

SUPPORTING INFORMATION

Stability of Extraframework Iron-containing Complexes in ZSM-5

Zeolite

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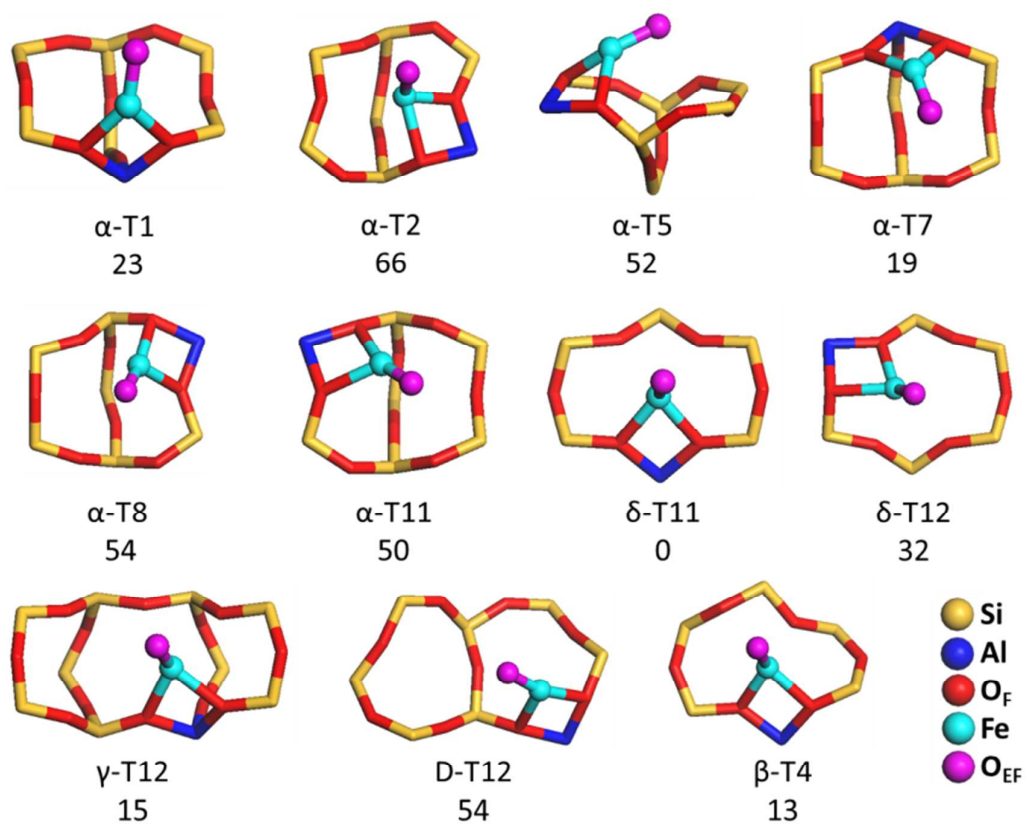


Figure S1: Local structures and relative energies (kJ/mol) of high spin state ($S=5/2$) $[\text{FeO}]^+$ at different positions of ZSM-5.

