Electronic Supplementary information for:

The Interaction of Pu(IV) with the Hematite (001) Terminations: A Periodic Boundary Condition DFT Study

Ryan L. Dempsey[1] and Nikolas Kaltsoyannis[1]*

[1]Department of Chemistry, The University of Manchester, Oxford Road, Manchester, UK M13 9PL.

Supplementary Figures

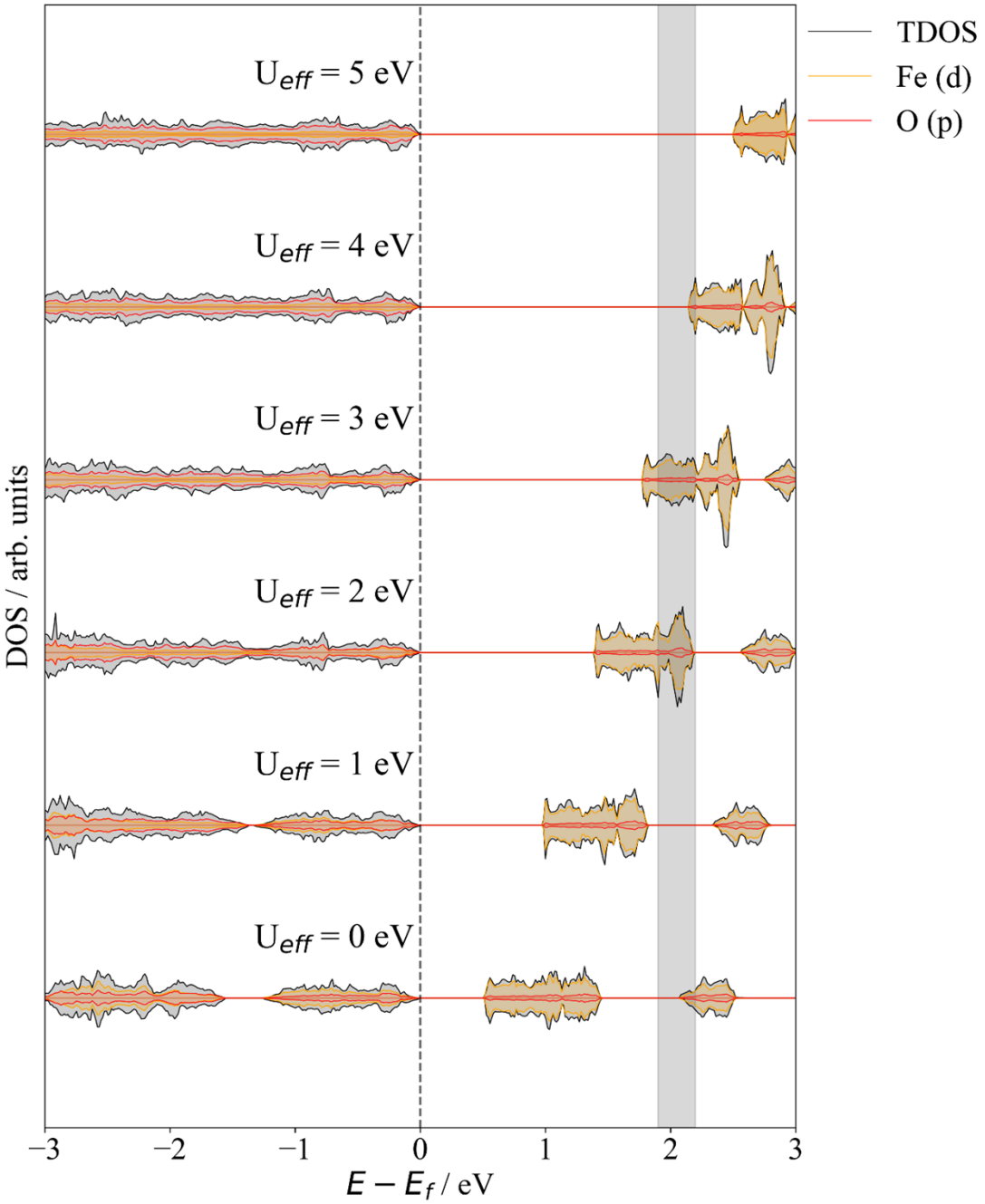

Figure S1: The effect of U_{eff} on the bulk Fe(d) and O(p) density of states. E = 0 eV represents the Fermi level. The grey region shows a range of experimentally determined band gaps.

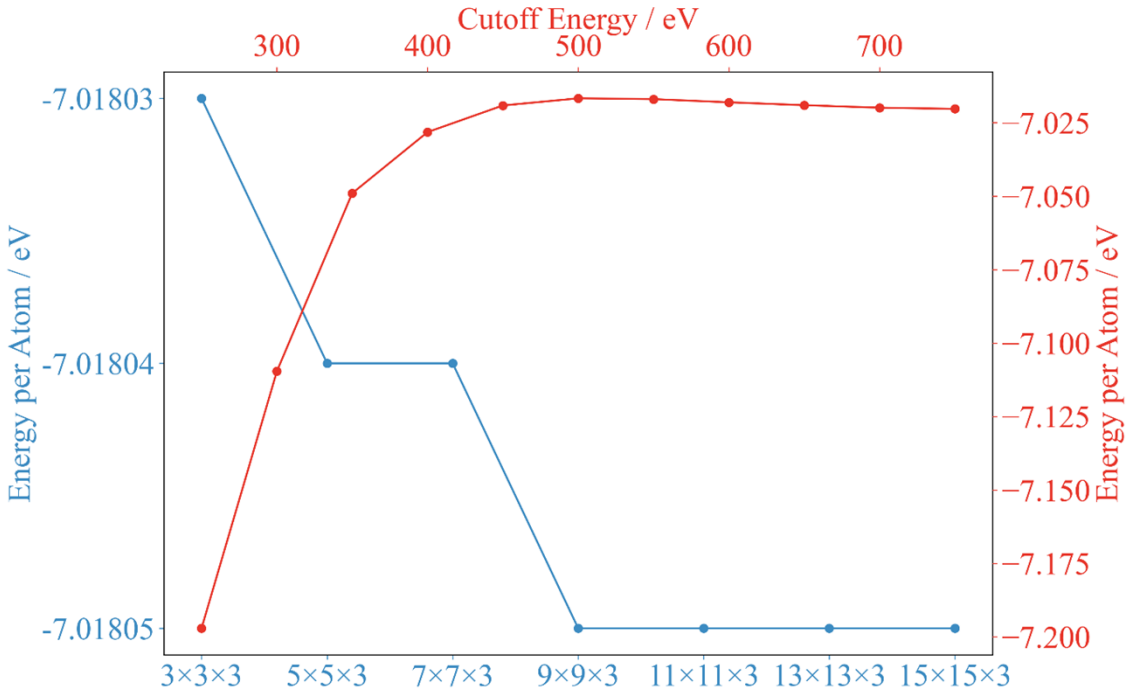

Figure S2: Convergence of the total energy of bulk hematite with respect to ***k***-point sampling and plane wave cutoff energy (see Tables S1 and S2).

