

Electronic Supplementary Information

Dissolution Mechanism of Fe₃O₄ Scale by 1-Hydroxyethane-1,1-Diphosphonic Acid: an *Ab Initio* Molecular Metadynamics Study

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Table S1 Experimental results of dissolution of iron scale by organic acid

Abbreviation	Name	Whether iron scale is dissolved
HEDP	1-Hydroxyethane-1,1-diphosphonic Acid	Yes
PBTCA	2-Phosphonobutane-1,2,4-tricarboxylic Acid	No
ATMP	Amino Trimethylene Phosphonic Acid	No
EDTMP	Ethylenediamine Tetramethylenephosphonic Acid	No
BHMTMPMPA	Bis(Hexamethylene Triamine Penta (Methylene Phosphonic Acid))	No
DTPMP	Diethylenetriaminepenta(methylene-phosphonic acid)	No
HDTMP	Hexamethylenediamine-N,N,N',N'-tetrakis(methylenephosphonic acid)	No
PAPEMP	Polyamino Polyether Methylene Phosphonate	No

Note: The iron scale was collected from Pingdingshan Halon Salt Co. Ltd. After chemical analysis, the purity of Fe₃O₄ is 98.5 wt%. The samples were stored in a dry and cool place before use. The organic acids were obtained from Shandong Taihe Technologies Co., Ltd. with a purity of 97 %. At room temperature, 200 ml of 5 wt% organic acid solution and 3.00 g iron scale samples were added to the beaker for 12 hours. In addition to HEDP, the iron scale cannot be dissolved after 30 days of soaking with other organic acids. The entire process was conducted at room temperature. The experimental results are taken from Ref 1.

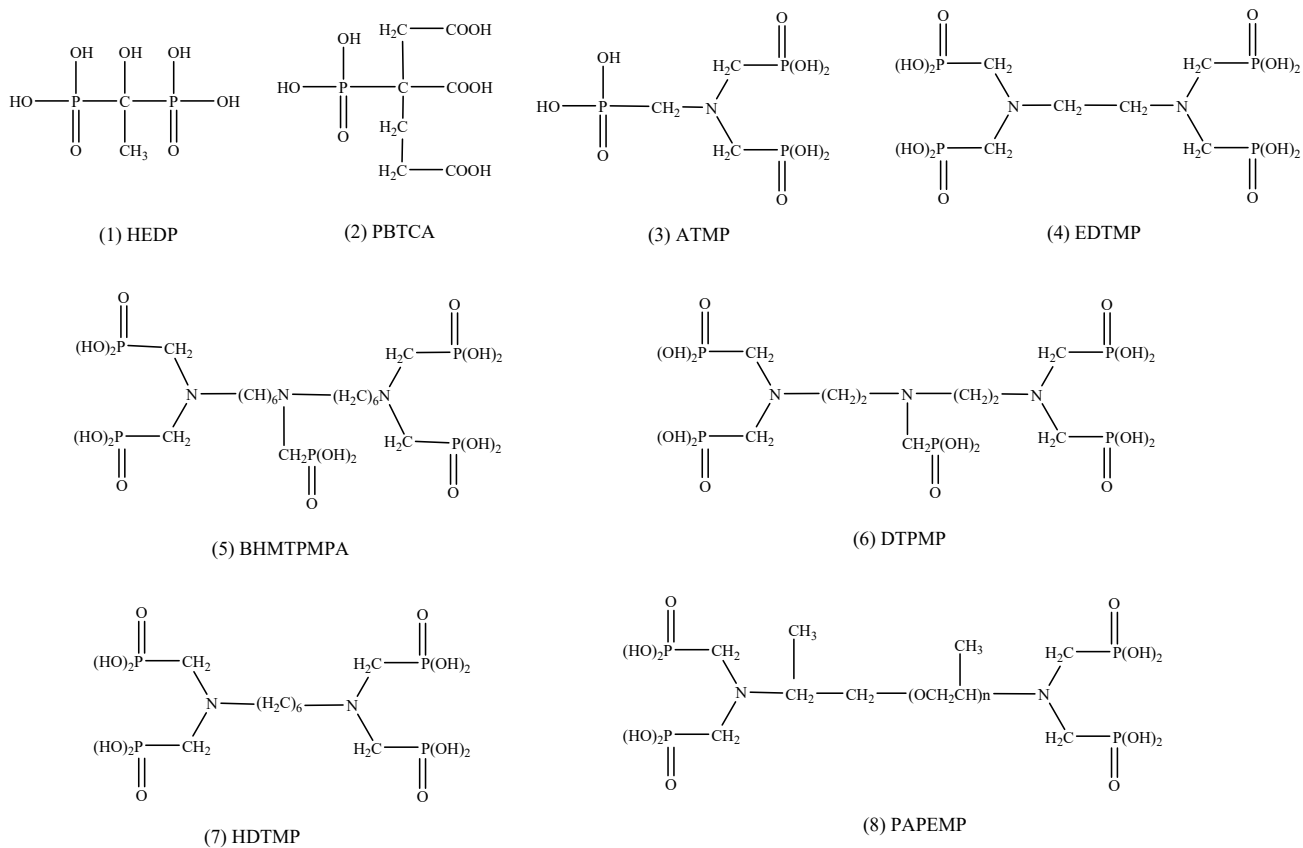


Figure S1. The structure formula of organic acid

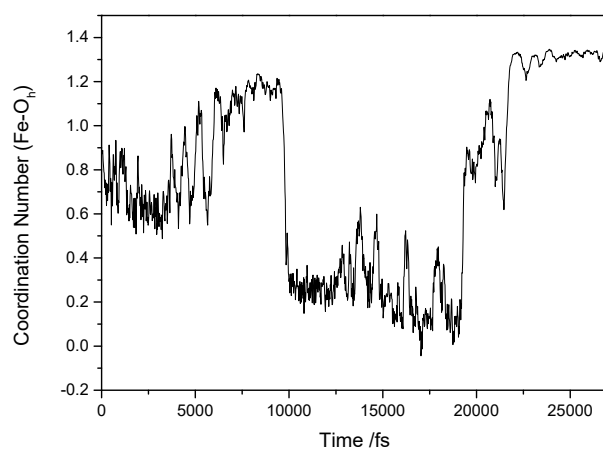


Figure S2. The change in coordination number between O atoms of HEDP and Fe³⁺ ion

