Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

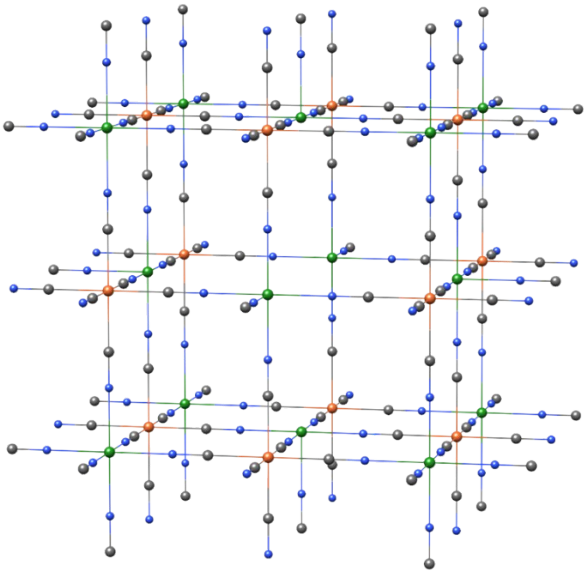

Figure S1. Defective Prussian blue (d-PB) with added cyanide ligand. The Fe^{III} ion is presented in green, Fe^{II} in orange, C in grey and N in blue. Those added ligand were removed before performing the 3D-RISM calculation.

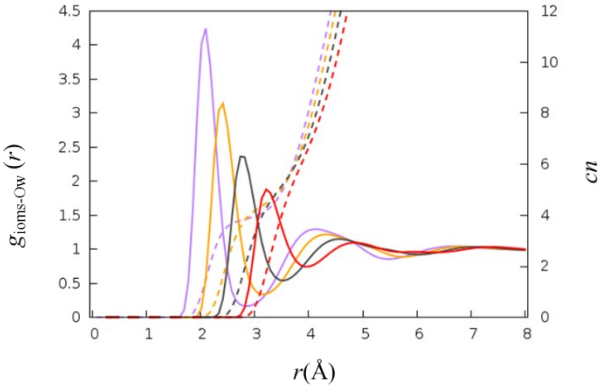

Fig. S2 Radial distribution functions (RDF) between oxygen of bulk water (O_w) and all cation species (full lines), Li^+ shown in pink, Na^+ in orange, K^+ in grey, and Cs^+ in red. The coordination number (*cn*) of each ion specie is indicated by a dashed line with the same defined colour.

Table S1. Atomic coordinates and ESP charges from B3LYP/6-31G(d) level of theory.

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
1	Fe	-5.083	-5.083	-5.083	-0.2564
2	Fe	-5.083	-5.083	0.000	-2.1587
3	Fe	-5.083	-5.083	5.083	-0.2564
4	Fe	-5.083	0.000	-5.083	-2.1105
5	Fe	-5.083	0.000	0.000	1.7042
6	Fe	-5.083	0.000	5.083	-2.1105
7	Fe	-5.083	5.083	-5.083	-0.2564
8	Fe	-5.083	5.083	0.000	-2.1587
9	Fe	-5.083	5.083	5.083	-0.2564
10	Fe	0.000	-5.083	-5.083	-2.1360
11	Fe	0.000	-5.083	0.000	1.7074
12	Fe	0.000	-5.083	5.083	-2.1360
13	Fe	0.000	0.000	-5.083	1.5468
14	Fe	0.000	0.000	5.083	1.5468
15	Fe	0.000	5.083	-5.083	-2.1360
16	Fe	0.000	5.083	0.000	1.7074
17	Fe	0.000	5.083	5.083	-2.1360
18	Fe	5.083	-5.083	-5.083	-0.2564
19	Fe	5.083	-5.083	0.000	-2.1587
20	Fe	5.083	-5.083	5.083	-0.2564
21	Fe	5.083	0.000	-5.083	-2.1105
22	Fe	5.083	0.000	0.000	1.7042
23	Fe	5.083	0.000	5.083	-2.1105
24	Fe	5.083	5.083	-5.083	-0.2564
25	Fe	5.083	5.083	0.000	-2.1587
26	Fe	5.083	5.083	5.083	-0.2564
27	C	-5.083	-5.083	-1.923	0.2428
28	C	-5.083	-5.083	1.923	0.2428
29	C	-5.083	-3.160	0.000	0.9015
30	C	-5.083	-1.923	-5.083	0.2347
31	C	-5.083	-1.923	5.083	0.2347
32	C	-5.083	0.000	-3.160	0.8860
33	C	-5.083	0.000	3.160	0.8860
34	C	-5.083	1.923	-5.083	0.2347
35	C	-5.083	1.923	5.083	0.2347
36	C	-5.083	3.160	0.000	0.9015
37	C	-5.083	5.083	-1.923	0.2428
38	C	-5.083	5.083	1.923	0.2428