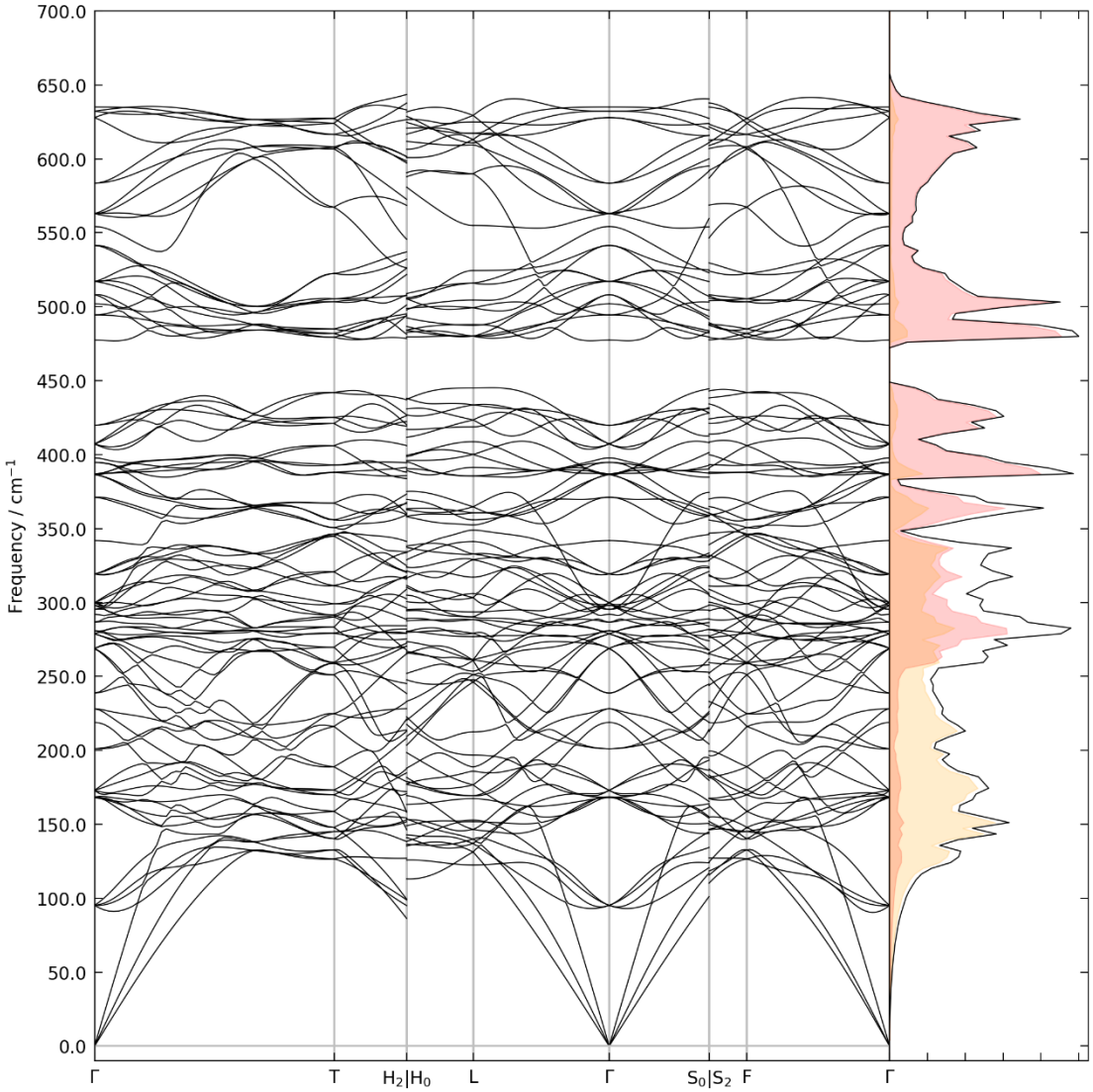

Figure S3: Phonon band structure and projected density of states calculated for a 2 × 2 × 1 supercell expansion of the relaxed hematite bulk unit cell. Colour scheme: Fe, orange; O, red.

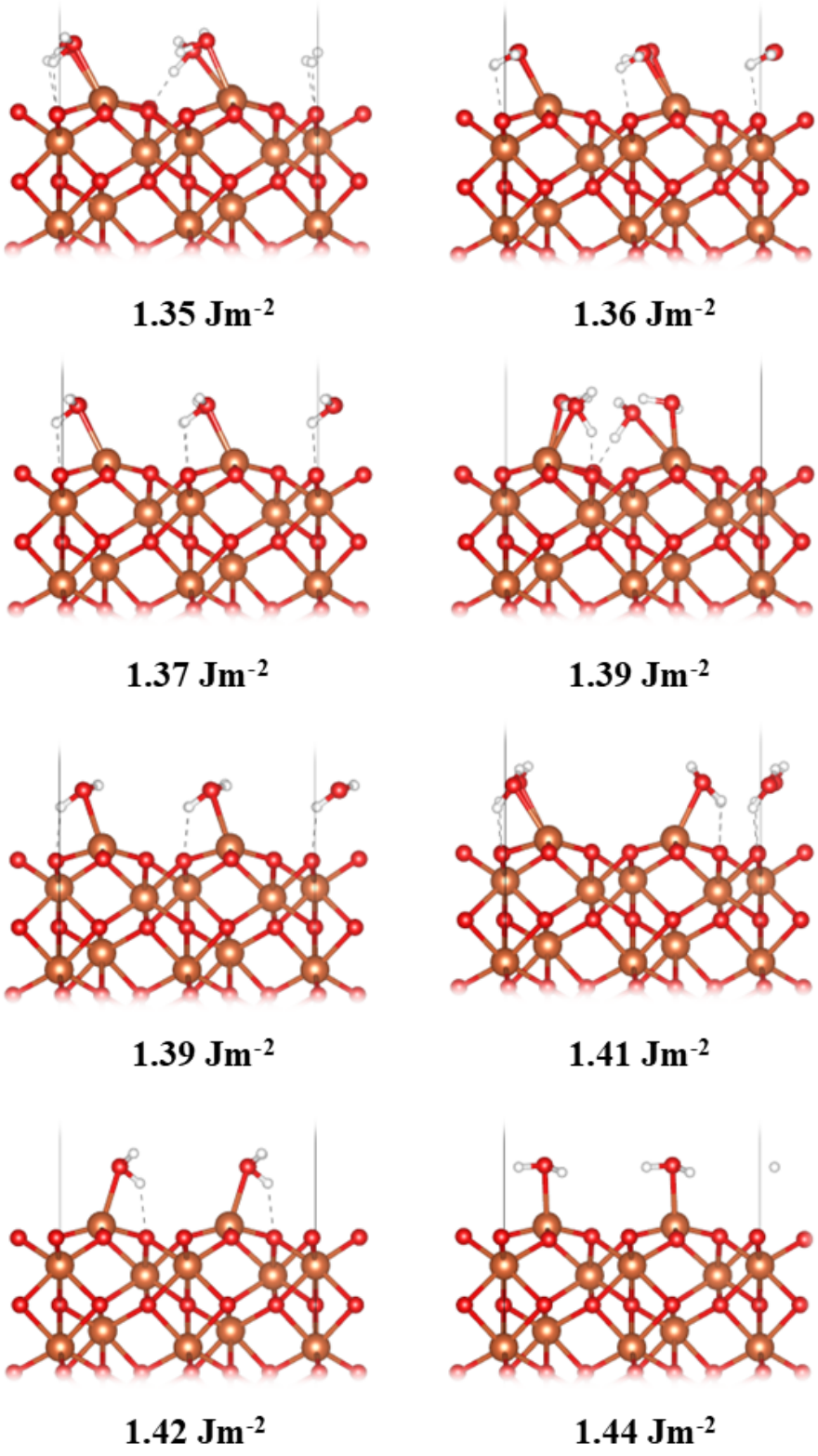

Figure S4: Hydrated Fe terminations and their corresponding γ_{hydr} surface energies. Colour scheme: Fe, orange; O, red; H, white.

