Supporting Information:

Effect of the Al Siting on the Structure of Co(II) and Cu(II) Cationic Sites in Ferrierite. A Periodic DFT Molecular Dynamics and FTIR study

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Figure Captions

Figure S1. Optimized structures of the β – 1 site of Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and cobalt atom in violet.

Figure S2. Optimized structures of the β – 1 site of Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and copper atom in pink.

Figure S3. Optimized structures of the α site of Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and cobalt atom in violet.

Figure S4. Optimized structures of the α site of Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and copper atom in pink.

Figure S5. Optimized structures of the β – 2 site of Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and cobalt atom in violet.

Figure S6. Optimized structures of the β – 2 site of Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, and copper atom in pink.

Figure S7. Optimized structures of the β – 1 site of NO–Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and cobalt atom in violet.

Figure S8. Optimized structures of the β – 1 site of NO–Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and copper atom in pink.

Figure S9. Optimized structures of the α site of NO–Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and cobalt atom in violet.

Figure S10. Optimized structures of the α site of NO–Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and copper atom in pink.

Figure S11. Optimized structures of the β – 2 site of NO–Co–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and cobalt atom in violet.

Figure S12. Optimized structures of the β – 2 site of NO–Cu–ferrierite before (left) and after (right) molecular dynamics simulations. The distances are in Å and the bond angle in degrees. Silicon atoms are in gray, oxygen atoms in red, aluminum atoms in yellow, nitrogen atom in blue, and copper atom in pink.