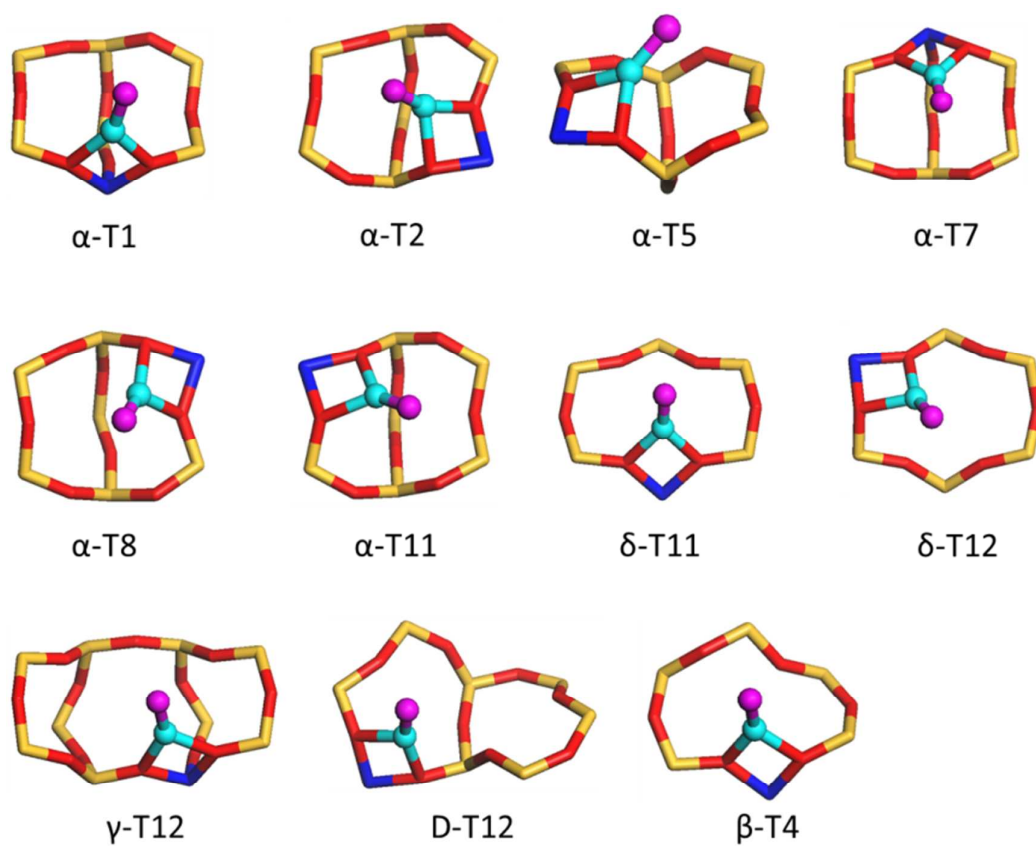


Figure S2: Local structures of low spin state ($S=3/2$) $[\text{FeO}]^+$ at different positions of ZSM-5.

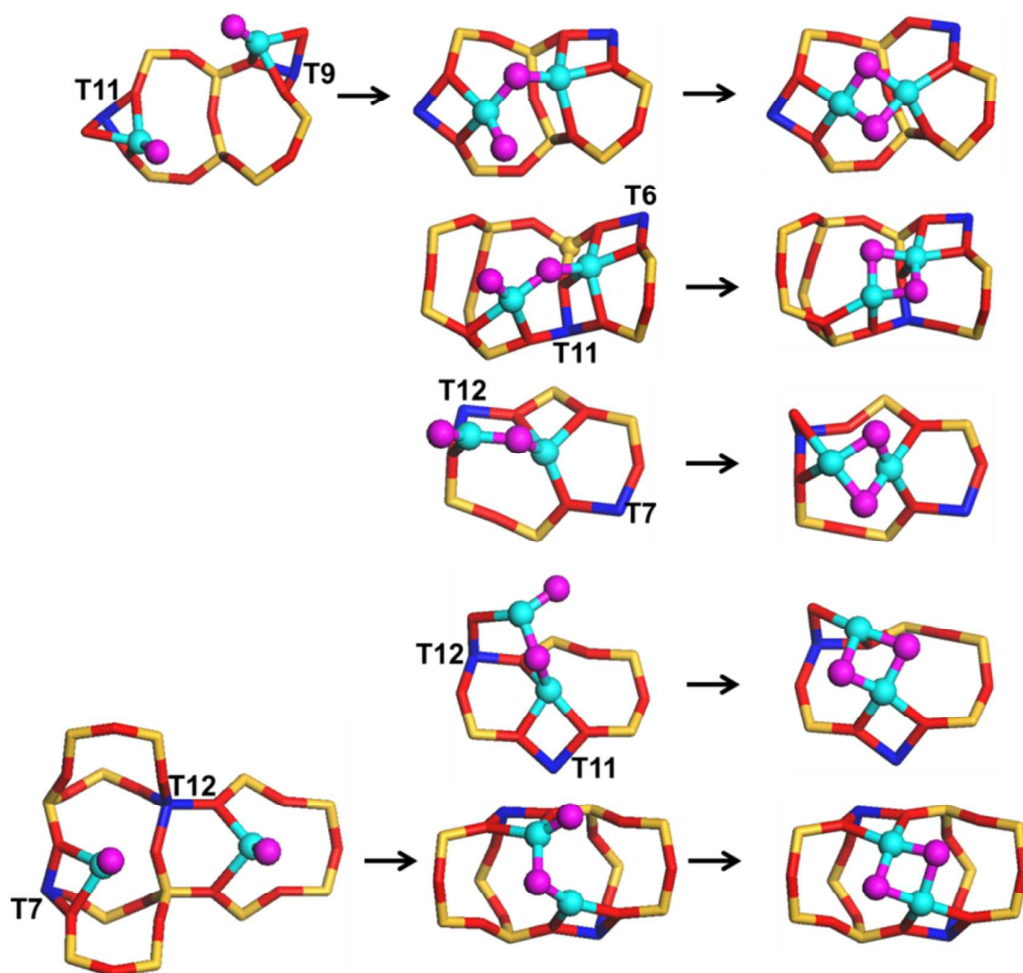
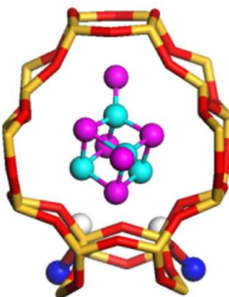
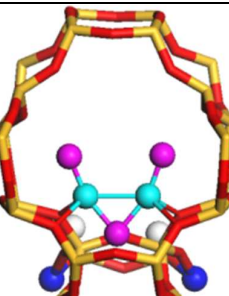
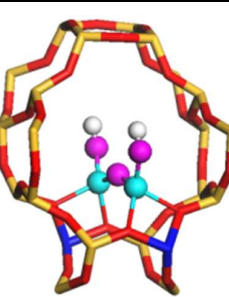
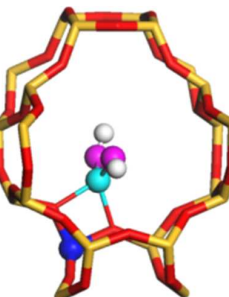
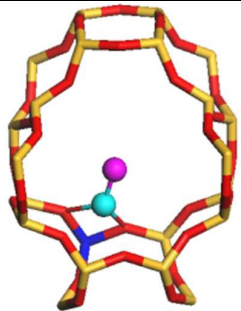
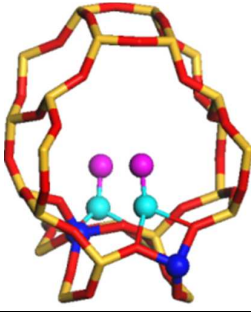
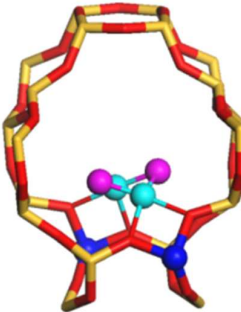
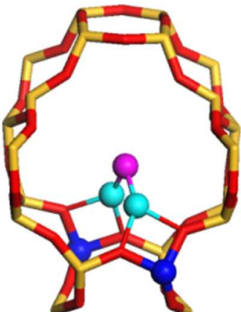
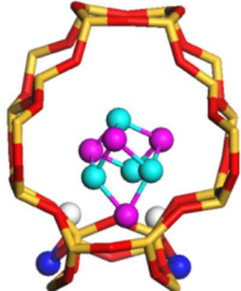
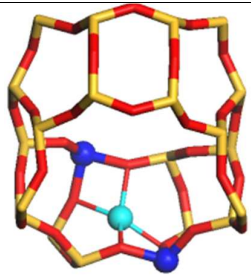
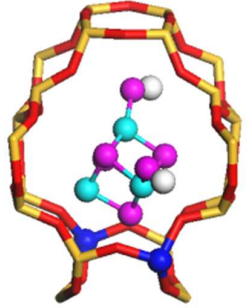
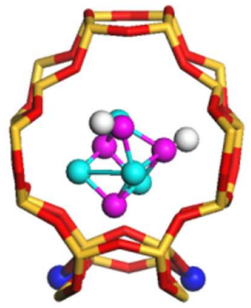
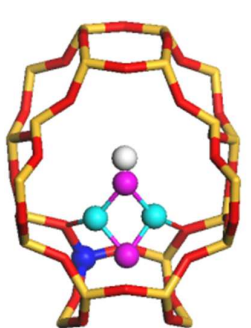


