

Supplementary Information

Interaction of FeO^- with water: Anion photoelectron spectroscopy and theoretical calculations

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Table S1 Relative energies, ADEs and VDEs (in eV) of the typical low-lying isomers of FeO^- and $\text{FeO}_2\text{H}_2(\text{H}_2\text{O})_{n-1}^-$ ($n = 1-4$) clusters calculated at the B3LYP/6-311+G(d, p) level, as compared to the experimental ADEs and VDEs.

Isomer	$\Delta E(\text{eV})$	ADE(eV)		VDE(eV)	
		Theo.	Expt.	Theo.	Expt.
FeO^-	0.00	1.48	1.52 ± 0.04	1.50	1.52 ± 0.04
FeO_2H_2^-	1A	0.00	1.18	1.10 ± 0.04	1.36
	1B	0.00	1.18		1.36
	1C	1.29	2.62		2.80
	1D	2.01	1.29		2.01
$\text{FeO}_2\text{H}_2(\text{H}_2\text{O})^-$	2A	0.00	1.29	1.48 ± 0.04	1.85
	2B	0.00	1.29		1.85
	2C	0.79	2.53		3.05
	2D	0.89	2.36		3.13
$\text{FeO}_2\text{H}_2(\text{H}_2\text{O})_2^-$	3A	0.00	1.45	1.85 ± 0.04	2.30
	3B	0.07	1.13		2.22
	3C	0.11	1.09		2.32
	3D	0.61	3.11		3.64
	3E	0.77	2.78		3.61
$\text{FeO}_2\text{H}_2(\text{H}_2\text{O})_3^-$	4A	0.00	1.30	2.11 ± 0.04	2.67
	4B	0.02	2.09		2.58
	4C	0.04	1.25		2.58
	4D	0.05	1.28		2.79
	4E	0.06	1.16		2.52
	4F	0.07	1.06		2.41
	4G	0.12	1.10		2.48
	4H	0.15	0.98		2.55
	4I	0.20	1.61		2.38
	4J	0.55	2.86		4.00