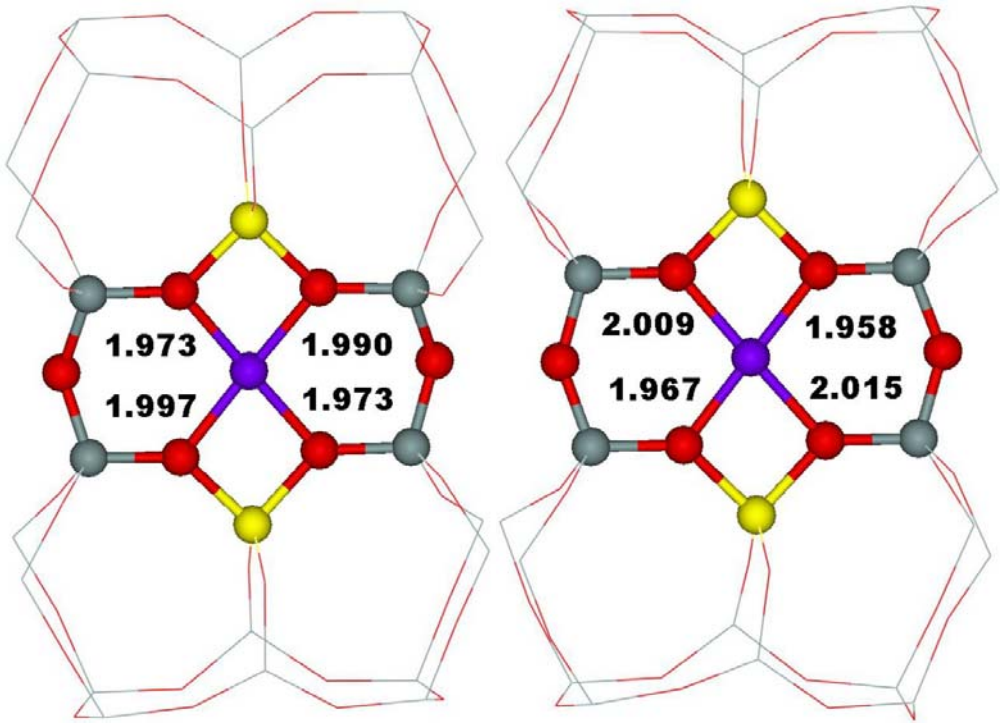


Figure S1

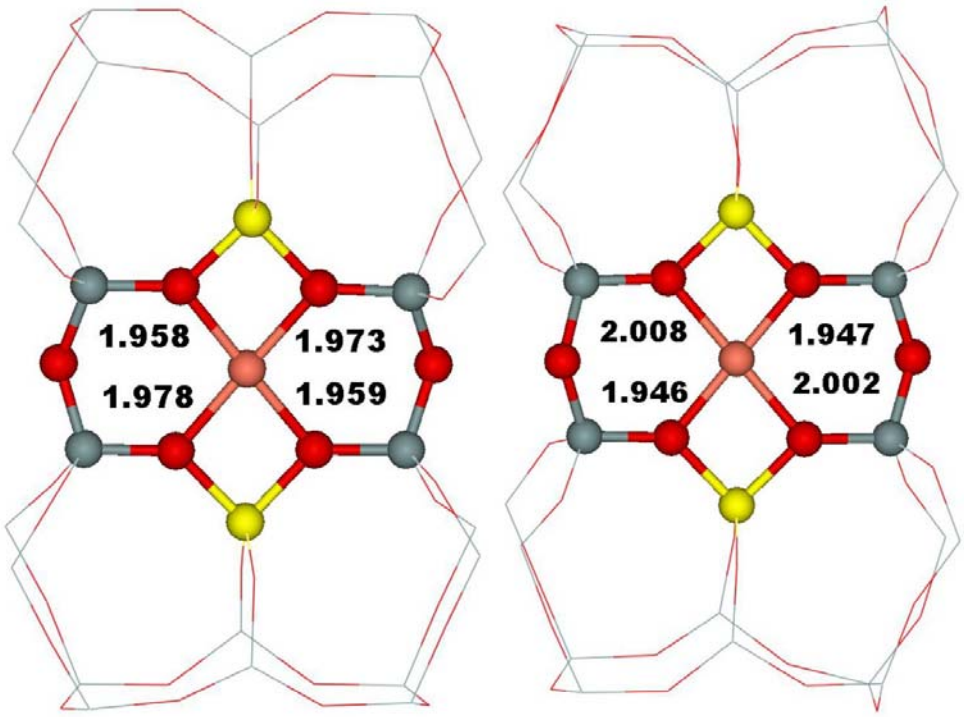