Figure S3: Local structures of isolated dual $[\text{FeO}]^+$ and their self-organization at different positions of ZSM-5.

Table S1. Geometric parameters of iron-containing specie involved in Figure 11.

No. (according to Figure 11)	local structures	$r(\text{Fe-O}_{\text{EF}})/\text{\AA}$	$r(\text{Fe-O}_{\text{F}})/\text{\AA}$
1		1.971, 2.009 1.940, 2.017 1.891, 1.840 1.954, 1.871 2.135, 1.823 1.859, 1.908 1.620, 1.645	2.131 2.251 2.146
2		1.667 1.665 1.855 1.851	2.161 2.213 2.197 2.193
3		1.770 1.764 1.771 1.780	2.030 2.118 2.129 2.003
4		1.806 1.799	2.077 2.052

5		1.673	2.107 2.104
5'		1.680 1.679	2.099 2.168 2.102 2.285
6		1.722 1.956 1.853 1.782	2.003 1.996 2.051 2.075
7		1.794 1.795	2.013 2.065 2.058 2.018
8		1.998, 2.022 1.844, 2.853 2.010, 1.935 1.821, 2.028 2.006, 1.917 1.920, 2.054	2.183 1.951 2.109 2.196

9		—	2.116 2.005 2.072 2.062
10		1.952, 2.046 1.799, 1.846 1.956, 1.921 1.821, 1.908 1.896, 1.873 1.867, 2.269 1.782, 1.773	2.017 2.750 2.263 2.794 2.058 2.055 2.129
11		1.940, 1.929 1.954, 2.004 1.872, 3.270 1.920, 2.017 1.973, 1.979 2.095, 2.055	2.133 2.542 2.540 2.178 2.200
12		1.880 1.858 1.954 1.928	2.029 2.128