

SPECIES			
Ion	Charges (e)		Core-shell int. (eV Å ⁻²)
	Core	Shell	
Iron (Fe)	3.000	-	-
Chlorine (Cl)	1.485	-2.485	29.38
Sodium (Na)	1.000	-	-
Oxygen (O)	0.210	-2.210	27.4000
Water Oxygen (Ow)	1.250	-2.050	209.45
Hydroxide Oxygen (Oh)	0.900	-2.300	74.9204
Hydrogen (H)	0.400	-	-
Calcium (Ca)	2.000	-	-
Carbon (C)	1.135	-	-
Carbonate Oxygen (Oc)	0.587	-1.632	507.4

BUCKINGHAM POTENTIALS $A_{ij}\exp(-r_{ij}/\rho_{ij}) - (C_{ij}/r_{ij}^6)$			
Ion pair (<i>ij</i>)	A_{ij} (eV)	ρ_{ij} (Å)	C_{ij} (eV Å ⁶)
Na-O	1226.840	0.3065	-
Na-Oh	858.790	0.3065	-
Na-Ow	2334.720	0.2387	-
Na-Cl	2314.700	0.2903	-
Fe-O	1102.400	0.3299	-
Fe-Oh	771.400	0.3299	-
Fe-Ow	440.800	0.3372	-
Fe-Cl	738.400	0.4161	-
H-O	396.270	0.2500	-
H-Oh	311.970	0.2500	-
Cl-O	1272.249	0.2352	34.99827
Cl-Oh	1272.249	0.2352	34.99827
Cl-Cl	1227.200	0.3214	29.06000
Oh-Oh	22764.30	0.1490	6.97
Oh-O	22764.30	0.1490	13.94
Oh-Ow	22764.30	0.1490	15.46
O-O	22764.30	0.1490	27.88
O-Ow	22764.30	0.1490	15.46
Ca-Oc	1550.0	0.2970	-
Oc-Oc	16372.0	0.2130	3.47
C-Ow	435.00	0.3400	0.00
Ca-Ow	1186.60	0.2970	0.00
Oc-Ow	12533.60	0.2130	12.09

LENNARD-JONES POTENTIALS $(A_{ij}/r_{ij}^n) - (B_{ij}/r_{ij}^m)$				
Ion pair (<i>ij</i>)	A_{ij} (eV Å ^{<i>n</i>})	B_{ij} (eV Å ^{<i>m</i>})	<i>n</i>	<i>m</i>
H-Ow	24.0	6.0	9	6
H-Cl	147.01	16.36	9	6
Cl-Ow	141959.17	159.85	12	6
Ow-Ow	39344.98	42.15	12	6
Hw-Oc	26.0	1.8	12	10

MORSE POTENTIALS $D_{ij}(1 - \exp(-\alpha_{ij}(r_{ij} - r_0))) - D_{ij} - C_{ij}(Q_i Q_j / r_{ij})$				
Ion pair (<i>ij</i>)	D_{ij} (eV)	α_{ij} (Å ⁻¹)	r_0 (Å)	C_{ij} (%)
Oh-H	7.052500	3.17490	0.92580	100
Ow-H	6.203713	2.22003	0.92376	50
H-H	0.00	2.8405	1.50000	50
C-Oc	4.71	3.80	1.18	0

THREE-BODY POTENTIALS $(k_{ijk}/2)(\theta_{ijk} - \theta_0)^2$			
Ions	k (eV rad ²)	θ (°)	
H-Ow-H	4.19978	108.69	
Oc-C-Oc	1.69	120	
FOUR BODY POTENTIALS $A[1 + \cos(m\phi_{ijkl} - \delta)]$			
Ions	A (eV)	δ (°)	m
Oc-C-Oc-Oc	0.11290	180	2.0