Figure S2

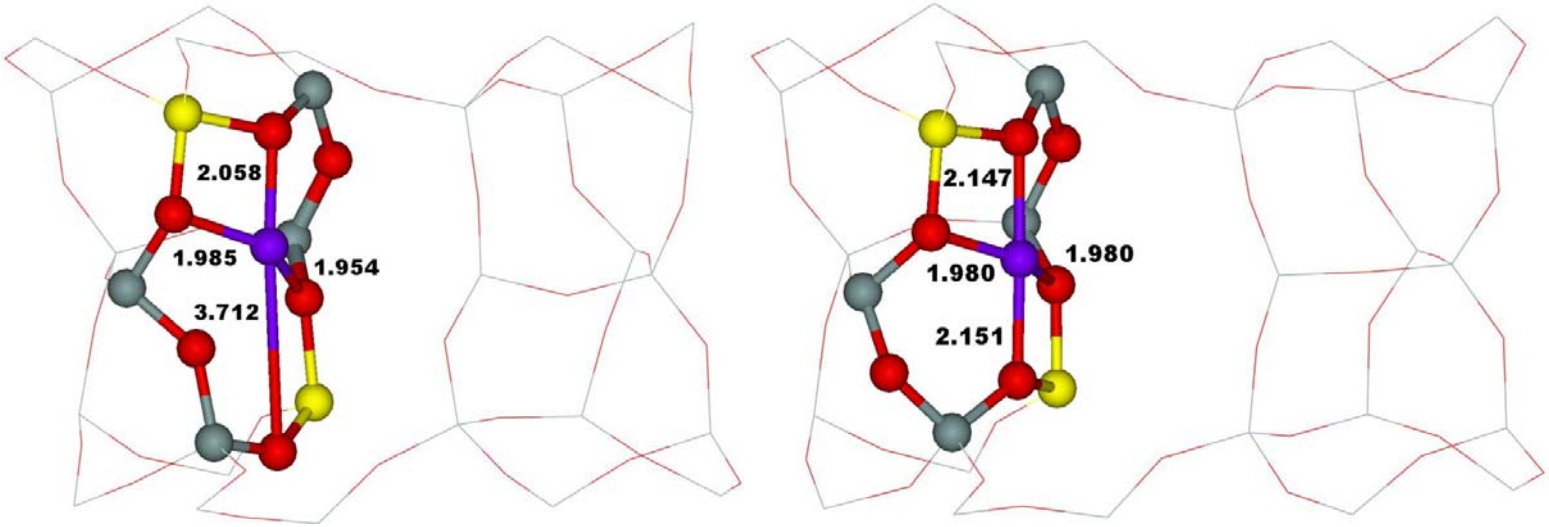


Figure S3