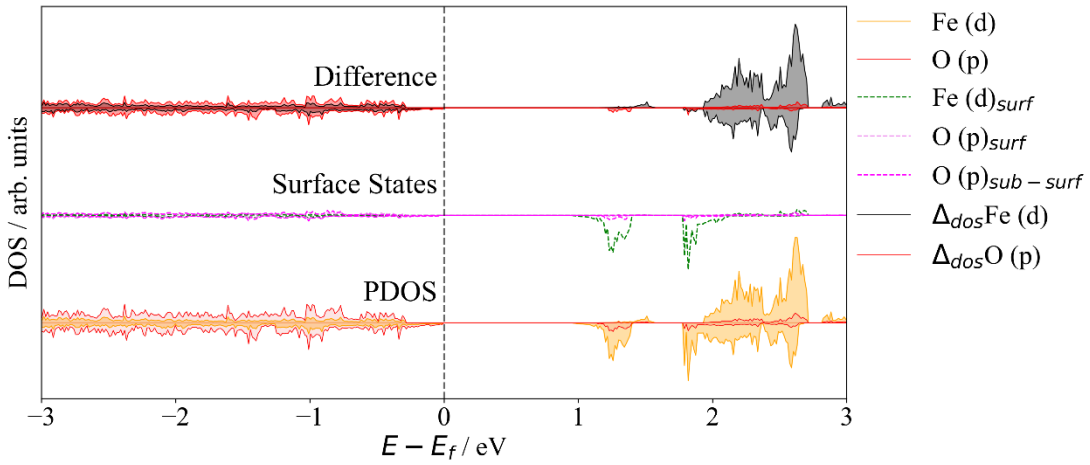

Figure S5: Atom-projected density of states showing the source of surface states in the band gap for the Fe termination. Subscripts "surf" and "sub-surf" refer to the top layer and second layer of Fe and O.

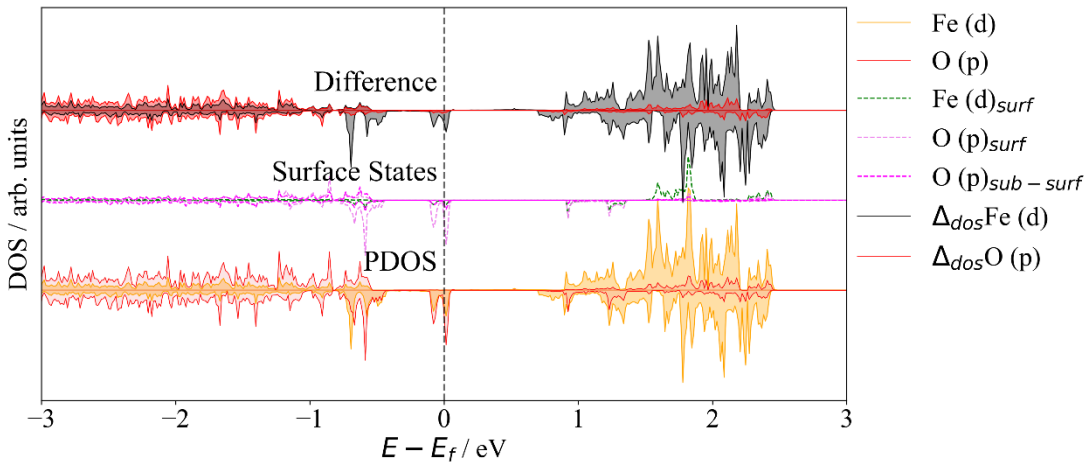

Figure S6: Atom-projected density of states showing the source of surface states in the band gap for the O_3 termination. Subscripts "surf" and "sub-surf" refer to the top layer and second layer of Fe and O.

