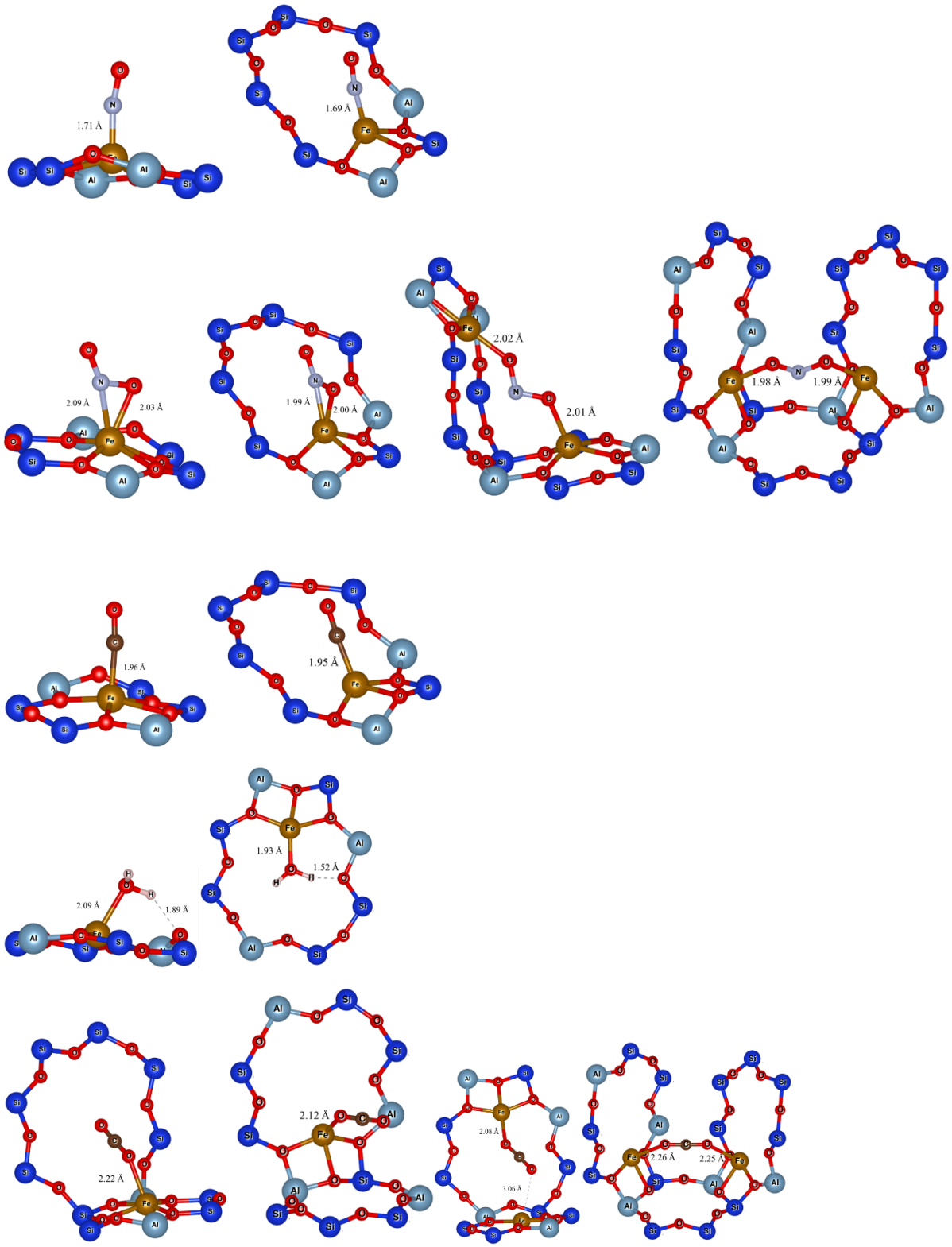


Figure SVI: Adsorption modes of the gases NO, $NO_2$, CO, $H_2O$, $CO_2$, over Fe-CHA (Si/Al=3) on the 6MR and 8MR. Cross adsorptions are feasible for the dioxides. The bond length is also mentioned.

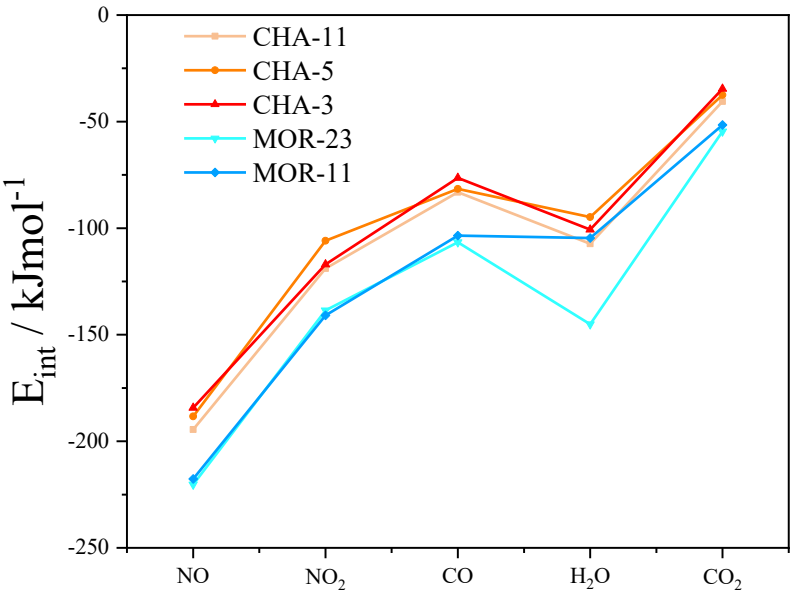


Figure SVII: Interaction energy of the gases with the various structures. Blue hues are selected for MOR and orange hues for CHA.