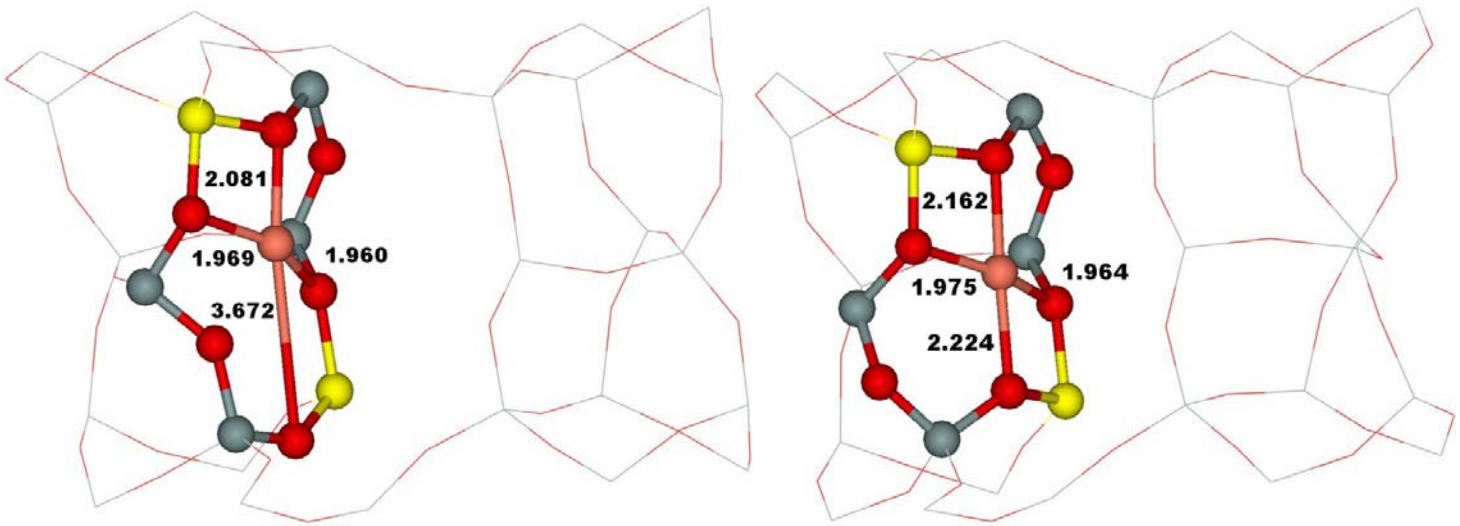


Figure S4

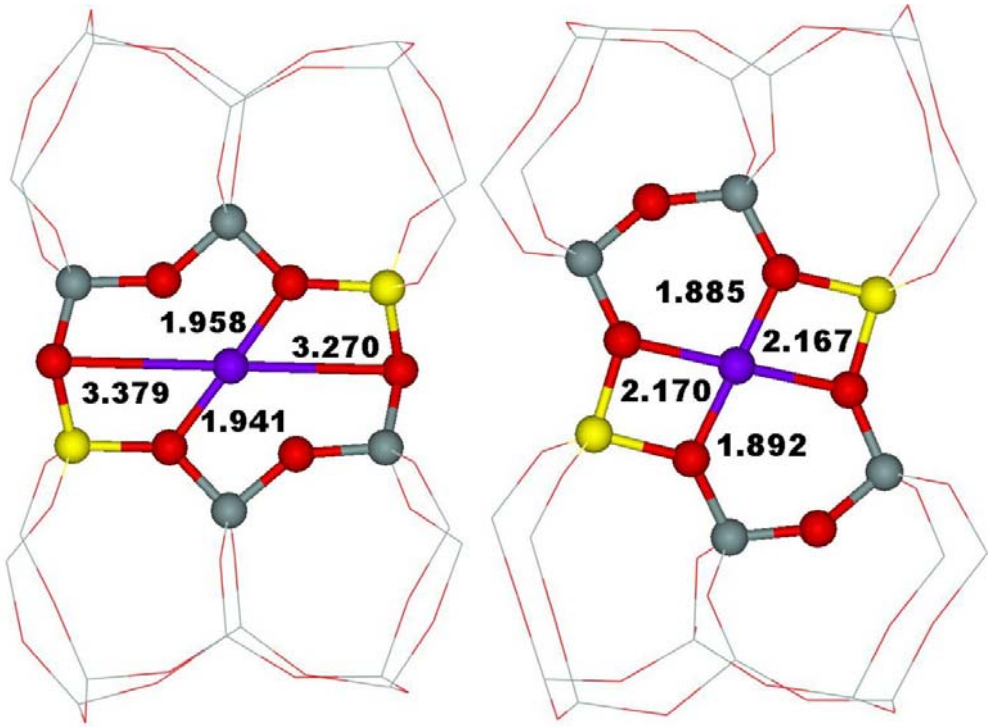


Figure S5