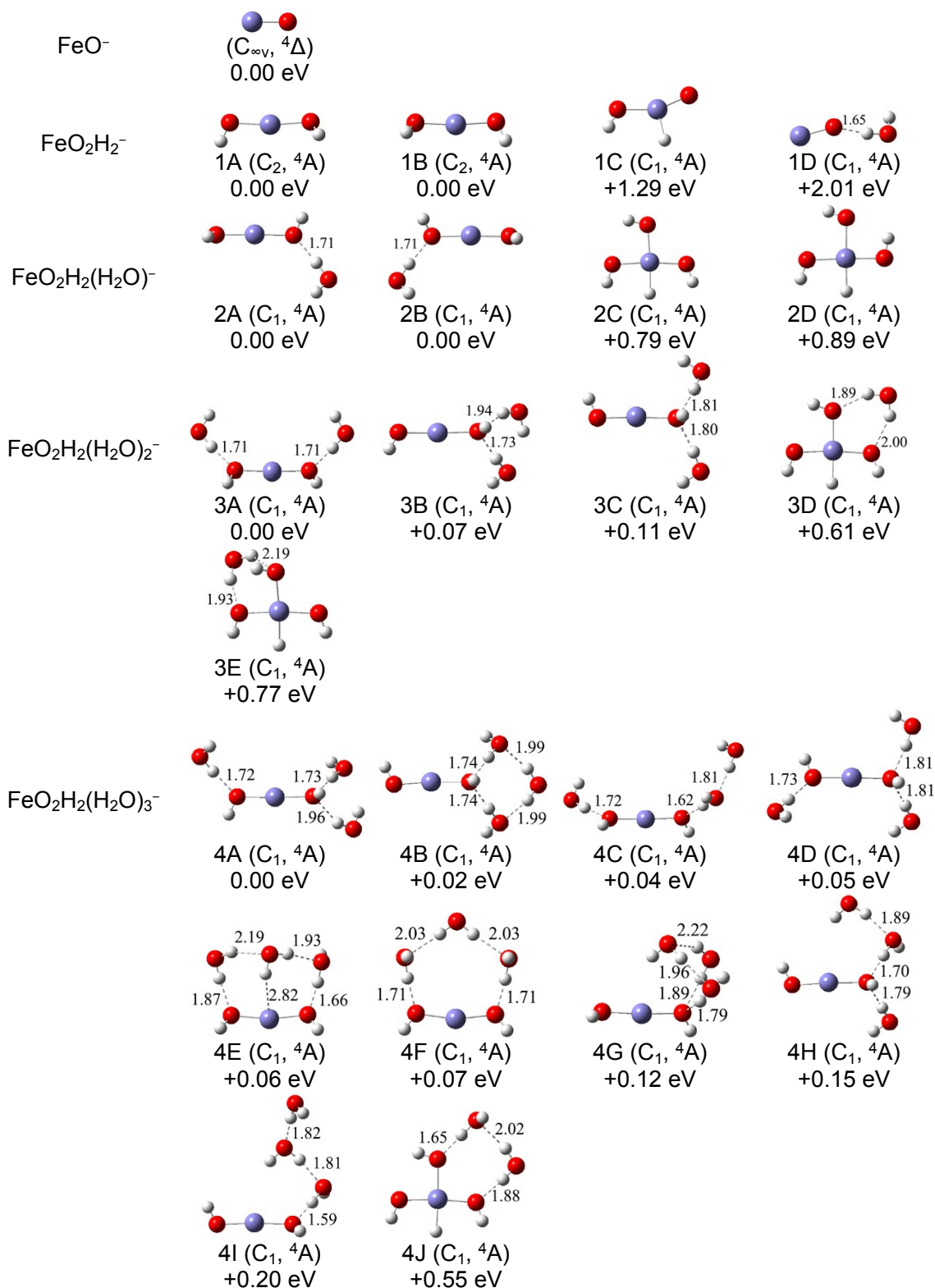


Fig. S1 Typical low-lying isomers of FeO^- and $\text{FeO}_2\text{H}_2(\text{H}_2\text{O})_{n-1}^-$ ($n = 1-4$) clusters. The $\text{O}\cdots\text{H}$ bond distances (in Å) are labeled. The symmetries and spin multiplicities are shown under the structures. Their relative energies (in eV) to the most stable isomers at the B3LYP/6-311+G(d, p) level are listed.