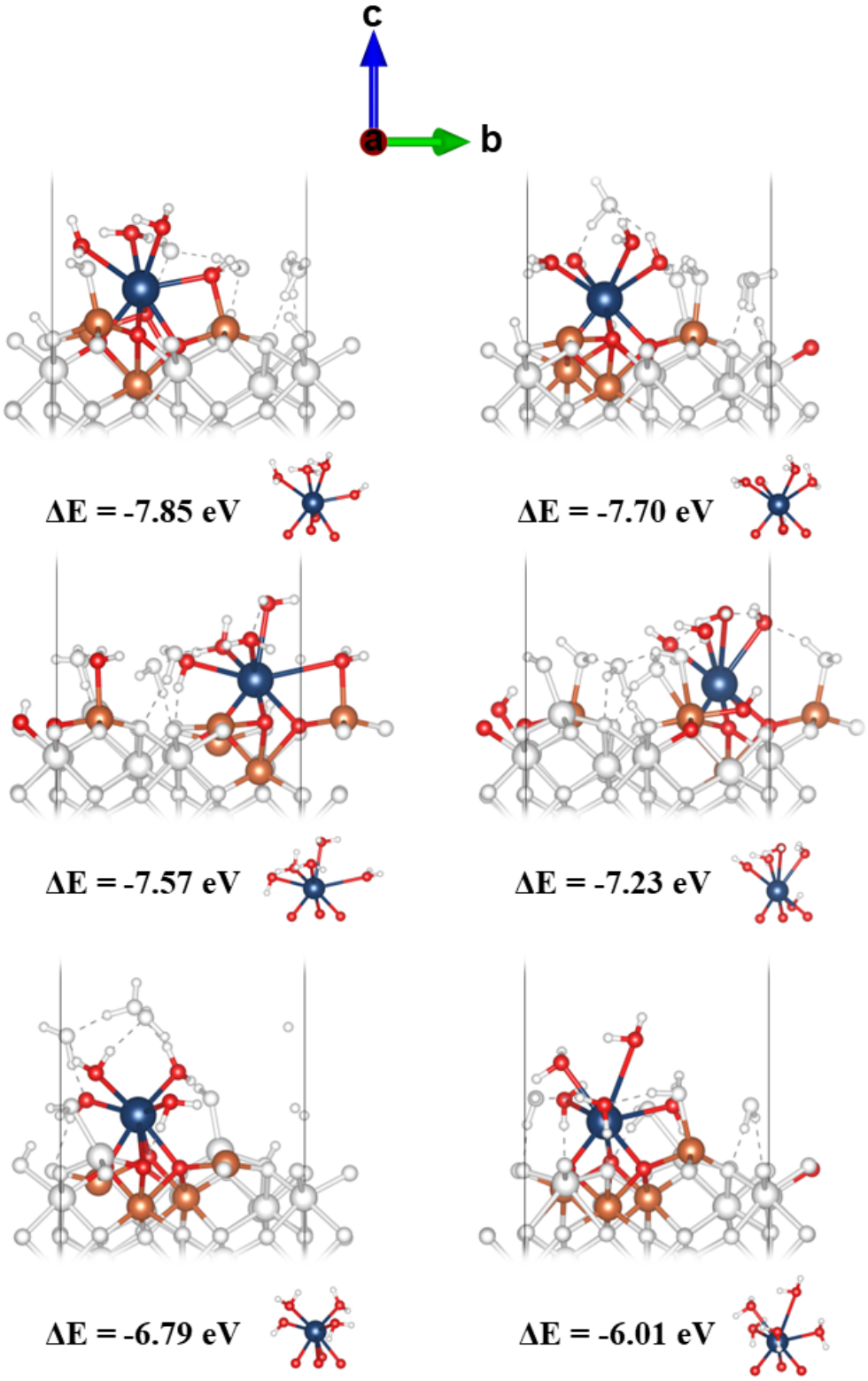

Figure S7: Pu@Hem(001) Fe-term complexes and their corresponding reaction energies, ΔE. The closest eight O atoms and four Fe atoms are coloured and the Pu-O coordination is highlighted separately. Colour scheme: Fe, orange; O, red; H, white.

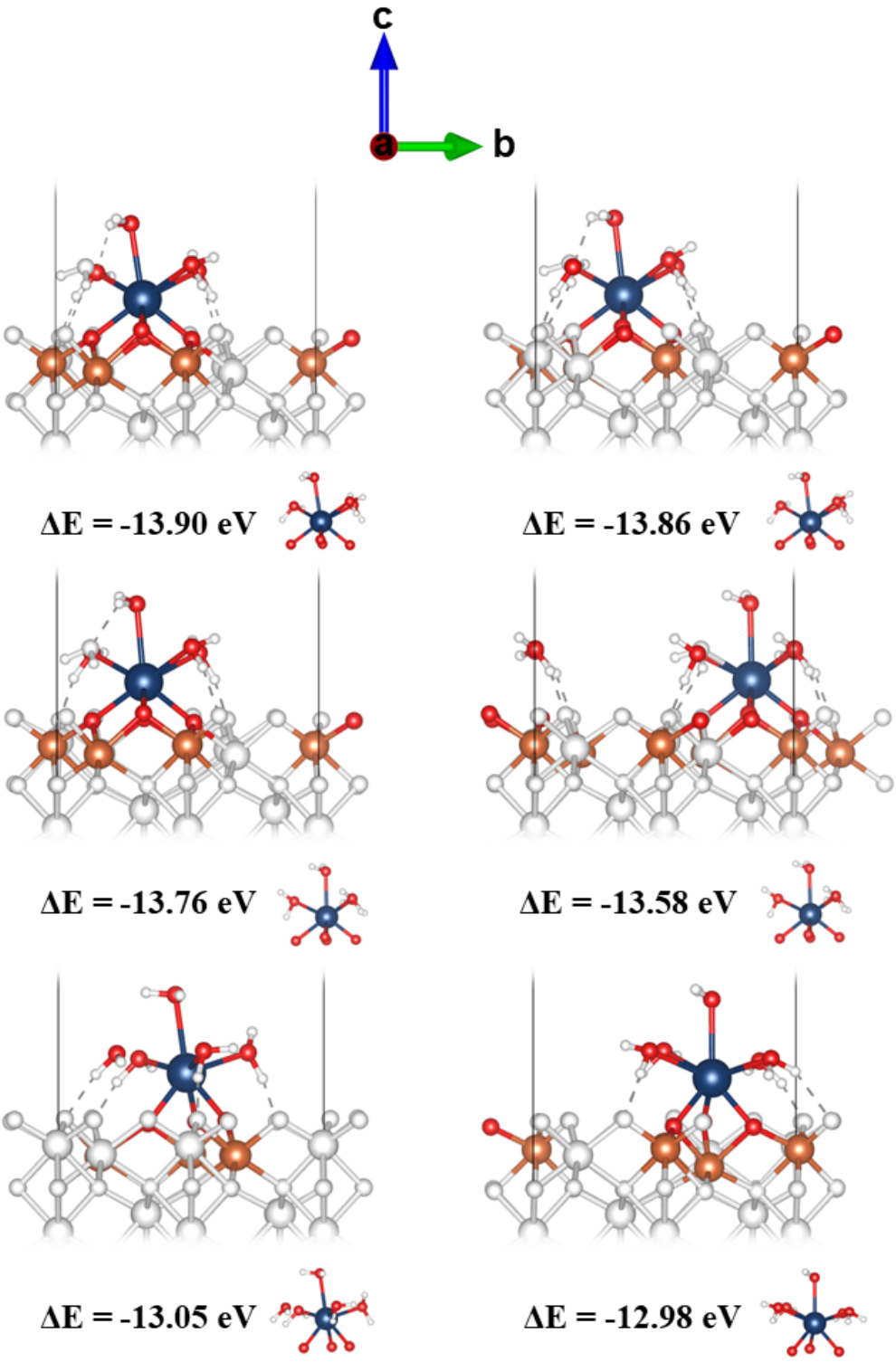

Figure S8: Pu@Hem(001) O_3-term complexes and their corresponding reaction energies, ΔE. The closest eight O atoms and four Fe atoms are coloured and the Pu-O coordination is highlighted separately. Colour scheme: Fe, orange; O, red; H, white.

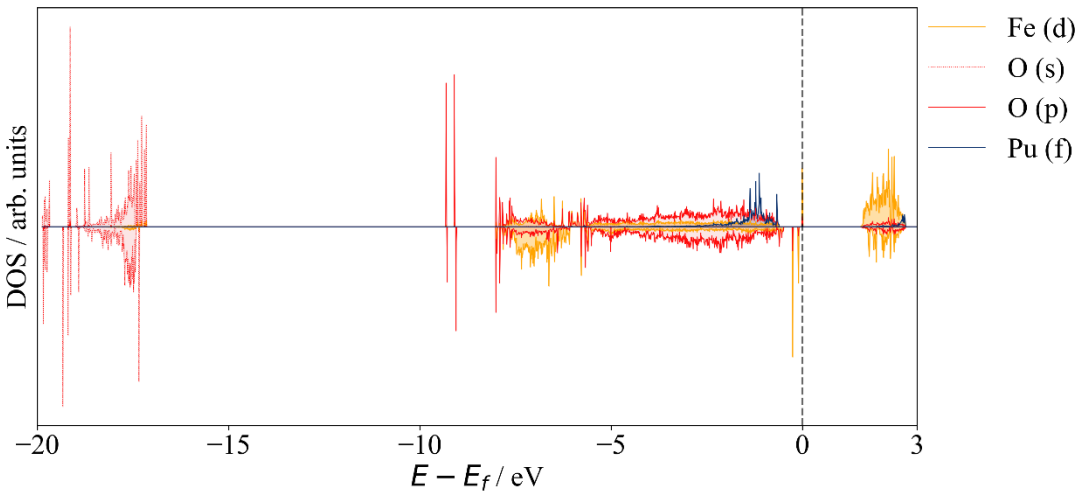

Figure S9: Extended atom-projected density of states showing the full valence region and semicore O(s) states for the lowest energy Pu@Fe-term complex.