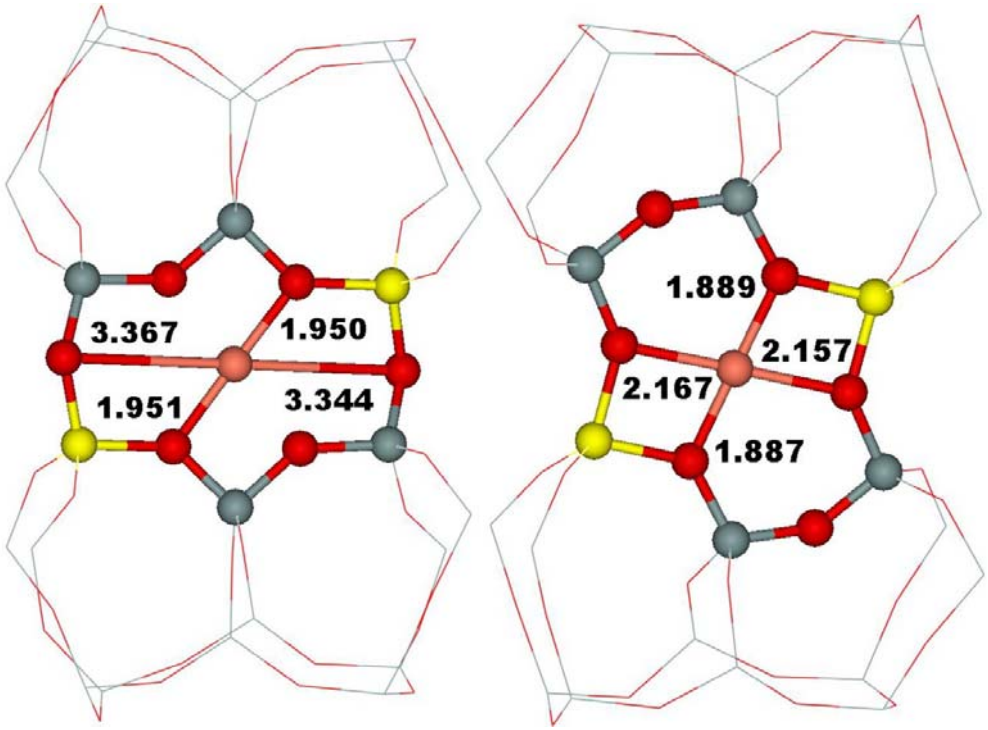
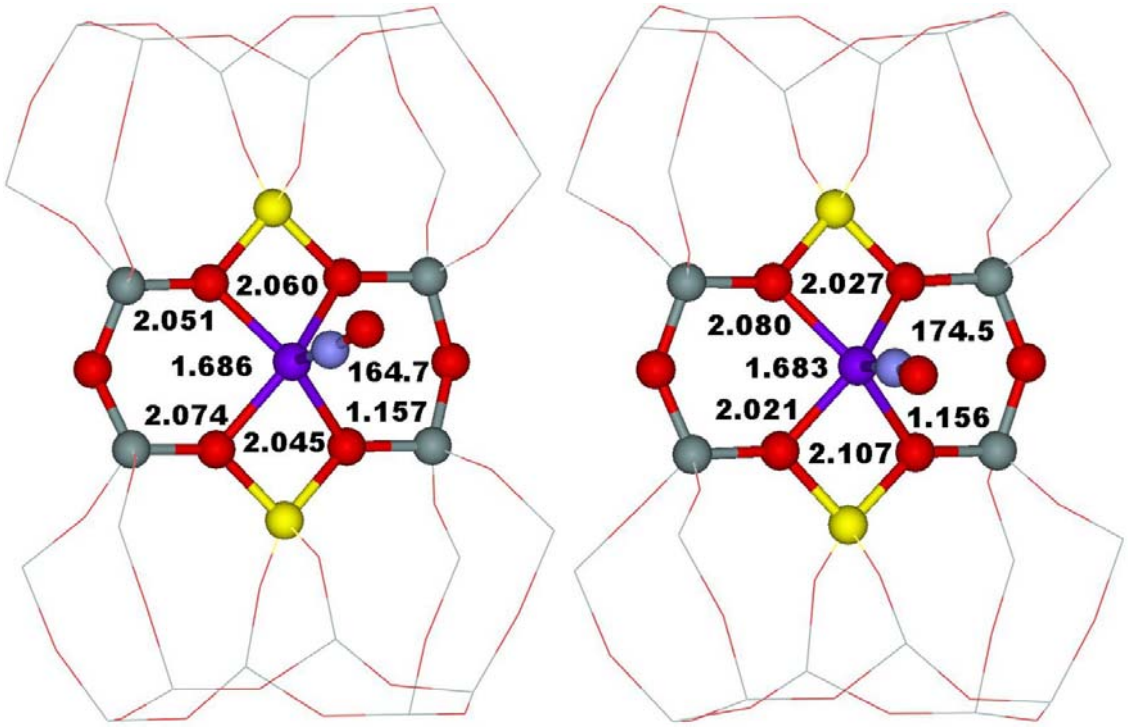