39	C	-3.160	-5.083	0.000	0.9010
40	C	-3.160	0.000	-5.083	0.8637
41	C	-3.160	0.000	5.083	0.8637

Table S1 (continued)

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
42	C	-3.160	5.083	0.000	0.9010
43	C	-1.923	-5.083	-5.083	0.2399
44	C	-1.923	-5.083	5.083	0.2399
45	C	-1.923	5.083	-5.083	0.2399
46	C	-1.923	5.083	5.083	0.2399
47	C	0.000	-5.083	-3.160	0.8899
48	C	0.000	-5.083	3.160	0.8899
49	C	0.000	-3.160	-5.083	0.8851
50	C	0.000	-3.160	5.083	0.8851
51	C	0.000	3.160	-5.083	0.8851
52	C	0.000	3.160	5.083	0.8851
53	C	0.000	5.083	-3.160	0.8899
54	C	0.000	5.083	3.160	0.8899
55	C	1.923	-5.083	-5.083	0.2399
56	C	1.923	-5.083	5.083	0.2399
57	C	1.923	5.083	-5.083	0.2399
58	C	1.923	5.083	5.083	0.2399
59	C	3.160	-5.083	0.000	0.9010
60	C	3.160	0.000	-5.083	0.8637
61	C	3.160	0.000	5.083	0.8637
62	C	3.160	5.083	0.000	0.9010
63	C	5.083	-5.083	-1.923	0.2428
64	C	5.083	-5.083	1.923	0.2428
65	C	5.083	-3.160	0.000	0.9015
66	C	5.083	-1.923	-5.083	0.2347
67	C	5.083	-1.923	5.083	0.2347
68	C	5.083	0.000	-3.160	0.8860
69	C	5.083	0.000	3.160	0.8860
70	C	5.083	1.923	-5.083	0.2347
71	C	5.083	1.923	5.083	0.2347
72	C	5.083	3.160	0.000	0.9015
73	C	5.083	5.083	-1.923	0.2428
74	C	5.083	5.083	1.923	0.2428
75	C *	7.006	0.000	5.083	0.9315
76	C *	5.083	0.000	7.006	0.9306

77	C *	8.243	5.083	-5.083	-1.2970
78	C *	5.083	8.243	-5.083	-1.2973
79	C *	5.083	5.083	-8.243	-1.2829
80	C *	5.083	5.083	8.243	-1.2829
81	C *	5.083	8.243	5.083	-1.2973
82	C *	8.243	5.083	5.083	-1.2970

Table S1 (continued)