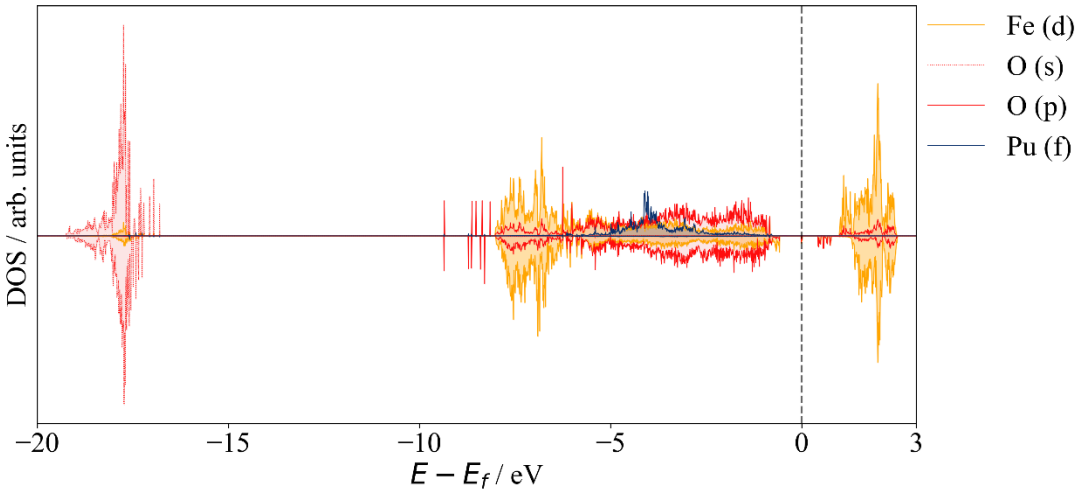

Figure S10: Extended atom-projected density of states showing the full valence region and semicore O(s) states for the lowest energy Pu@O_3-term complex.

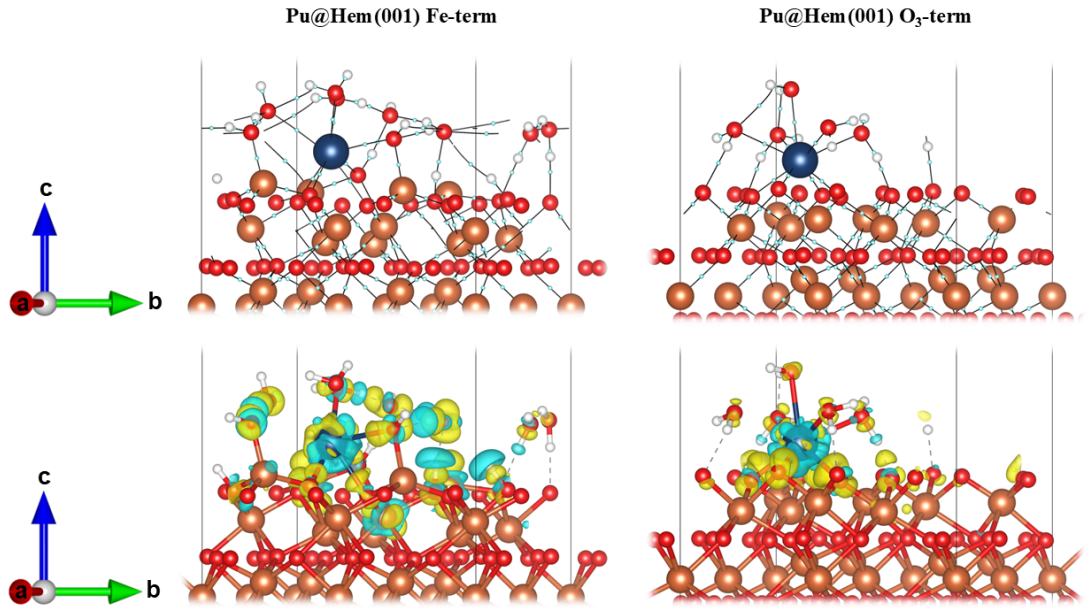

Figure S11: Analysis of the charge density surrounding the adsorbed Pu atom in the lowest energy Pu@Hem complexes. Upper; QTAIM molecular graph with BCPs coloured cyan. Lower; Charge density difference. Regions of charge accumulation and charge depletion are yellow and blue respectively. Surface presented with an isovalue = 0.01 eÅ^{-3}.

Supplementary Tables

Table S1: Hematite bulk lattice parameters relaxed while varying U_{eff} and keeping a fixed 9×9×3 ***k***-point mesh and plane wave cutoff of 600 eV.

U_{eff} / eV	a = b / Å	c / Å	c/a	μ / μ_B	E_g / eV
No U_{eff}	4.99	13.81	2.77	±3.49	0.54
1	5.03	13.85	2.76	±3.76	0.99
2	5.04	13.86	2.75	±3.91	1.40
3	5.05	13.86	2.74	±4.03	1.78
4	5.05	13.84	2.74	±4.12	2.16
5	5.06	13.82	2.73	±4.21	2.52

Table S2: Convergence of the total energy of bulk hematite with respect to plane wave energy cutoff at a fixed ***k***-point sampling of 9×9×3 and U_{eff} = 4eV on Fe.

ENCUT	SCF Energy / eV	SCF Energy per atom / eV
250	-215.91179	-7.19706
300	-213.28817	-7.10961
350	-211.47016	-7.04901
400	-210.84601	-7.02820
450	-210.57390	-7.01913
500	-210.50087	-7.01670
550	-210.50918	-7.01697
600	-210.54137	-7.01805
650	-210.57102	-7.01903
700	-210.59664	-7.01989

Table S3: Convergence of the total energy of bulk hematite with respect to ***k***-point sampling at a fixed plane wave energy cutoff of 600 eV and U_{eff} = 4eV on Fe.

k-points	SCF Energy / eV	SCF Energy per atom / eV
3×3×3	-210.54101	-7.01803
5×5×3	-210.54107	-7.01804
7×7×3	-210.54123	-7.01804
9×9×3	-210.54137	-7.01805
11×11×3	-210.54142	-7.01805
13×13×3	-210.54135	-7.01805
15×15×3	-210.54137	-7.01805

Table S4: Convergence of the total energy of Hem(001) Fe-term with respect to ***k***-point sampling at a fixed plane wave energy cutoff of 600 eV.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
3×3×1	-821.17737	-6.84314
5×5×1	-821.17686	-6.84314
7×7×1	-821.17703	-6.84314
9×9×1	-821.17725	-6.84314

Table S5: Convergence of the total energy of Hem(001) O_3-term with respect to ***k***-point sampling at a fixed plane wave energy cutoff of 600 eV.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
3×3×1	-794.52180	-6.62102
5×5×1	-794.51865	-6.62099
7×7×1	-794.51984	-6.62100
9×9×1	-794.52038	-6.62100

Table S6: Convergence of the total energy of Hem(001) Fe-term with respect to layer relaxation.