Figure S6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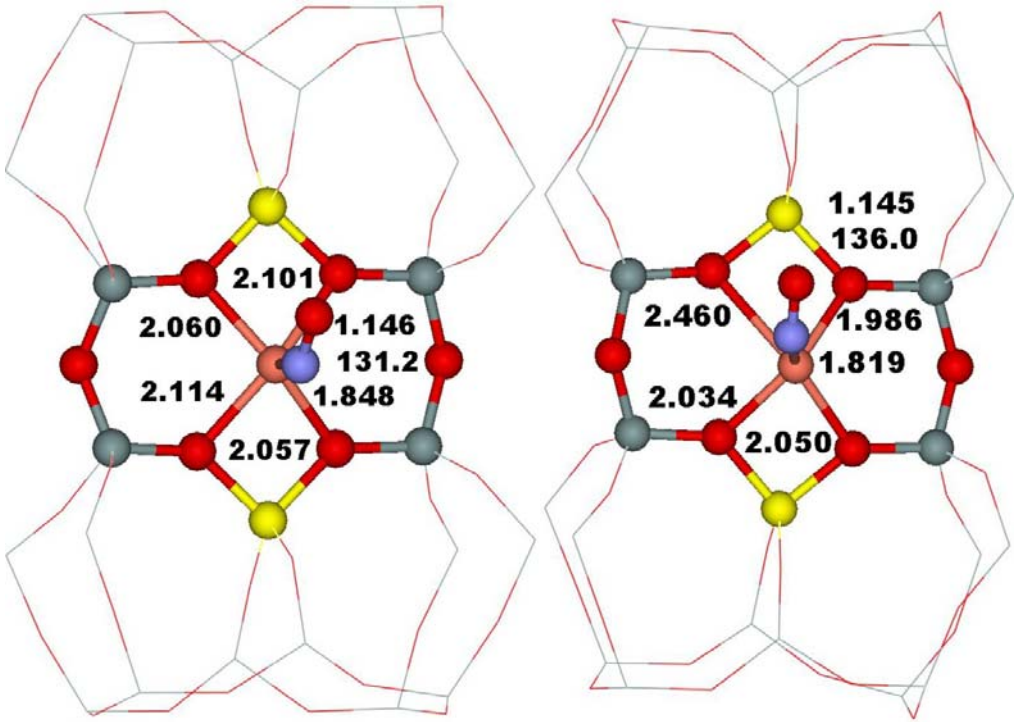
2.051
1.686
164.7
2.074
1.157
2.045
2.027
2.080
174.5
1.683
2.021
1.156
2.107

Figure S7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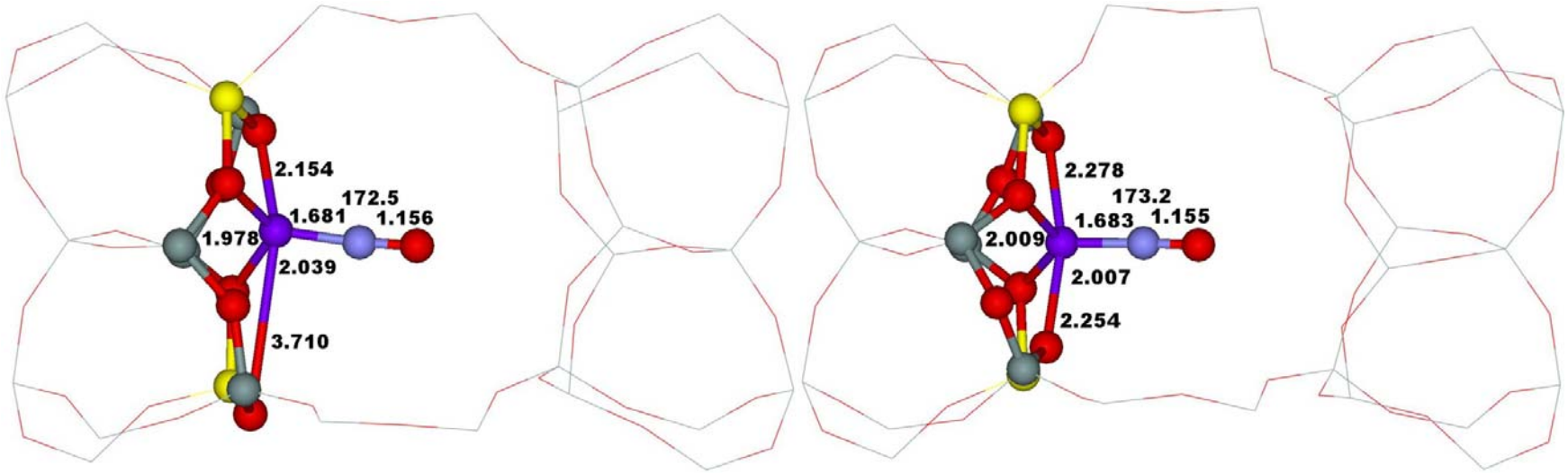
2.060
1.146
131.2
2.114
1.848
2.057
1.145
136.0
2.460
1.986
1.819
2.034
2.050