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
83	C *	7.006	5.083	0.000	0.9426
84	C *	5.083	7.006	0.000	0.9427
85	C *	8.243	0.000	0.000	-0.7388
86	C *	5.083	0.000	-7.006	0.9306
87	C *	7.006	0.000	-5.083	0.9315
88	C *	5.083	-5.083	8.243	-1.2829
89	C *	5.083	-8.243	5.083	-1.2973
90	C *	8.243	-5.083	5.083	-1.2970
91	C *	5.083	-7.006	0.000	0.9427
92	C *	7.006	-5.083	0.000	0.9426
93	C *	5.083	-5.083	-8.243	-1.2829
94	C *	5.083	-8.243	-5.083	-1.2973
95	C *	8.243	-5.083	-5.083	-1.2970
96	C *	0.000	5.083	7.006	0.9336
97	C *	0.000	7.006	5.083	0.9391
98	C *	0.000	8.243	0.000	-0.7356
99	C *	0.000	5.083	-7.006	0.9336
100	C *	0.000	7.006	-5.083	0.9391
101	C *	0.000	0.000	8.243	-0.7841
102	C *	0.000	0.000	-8.243	-0.7841
103	C *	0.000	-5.083	7.006	0.9336
104	C *	0.000	-7.006	5.083	0.9391
105	C *	0.000	-8.243	0.000	-0.7356
106	C *	0.000	-5.083	-7.006	0.9336
107	C *	0.000	-7.006	-5.083	0.9391
108	C *	-5.083	5.083	8.243	-1.2829
109	C *	-5.083	7.006	0.000	0.9427
110	C *	-5.083	8.243	5.083	-1.2973
111	C *	-8.243	5.083	5.083	-1.2970
112	C *	-5.083	-5.083	-8.243	-1.2829
113	C *	-5.083	-8.243	-5.083	-1.2973
114	C *	-8.243	-5.083	-5.083	-1.2970

115	C *	-7.006	-5.083	0.000	0.9426
116	C *	-5.083	-5.083	8.243	-1.2829
117	C *	-5.083	-8.243	5.083	-1.2973
118	C *	-8.243	-5.083	5.083	-1.2970
119	C *	-5.083	0.000	-7.006	0.9306
120	C *	-7.006	0.000	-5.083	0.9315
121	C *	-8.243	0.000	0.000	-0.7388
122	C *	-5.083	0.000	7.006	0.9306
123	C *	-7.006	0.000	5.083	0.9315

Table S1 (continued)

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
124	C *	-5.083	5.083	-8.243	-1.2829
125	C *	-5.083	8.243	-5.083	-1.2973
126	C *	-8.243	5.083	-5.083	-1.2970
127	C *	-5.083	-7.006	0.000	0.9427
128	C *	-7.006	5.083	0.000	0.9426
129	N	-5.083	-5.083	-3.054	-0.0333
130	N	-5.083	-5.083	3.054	-0.0333
131	N	-5.083	-3.054	-5.083	-0.0307
132	N	-5.083	-3.054	5.083	-0.0307
133	N	-5.083	-2.029	0.000	-0.8976
134	N	-5.083	0.000	-2.029	-0.8971
135	N	-5.083	0.000	2.029	-0.8971
136	N	-5.083	2.029	0.000	-0.8976
137	N	-5.083	3.054	-5.083	-0.0307
138	N	-5.083	3.054	5.083	-0.0307
139	N	-5.083	5.083	-3.054	-0.0333
140	N	-5.083	5.083	3.054	-0.0333
141	N	-3.054	-5.083	-5.083	-0.0325
142	N	-3.054	-5.083	5.083	-0.0325
143	N	-3.054	5.083	-5.083	-0.0325
144	N	-3.054	5.083	5.083	-0.0325
145	N	-2.029	-5.083	0.000	-0.8963
146	N	-2.029	0.000	-5.083	-0.8490
147	N	-2.029	0.000	5.083	-0.8490
148	N	-2.029	5.083	0.000	-0.8963
149	N	0.000	-5.083	-2.029	-0.8968
150	N	0.000	-5.083	2.029	-0.8968
151	N	0.000	-2.029	-5.083	-0.8755
152	N	0.000	-2.029	5.083	-0.8755

153	N	0.000	2.029	-5.083	-0.8755
154	N	0.000	2.029	5.083	-0.8755
155	N	0.000	5.083	-2.029	-0.8968
156	N	0.000	5.083	2.029	-0.8968
157	N	2.029	-5.083	0.000	-0.8963
158	N	2.029	0.000	-5.083	-0.8490
159	N	2.029	0.000	5.083	-0.8490
160	N	2.029	5.083	0.000	-0.8963
161	N	3.054	-5.083	-5.083	-0.0325
162	N	3.054	-5.083	5.083	-0.0325
163	N	3.054	5.083	-5.083	-0.0325
164	N	3.054	5.083	5.083	-0.0325

