Electronic supplementary information for:

"A Computational Study of the Interaction of Organic Surfactants with Goethite α-FeO(OH) Surfaces"

David Santos-Carballal,[*ab] Zhimei Du,[a] Helen E. King[c] and Nora H. de Leeuw[*abc]

Electronic supplementary information (ESI) contains the interatomic potentials for the interaction of methanoic acid, hydroxamic acid and hydroxyethanal with goethite.

[a] *School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, United Kingdom. (D.S.-C.) E-mail: SantosCarballalD@cardiff.ac.uk; Tel: +44 (0)29 2087 0827. (N.H.d.L.) E-mail: DeLeeuwN@cardiff.ac.uk; Tel: +44 (0)29 2087 0658*
[b] *Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom*
[c] *Department of Earth Sciences, Utrecht University, Budapestlaan 4, 3584 CD Utrecht, The Netherlands*

Table ESI-1 Interatomic potential parameters for the interaction between methanoic acid (MA) and goethite (G) surfaces (short-range cut-off 20 Å)

Ion	Charges (e)		
	Core	Shell	Core-shell interaction (eV Å^{-2})
Fe	+3.000		
H	+0.400		
OX	+1.000	−3.000	60.78000
OH	+0.900	−2.300	74.92038
OD	−0.380		
OH1	−0.380		
C	+0.310		
HC	+0.100		
HO	+0.350		
Ion pair	Buckingham potential parameters		
	A (eV)	ρ (Å)	C (eV Å^6)
Fe – OD	209.50	0.3299	0.00
Fe – OH1	209.50	0.3299	0.00
OX (shell) − OD	11994.00	0.2130	24.55
OX (shell) – OH1	11994.00	0.2130	24.55
OH (shell) − OD	8395.80	0.2130	12.27
OH (shell) – OH1	8395.80	0.2130	12.27
OX (shell) − C	2237.50	0.2600	0.00
OH (shell) − C	1566.25	0.2600	0.00
OX (shell) − HO	396.27	0.2500	0.00
OX (shell) − HC	396.27	0.2500	0.00
OH (shell) − HO	311.97	0.2500	0.00
OH (shell) − HC	311.97	0.2500	0.00
Ion pair	Lennard-Jones potential parameters		
	A (eV Å^{12})		B (eV Å^6)
H − OD	1908.1		5.55
H − O	1908.1		5.55

H G hydroxy hydrogen atom, *OX* G oxygen ion, *OH* G hydroxy oxygen atom, *OD* MA carbonyl oxygen atom, *OH1* MA hydroxy oxygen atom, *HC* MA hydrogen attached to carbon atom, *HO* MA hydroxy hydrogen atom.

Table ESI-2 Interatomic potential parameters for the interaction between hydroxamic acid (HA) and goethite (G) surfaces (short-range cut-off 20 Å)

Ion	Charges (e)		
	Core	Shell	Core-shell interaction (eV Å^{-2})
Fe	+3.000		
H	+0.400		
OX	+1.000	−3.000	60.78000
OH	+0.900	−2.300	74.92038
OD	−0.380		
OH1	−0.208		
CD	+0.167		
HC	+0.213		
HO	+0.350		
N	−0.422		
HN	+0.280		
Ion pair	Buckingham potential parameters		
	A (eV)	*ϱ* (Å)	*C* (eV Å^6)
Fe – OH1	114.65	0.3299	0.00
Fe – OD	209.46	0.3299	0.00
Fe – N	232.61	0.3299	0.00
OX (shell) – OH1	6565.14	0.2130	24.54
OX (shell) – OD	11994.00	0.2130	24.54
OX (shell) – N	13319.65	0.2130	24.54
OH (shell) – OH1	4595.60	0.2130	12.27
OH (shell) – OD	8395.80	0.2130	12.27
OH (shell) – N	9323.76	0.2130	12.27
OX (shell) – CD	2237.50	0.2600	0.00
OH (shell) – CD	1566.25	0.2600	0.00
OX (shell) – HC	396.27	0.2500	0.00
OX (shell) – HN	396.27	0.2500	0.00
OX (shell) – HO	396.27	0.2500	0.00
OH (shell) – HC	311.97	0.2500	0.00
OH (shell) – HN	311.97	0.2500	0.00
OH (shell) – HO	311.97	0.2500	0.00
Ion pair	Lennard-Jones potential parameters		
	A (eV Å^{12})		*B* (eV Å^6)
H – O	1908.1		5.55
H – OD	1908.1		5.55
H – N	5499.1		8.71

H G hydroxy hydrogen atom, *OX* G oxygen ion, *OH* G hydroxy oxygen atom, *OD* HA carbonyl oxygen atom, *OH1* HA hydroxy oxygen atom, *HC* HA hydrogen attached to carbon atom, *HO* HA hydroxy hydrogen atom, *HN* HA hydrogen attached to nitrogen atom.

Table ESI-3 Interatomic potential parameters for the interaction between hydroxyethanal (HE) and goethite (G) surfaces (short-range cut-off 20 Å)

Ion	Charges (e)		
	Core	Shell	Core-shell interaction (eV Å^{-2})
Fe	+3.000		
H	+0.400		
OX	+1.000	−3.000	60.78000
OH	+0.900	−2.300	74.92038
COH	−0.170		
HCO	+0.213		
OD	−0.380		
OH1	−0.380		
CD	+0.167		
HC	+0.100		
HO	+0.350		
Ion pair	Buckingham potential parameters		
	A (eV)	ϱ (Å)	C (eV Å^6)
Fe − COH	93.70	0.3299	0.00
Fe − OD	209.50	0.3299	0.00
Fe − OH1	209.50	0.3299	0.00
OX (shell) − COH	5365.73	0.2130	25.26
OX (shell) − OD	11994.00	0.2130	24.54
OX (shell) − OH1	11994.00	0.2130	24.54
OH (shell) − COH	3756.00	0.2130	12.63
OH (shell) − OD	8395.80	0.2130	12.27
OH (shell) − OH1	8395.80	0.2130	12.27
OX (shell) − CD	2237.50	0.2600	0.00
OH (shell) − CD	1566.25	0.2600	0.00
OX (shell) − HCO	396.27	0.2500	0.00
OX (shell) − HO	396.27	0.2500	0.00
OX (shell) − HC	396.27	0.2500	0.00
OH (shell) − HCO	311.97	0.2500	0.00
OH (shell) − HO	311.97	0.2500	0.00
OH (shell) − HC	311.97	0.2500	0.00
Ion pair	Lennard-Jones potential parameters		
	A (eV Å^{12})		B (eV Å^6)
H − COH	1908.1		5.55
H − OD	1908.1		5.55
H − OH1	1908.1		5.55

H G hydroxy hydrogen atom, *OX* G oxygen ion, *OH* G hydroxy oxygen atom, *COH* HE carbon atom attached to hydroxy group, *HCO* HE hydrogen atom attached to carbonyl carbon atom, *OD* HE carbonyl oxygen atom, *OH1* HE hydroxy oxygen atom, *CD* HE carbonyl carbon atom, *HC* HE hydrogen atom attached to *COH*, *HO* HE hydroxy hydrogen atom.