#Layers Relaxed	**SCF Energy / eV**	**SCF Energy per atom / eV**	**γ / Jm^{-2}**
0	-821.17703	-6.84314	1.91
1	-822.53012	-6.85442	1.67
2	-822.52955	-6.85441	1.67
3	-822.59031	-6.85492	1.66
4	-822.83022	-6.85692	1.61
5	-822.90256	-6.85752	1.60
6	-822.90512	-6.85754	1.60

Table S7: Convergence of the total energy of Hem(001) O_3-term with respect to layer relaxation.

#Layers Relaxed	**SCF Energy / eV**	**SCF Energy per atom / eV**	**γ / Jm^{-2}**
0	-794.51985	-6.62100	4.33
1	-798.64000	-6.65533	3.58
2	-798.64940	-6.65541	3.58
3	-799.19403	-6.65995	3.48
4	-799.22818	-6.66023	3.47
5	-799.27766	-6.66065	3.46
6	-799.27857	-6.66065	3.46

Table S8: Total energies and surface energies of the hydrated Hem(001) Fe-term models with 100% coverage, corresponding to the structures in Figures S4.

Surface ID	SCF Energy / eV	γ_{hydr} / Jm^{-2}
1	-881.14952	1.35
2	-881.14646	1.36
3	-881.05962	1.37
4	-880.95768	1.39
5	-880.93199	1.39
6	-880.82485	1.41
7	-880.79723	1.42
8	-880.67543	1.44

Table S9: Optimised interlayer spacing (Å) in the Hem(001) Fe-term.

Layers	Unrelaxed	Relaxed	% Difference
Fe-O	0.87	0.31	-64%
O-Fe	0.87	0.94	8%
Fe-Fe	0.57	0.35	-38%
Fe-O	0.87	1.01	16%
O-Fe	0.87	0.89	3%
Fe-Fe	0.57	0.57	0%

Table S10: Optimised interlayer spacing (Å) in the Hem(001) O_3-term.

Layers	Unrelaxed	Relaxed	% Difference
O-Fe	0.87	0.81	-7%
Fe-Fe	0.57	0.26	-55%
Fe-O	0.87	1.10	27%
O-Fe	0.87	0.81	-6%
Fe-Fe	0.57	0.62	9%
Fe-O	0.87	0.87	0%

Table S11: Pu@Hem(001) reaction energies, charge, and average Pu-O/Fe distances corresponding to the structures in Figures S8 and S9.

Surface ID	ΔE_r / eV	q(Pu)	Average distance to n closest Pu-O / Å			Average distance to 4 closest Pu-Fe / Å	Binding Mode
			n = 6	n = 7	n = 8		
Fe-term							
1	-7.85	2.15	2.47	2.51	2.54	3.37	Pentadentate
2	-7.70	2.13	2.45	2.51	2.59	3.47	Tetradentate
3	-7.57	2.12	2.49	2.54	2.62	3.44	Tetradentate
4	-7.23	2.07	2.46	2.58	2.68	3.39	Tetradentate
5	-6.79	2.14	2.44	2.47	2.61	3.53	Tetradentate
6	-6.01	2.09	2.45	2.55	2.64	3.36	Tridentate
O_3-term							
1	-13.90	2.54	2.38	2.41	2.44	3.62	Tetradentate
2	-13.86	2.54	2.39	2.42	2.44	3.63	Tetradentate
3	-13.76	2.54	2.38	2.41	2.44	3.62	Tetradentate
4	-13.58	2.54	2.40	2.43	2.45	3.64	Tetradentate
5	-13.05	2.43	2.64	2.64	2.65	3.70	Tridentate
6	-12.98	2.49	2.37	2.41	2.44	3.59	Tridentate

Table S12: Average Pu-O QTAIM bond critical point properties (a.u.) for the Pu@Hem(001) complexes.

Surface ID	Pu-O_{surf}			Pu-O_{water}			Overall Pu-O		
	ρ	H	$-G/V$	ρ	H	$-G/V$	ρ	H	$-G/V$
Fe-term									
1	0.06	-0.01	0.88	0.04	0.00	0.98	0.05	0.00	0.93
2	0.06	-0.01	0.93	0.04	0.00	0.98	0.05	-0.01	0.96
3	0.06	-0.02	0.93	0.03	0.00	1.02	0.05	-0.01	0.97
4	0.08	-0.03	0.80	0.04	0.00	0.98	0.06	-0.01	0.89
5	0.06	-0.01	0.87	0.05	-0.01	0.91	0.06	-0.01	0.89
6	0.08	-0.02	0.79	0.03	0.00	1.08	0.05	-0.01	0.94
O_3-term									
1	0.08	-0.03	0.79	0.05	-0.01	0.89	0.07	-0.02	0.84
2	0.08	-0.03	0.79	0.05	-0.01	0.89	0.07	-0.02	0.84
3	0.08	-0.03	0.78	0.05	-0.01	0.89	0.06	-0.02	0.84
4	0.08	-0.03	0.80	0.05	-0.01	0.89	0.06	-0.02	0.84
5	0.10	-0.04	0.74	0.05	-0.01	0.91	0.08	-0.02	0.83
6	0.11	-0.05	0.76	0.04	0.00	0.92	0.08	-0.03	0.84

Optimised Coordinates

All coordinates given in the VASP POSCAR format.

Bulk Hematite – Fe12O18

```
1.0
     5.0548567772    0.0000000000    0.0000000000
    -2.5274283886    4.3776343815    0.0000000000
     0.0000000000    0.0000000000   13.8361234665
  Fe   O
  12  18
Direct
   0.333333343     0.666666687     0.520679235
   0.000000000     0.000000000     0.645987451
   0.333333343     0.666666687     0.812654138
   0.666666687     0.333333343     0.687345862
   0.000000000     0.000000000     0.854012549
   0.666666687     0.333333343     0.979320765
   0.000000000     0.000000000     0.145987451
   0.333333343     0.666666687     0.020679217
   0.666666687     0.333333343     0.187345877
   0.333333343     0.666666687     0.312654108
   0.666666687     0.333333343     0.479320794
   0.000000000     0.000000000     0.354012549
   0.693498433     0.693498433     0.750000000
   0.306501538     0.000000000     0.750000000
   0.666666687     0.026831781     0.583333313
   0.360165119     0.333333343     0.583333313
   0.973168194     0.639834881     0.583333313
   0.000000000     0.306501538     0.750000000
   0.360165119     0.026831781     0.083333336
   0.973168194     0.333333343     0.083333336
   0.333333343     0.360165119     0.916666687
   0.026831781     0.666666687     0.916666687
   0.639834881     0.973168194     0.916666687
   0.666666687     0.639834881     0.083333336
   0.026831781     0.360165119     0.416666657
   0.639834881     0.666666687     0.416666657
   0.000000000     0.693498433     0.250000000
   0.693498433     0.000000000     0.250000000
   0.306501538     0.306501538     0.250000000
   0.333333343     0.973168194     0.416666657
```