Table S1 (continued)

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
165	N	5.083	-5.083	-3.054	-0.0333
166	N	5.083	-5.083	3.054	-0.0333
167	N	5.083	-3.054	-5.083	-0.0307
168	N	5.083	-3.054	5.083	-0.0307
169	N	5.083	-2.029	0.000	-0.8976
170	N	5.083	0.000	-2.029	-0.8971
171	N	5.083	0.000	2.029	-0.8971
172	N	5.083	2.029	0.000	-0.8976
173	N	5.083	3.054	-5.083	-0.0307
174	N	5.083	3.054	5.083	-0.0307
175	N	5.083	5.083	-3.054	-0.0333
176	N	5.083	5.083	3.054	-0.0333
177	N *	5.083	5.083	-7.112	0.4886
178	N *	5.083	8.137	0.000	-0.9903
179	N *	5.083	5.083	7.112	0.4886
180	N *	7.112	5.083	5.083	0.4929
181	N *	5.083	7.112	5.083	0.4931
182	N *	8.137	5.083	0.000	-0.9908
183	N *	5.083	7.112	-5.083	0.4931
184	N *	7.112	5.083	-5.083	0.4929
185	N *	5.083	0.000	8.137	-0.9916
186	N *	8.137	0.000	5.083	-0.9876
187	N *	7.112	0.000	0.000	0.2842
188	N *	5.083	0.000	-8.137	-0.9916
189	N *	8.137	0.000	-5.083	-0.9876
190	N *	5.083	-5.083	7.112	0.4886

191	N *	5.083	-7.112	5.083	0.4931
192	N *	7.112	-5.083	5.083	0.4929
193	N *	5.083	-8.137	0.000	-0.9903
194	N *	8.137	-5.083	0.000	-0.9908
195	N *	5.083	-5.083	-7.112	0.4886
196	N *	5.083	-7.112	-5.083	0.4931
197	N *	7.112	-5.083	-5.083	0.4929
198	N *	0.000	5.083	8.137	-0.9924
199	N *	0.000	8.137	5.083	-0.9890
200	N *	0.000	7.112	0.000	0.2832
201	N *	0.000	5.083	-8.137	-0.9924
202	N *	0.000	8.137	-5.083	-0.9890
203	N *	0.000	0.000	7.112	0.3093
204	N *	0.000	0.000	-7.112	0.3093
205	N *	0.000	-5.083	8.137	-0.9924

Table S1 (continued)

No.	Atom	Coordinate (Å)			ESP Charge (a.u.)
		x	y	z	
206	N *	0.000	-8.137	5.083	-0.9890
207	N *	0.000	-7.112	0.000	0.2832
208	N *	0.000	-5.083	-8.137	-0.9924
209	N *	0.000	-8.137	-5.083	-0.9890
210	N *	-5.083	5.083	7.112	0.4886
211	N *	-5.083	7.112	5.083	0.4931
212	N *	-7.112	5.083	5.083	0.4929
213	N *	-5.083	-5.083	-7.112	0.4886
214	N *	-5.083	-7.112	-5.083	0.4931
215	N *	-7.112	-5.083	-5.083	0.4929
216	N *	-5.083	-8.137	0.000	-0.9903
217	N *	-8.137	-5.083	0.000	-0.9908
218	N *	-5.083	-5.083	7.112	0.4886
219	N *	-5.083	-7.112	5.083	0.4931
220	N *	-7.112	-5.083	5.083	0.4929
221	N *	-5.083	0.000	-8.137	-0.9916
222	N *	-8.137	0.000	-5.083	-0.9876
223	N *	-7.112	0.000	0.000	0.2842
224	N *	-5.083	0.000	8.137	-0.9916
225	N *	-8.137	0.000	5.083	-0.9876
226	N *	-5.083	5.083	-7.112	0.4886
227	N *	-5.083	7.112	-5.083	0.4931
228	N *	-7.112	5.083	-5.083	0.4929

229	N *	-5.083	8.137	0.000	-0.9903
230	N *	-8.137	5.083	0.000	-0.9908

*Removed atoms in 3DRISM calculation