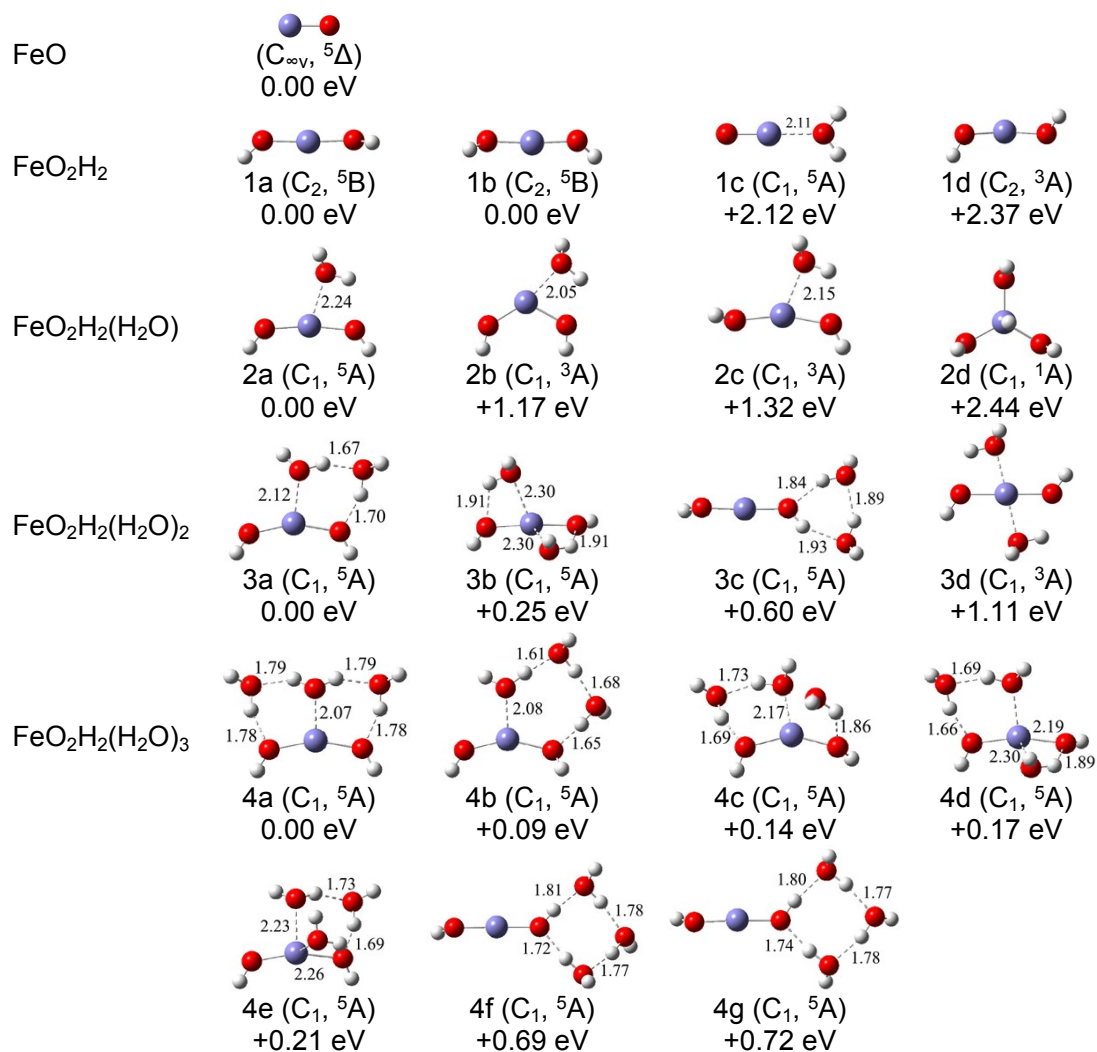


Fig. S2 Typical low-lying isomers of FeO and FeO₂H₂(H₂O)_{*n*-1}⁻ (*n* = 1–4) clusters. The O···H bond distances (in Å) are labeled. The symmetries and spin multiplicities are shown under the structures. Their relative energies (in eV) to the most stable isomers at the B3LYP/6-311+G(d, p) level are listed.

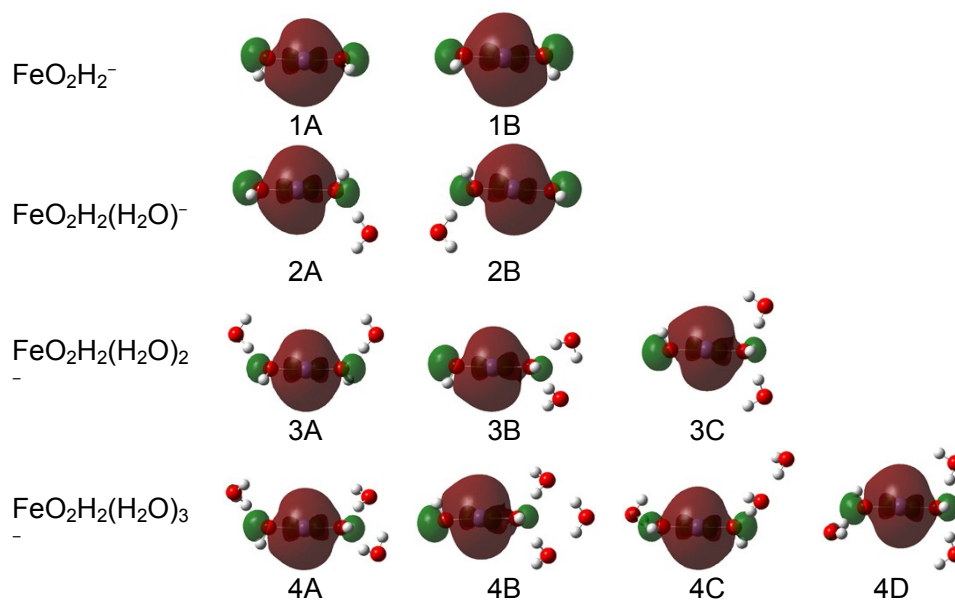


Fig. S3 Highest occupied molecular orbitals (HOMOs) of the typical isomers of $\text{FeO}_2\text{H}_2(\text{H}_2\text{O})_{n-1}^-$ ($n = 1-4$).