Figure S8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172.5
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1.156
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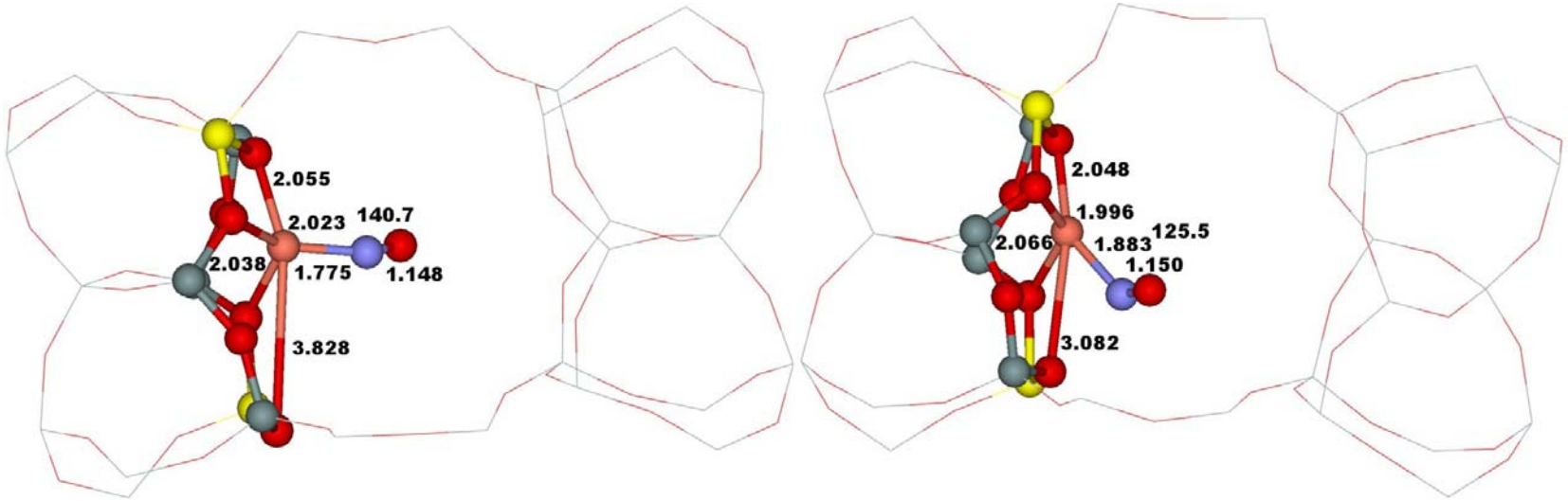
3.710
2.278
173.2
1.683
1.155
2.009
2.007
2.254

Figure S9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2.023
140.7
2.038
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3.828
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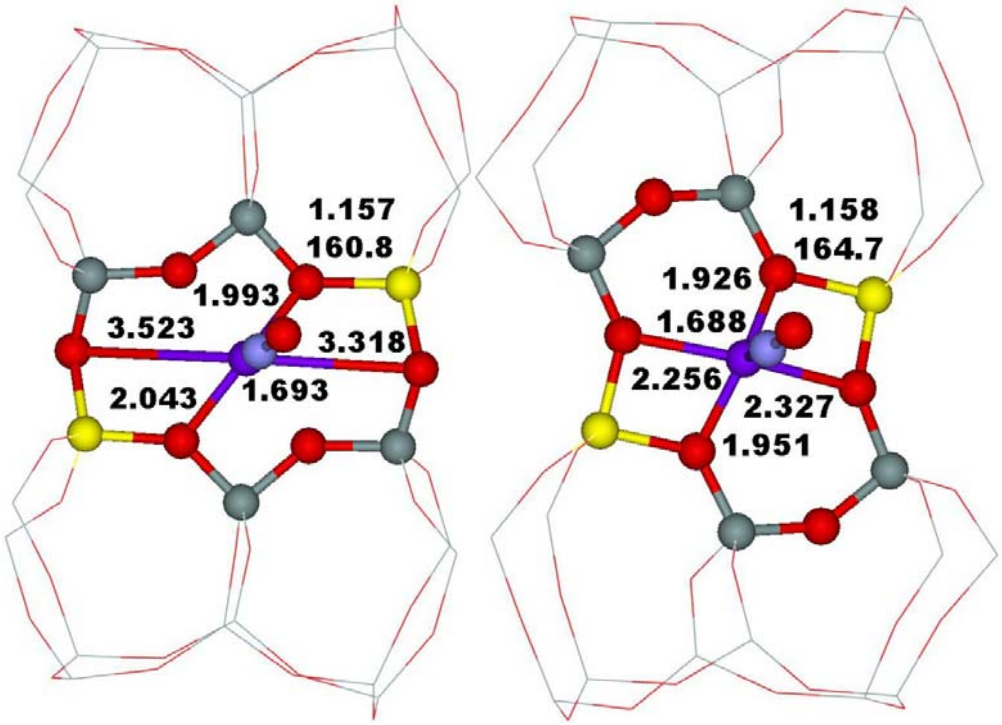
1.996
2.066
1.883
125.5
1.150
3.082