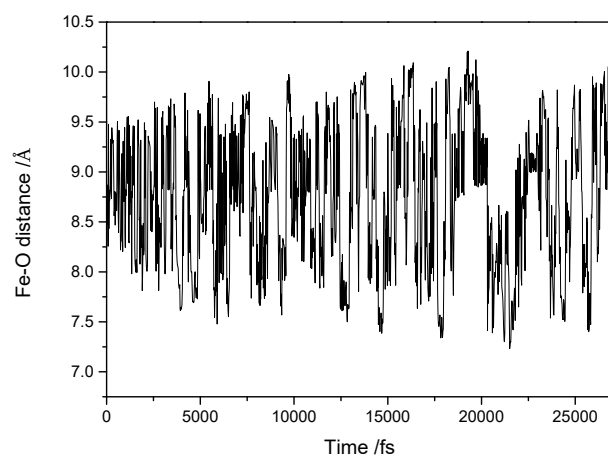
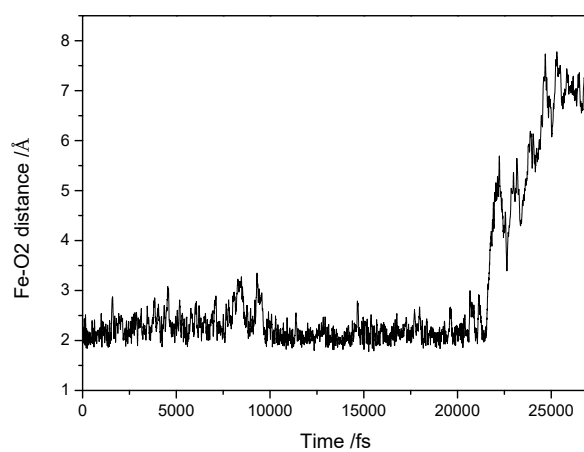
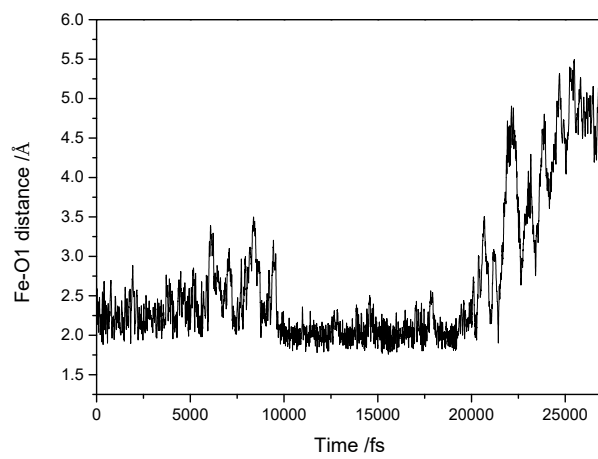


Figure S3. The change in four bond lengths between the Fe^{3+} ion and the four O atoms of HEDP



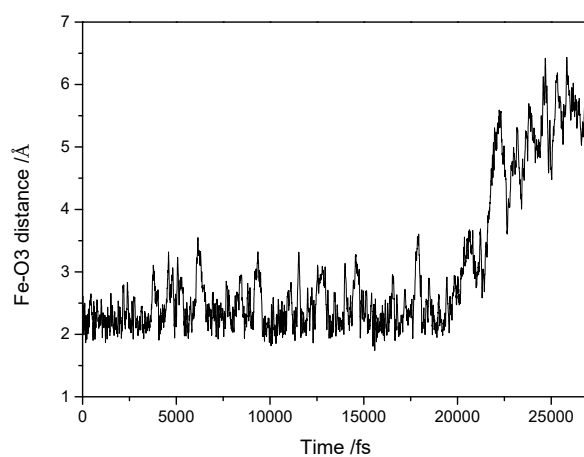


Figure S4. The change in bond lengths of the Fe^{3+} ion with the original O atoms

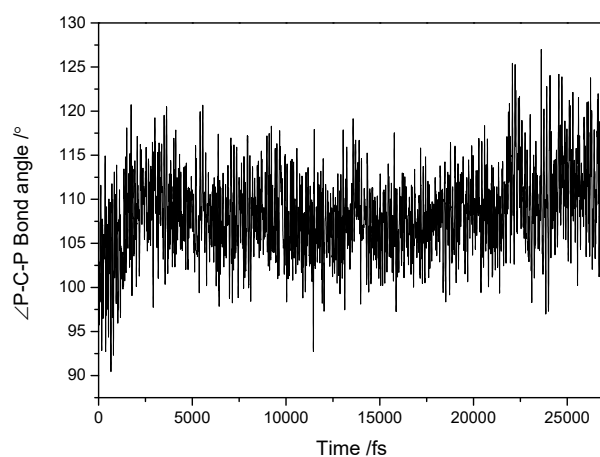


Figure S5. The change in bond angle of $\angle\text{P-C-P}$ angles of HEDP

Reference:

1. X. Zhao, S. Li, M. Su and S. Xu, *Journal of Molecular Science*, 2015, 31, 276-282. (In Chinese)