Relaxed Hematite(001)-Fe – Fe48O72

```
1.0
    10.1097135544    0.0000000000    0.0000000000
    -5.0548563004    8.7552679372    0.0000000000
     0.0000000000    0.0000000000   33.2638816833
  Fe   O
  48  72
Direct
   0.166666642     0.333333373     0.999995291
   0.166666642     0.833333373     0.999995291
   0.666666627     0.333333373     0.999995291
   0.666666627     0.833333373     0.999995291
   0.000000000     0.000000000     0.052117266
   0.000000000     0.500000000     0.052117266
   0.500000000     0.000000000     0.052117266
   0.500000000     0.500000000     0.052117266
   0.333333313     0.166666687     0.069320321
   0.333333313     0.666666687     0.069320321
   0.833333313     0.166666687     0.069320321
   0.833333313     0.666666687     0.069320321
   0.166666642     0.333333373     0.121442333
   0.166666642     0.833333373     0.121442333
   0.666666627     0.333333373     0.121442333
   0.666666627     0.833333373     0.121442333
   0.000000000     0.000000000     0.138645381
   0.000000000     0.500000000     0.138645381
   0.500000000     0.000000000     0.138645381
   0.500000000     0.500000000     0.138645381
   0.333333313     0.166666687     0.190767378
   0.333333313     0.666666687     0.190767378
   0.833333313     0.166666687     0.190767378
   0.833333313     0.666666687     0.190767378
   0.166666642     0.333333373     0.207970440
   0.166666642     0.833333373     0.207970440
   0.666666627     0.333333373     0.207970440
   0.666666627     0.833333373     0.207970440
   0.000000000     0.000000000     0.260092437
   0.000000000     0.500000000     0.260092437
   0.500000000     0.000000000     0.260092437
   0.500000000     0.500000000     0.260092437
   0.333333313     0.166666687     0.277295470
   0.333333313     0.666666687     0.277295470
   0.833333313     0.166666687     0.277295470
   0.833333313     0.666666687     0.277295470
   0.166666642     0.333333373     0.334440619
   0.166666642     0.833333373     0.334440619
   0.666666627     0.333333373     0.334440619
   0.666666627     0.833333373     0.334440619
   0.000000000     0.000000000     0.345099479
   0.000000000     0.500000000     0.345099479
   0.500000000     0.000000000     0.345099479
   0.500000000     0.500000000     0.345099479
   0.333333313     0.166666687     0.382709652
   0.333333313     0.666666687     0.382709652
   0.833333313     0.166666687     0.382709652
   0.833333313     0.666666687     0.382709652
   0.333333313     0.013415892     0.026056252
   0.333333313     0.513415873     0.026056252
   0.833333313     0.013415892     0.026056252
   0.833333313     0.513415873     0.026056252
   0.180082545     0.166666687     0.026056252
   0.180082545     0.666666687     0.026056252
   0.680082560     0.166666687     0.026056252
   0.680082560     0.666666687     0.026056252
   0.486584067     0.319917470     0.026056252
   0.486584067     0.819917440     0.026056252
   0.986584067     0.319917470     0.026056252
   0.986584067     0.819917440     0.026056252
   0.346749187     0.346749246     0.095381320
   0.346749187     0.846749246     0.095381320
   0.846749187     0.346749246     0.095381320
   0.846749187     0.846749246     0.095381320
   0.153250769     0.000000000     0.095381320
   0.153250769     0.500000000     0.095381320
   0.653250754     0.000000000     0.095381320
   0.653250754     0.500000000     0.095381320
   0.000000000     0.153250784     0.095381320
   0.000000000     0.653250813     0.095381320
   0.500000000     0.153250784     0.095381320
```

0.500000000	0.653250813	0.095381320
0.166666657	0.180082574	0.164706394
0.166666657	0.680082560	0.164706394
0.666666627	0.180082574	0.164706394
0.666666627	0.680082560	0.164706394
0.013415871	0.333333373	0.164706394
0.013415871	0.833333373	0.164706394
0.513415873	0.333333373	0.164706394
0.513415873	0.833333373	0.164706394
0.319917411	0.486584157	0.164706394
0.319917411	0.986584187	0.164706394
0.819917440	0.486584157	0.164706394
0.819917440	0.986584187	0.164706394
0.180082545	0.013415892	0.234031439
0.180082545	0.513415873	0.234031439
0.680082560	0.013415892	0.234031439
0.680082560	0.513415873	0.234031439
0.486584067	0.166666687	0.234031439
0.486584067	0.666666687	0.234031439
0.986584067	0.166666687	0.234031439
0.986584067	0.666666687	0.234031439
0.333333313	0.319917470	0.234031439
0.333333313	0.819917440	0.234031439
0.833333313	0.319917470	0.234031439
0.833333313	0.819917440	0.234031439
0.000501999	0.344547153	0.304074347
0.000501999	0.844547153	0.304074347
0.500501990	0.344547153	0.304074347
0.500501990	0.844547153	0.304074347
0.344045103	0.999498010	0.304074347
0.344045103	0.499498010	0.304074347
0.844045103	0.999498010	0.304074347
0.844045103	0.499498010	0.304074347
0.155452862	0.155954883	0.304074347
0.155452862	0.655954897	0.304074347
0.655452847	0.155954883	0.304074347
0.655452847	0.655954897	0.304074347
0.012146195	0.172969297	0.373314053
0.012146195	0.672969282	0.373314053
0.512146175	0.172969297	0.373314053
0.512146175	0.672969282	0.373314053
0.327030689	0.339176953	0.373314053
0.327030689	0.839176953	0.373314053
0.827030718	0.339176953	0.373314053
0.827030718	0.839176953	0.373314053
0.160823062	0.487853855	0.373314053
0.160823062	0.987853885	0.373314053
0.660823047	0.487853855	0.373314053
0.660823047	0.987853885	0.373314053

Hematite(001)-O_3 – Fe48O72

1.0

10.1097135544	0.0000000000	0.0000000000
-5.0548563004	8.7552679372	0.0000000000
0.0000000000	0.0000000000	32.9692344666