Figure S10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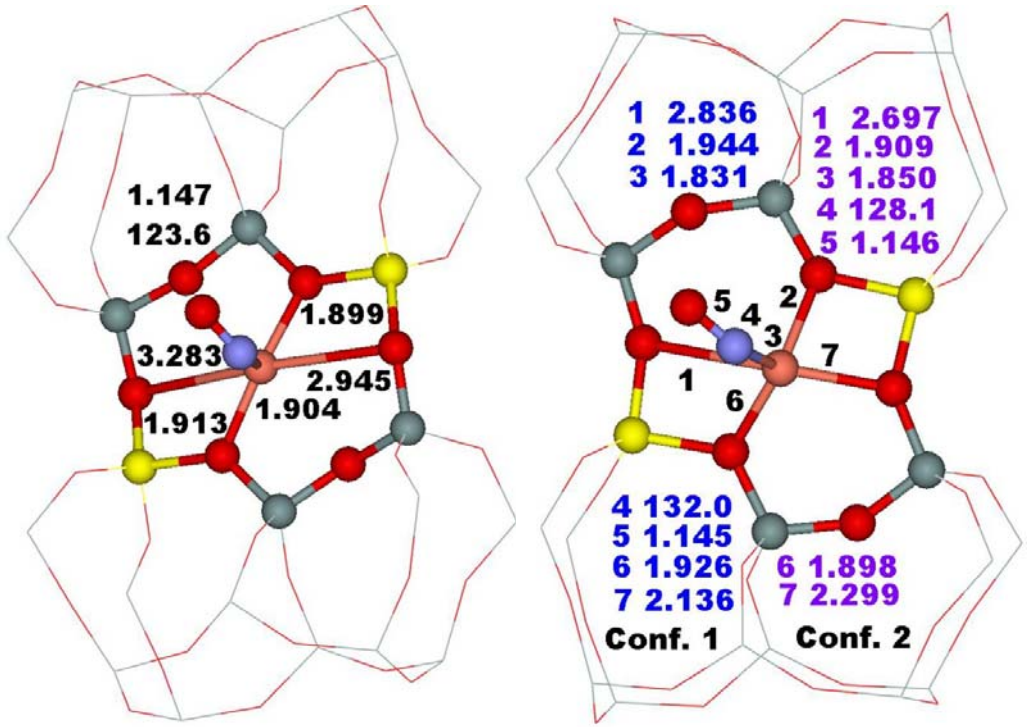
160.8
1.993
3.523
3.318
2.043
1.693
1.158
164.7
1.926
1.688
2.256
2.327
1.951

Figure S11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123.6
1.899
3.283
2.945
1.913
1.904
1 2.836
2 1.944
3 1.831
4 132.0
5 1.145
6 1.926
7 2.136
Conf. 1
1 2.697
2 1.909
3 1.850
4 128.1
5 1.146
6 1.898
7 2.299
Conf. 2
1
2
3
4
5
6
7

Figure S12