Fe	O
48	72

Direct

0.000000000	0.000000000	0.364565283
0.000000000	0.500000000	0.364565283
0.500000000	0.000000000	0.364565283
0.500000000	0.500000000	0.364565283
0.333333313	0.166666687	0.356679797
0.333333313	0.666666687	0.356679797
0.833333313	0.166666687	0.356679797
0.833333313	0.666666687	0.356679797
0.166666642	0.333333373	0.298661888
0.166666642	0.833333373	0.298661888
0.666666627	0.333333373	0.298661888
0.666666627	0.833333373	0.298661888
0.000000000	0.000000000	0.279781997
0.000000000	0.500000000	0.279781997
0.500000000	0.000000000	0.279781997
0.500000000	0.500000000	0.279781997
0.333333313	0.166666687	0.227194265
0.333333313	0.666666687	0.227194265
0.833333313	0.166666687	0.227194265
0.833333313	0.666666687	0.227194265
0.166666642	0.333333373	0.209837452
0.166666642	0.833333373	0.209837452
0.666666627	0.333333373	0.209837452
0.666666627	0.833333373	0.209837452
0.000000000	0.000000000	0.157249644
0.000000000	0.500000000	0.157249644
0.500000000	0.000000000	0.157249644
0.500000000	0.500000000	0.157249644
0.333333313	0.166666687	0.139892772
0.333333313	0.666666687	0.139892772
0.833333313	0.166666687	0.139892772
0.833333313	0.666666687	0.139892772
0.166666642	0.333333373	0.087305017
0.166666642	0.833333373	0.087305017
0.666666627	0.333333373	0.087305017
0.666666627	0.833333373	0.087305017
0.000000000	0.000000000	0.069948144
0.000000000	0.500000000	0.069948144
0.500000000	0.000000000	0.069948144
0.500000000	0.500000000	0.069948144
0.333333313	0.166666687	0.017360399
0.333333313	0.666666687	0.017360399
0.833333313	0.166666687	0.017360399
0.833333313	0.666666687	0.017360399
0.166666642	0.333333373	0.000003526
0.166666642	0.833333373	0.000003526
0.666666627	0.333333373	0.000003526
0.666666627	0.833333373	0.000003526
0.360481262	0.025585804	0.389088988
0.360481262	0.525585771	0.389088988
0.860481262	0.025585804	0.389088988
0.860481262	0.525585771	0.389088988
0.165104508	0.139518738	0.389088988
0.165104508	0.639518738	0.389088988
0.665104508	0.139518738	0.389088988
0.665104508	0.639518738	0.389088988
0.474414140	0.334895521	0.389088988
0.474414140	0.834895492	0.389088988
0.974414170	0.334895521	0.389088988
0.974414170	0.834895492	0.389088988
0.348586023	0.345543832	0.323274165
0.348586023	0.845543861	0.323274165
0.848586023	0.345543832	0.323274165
0.848586023	0.845543861	0.323274165
0.154456168	0.003042237	0.323274165
0.154456168	0.503042221	0.323274165
0.654456139	0.003042237	0.323274165
0.654456139	0.503042221	0.323274165
0.996957779	0.151413947	0.323274165
0.996957779	0.651413977	0.323274165
0.496957749	0.151413947	0.323274165
0.496957749	0.651413977	0.323274165
0.166666657	0.180082574	0.253488123
0.166666657	0.680082560	0.253488123
0.666666627	0.180082574	0.253488123
0.666666627	0.680082560	0.253488123

0.013415871 0.333333373 0.253488123
0.013415871 0.833333373 0.253488123
0.513415873 0.333333373 0.253488123
0.513415873 0.833333373 0.253488123
0.319917411 0.486584157 0.253488123
0.319917411 0.986584187 0.253488123
0.819917440 0.486584157 0.253488123
0.819917440 0.986584187 0.253488123
0.180082545 0.013415892 0.183543518
0.180082545 0.513415873 0.183543518
0.680082560 0.013415892 0.183543518
0.680082560 0.513415873 0.183543518
0.486584067 0.166666687 0.183543518
0.486584067 0.666666687 0.183543518
0.986584067 0.166666687 0.183543518
0.986584067 0.666666687 0.183543518
0.333333313 0.319917470 0.183543518
0.333333313 0.819917440 0.183543518
0.833333313 0.319917470 0.183543518
0.833333313 0.819917440 0.183543518
0.000000000 0.346749246 0.113598891
0.000000000 0.846749246 0.113598891
0.500000000 0.346749246 0.113598891
0.500000000 0.846749246 0.113598891
0.346749216 0.000000000 0.113598891
0.346749216 0.500000000 0.113598891
0.846749187 0.000000000 0.113598891
0.846749187 0.500000000 0.113598891
0.153250754 0.153250784 0.113598891
0.153250754 0.653250813 0.113598891
0.653250754 0.153250784 0.113598891
0.653250754 0.653250813 0.113598891
0.013415889 0.180082574 0.043654270
0.013415889 0.680082560 0.043654270
0.513415873 0.180082574 0.043654270
0.513415873 0.680082560 0.043654270
0.319917411 0.333333373 0.043654270
0.319917411 0.833333373 0.043654270
0.819917440 0.333333373 0.043654270
0.819917440 0.833333373 0.043654270
0.166666657 0.486584157 0.043654270
0.166666657 0.986584187 0.043654270
0.666666627 0.486584157 0.043654270
0.666666627 0.986584187 0.043654270

Hydrated Hematite(001)-Fe Fe48O72•4H2O

1.0

10.1097135544 0.0000000000 0.0000000000
-5.0548563004 8.7552679372 0.0000000000
0.0000000000 0.0000000000 33.2638816833

Fe O H
48 76 8

Direct

0.166666642 0.333333373 0.999995291
0.166666642 0.833333373 0.999995291
0.666666627 0.333333373 0.999995291
0.666666627 0.833333373 0.999995291
0.000000000 0.000000000 0.052117266
0.000000000 0.500000000 0.052117266
0.500000000 0.000000000 0.052117266
0.500000000 0.500000000 0.052117266
0.333333313 0.166666687 0.069320321
0.333333313 0.666666687 0.069320321
0.833333313 0.166666687 0.069320321
0.833333313 0.666666687 0.069320321
0.166666642 0.333333373 0.121442333
0.166666642 0.833333373 0.121442333
0.666666627 0.333333373 0.121442333
0.666666627 0.833333373 0.121442333
0.000000000 0.000000000 0.138645381
0.000000000 0.500000000 0.138645381
0.500000000 0.000000000 0.138645381
0.500000000 0.500000000 0.138645381
0.333333313 0.166666687 0.190767378
0.333333313 0.666666687 0.190767378
0.833333313 0.166666687 0.190767378
0.833333313 0.666666687 0.190767378
0.166666642 0.333333373 0.207970440
0.166666642 0.833333373 0.207970440
0.666666627 0.333333373 0.207970440
0.666666627 0.833333373 0.207970440
0.000000000 0.000000000 0.260092437
0.000000000 0.500000000 0.260092437
0.500000000 0.000000000 0.260092437
0.500000000 0.500000000 0.260092437
0.333333313 0.166666687 0.277295470
0.333333313 0.666666687 0.277295470
0.833333313 0.166666687 0.277295470
0.833333313 0.666666687 0.277295470
0.165037364 0.334758759 0.333752453
0.166305855 0.833188355 0.334018350
0.666554451 0.332892001 0.333845288
0.666716039 0.833850026 0.333798081
0.998828828 0.001018685 0.344727725
0.999034584 0.502725303 0.344598293
0.497467905 0.997376144 0.344777375
0.501088619 0.501301348 0.344074637
0.335785985 0.167972922 0.386407942
0.334917903 0.662667572 0.387960106
0.836545944 0.172125950 0.385657430
0.834102154 0.668572962 0.386182278
0.333333313 0.013415892 0.026056252
0.333333313 0.513415873 0.026056252
0.833333313 0.013415892 0.026056252
0.833333313 0.513415873 0.026056252
0.180082545 0.166666687 0.026056252
0.180082545 0.666666687 0.026056252
0.680082560 0.166666687 0.026056252
0.680082560 0.666666687 0.026056252
0.486584067 0.319917470 0.026056252
0.486584067 0.819917440 0.026056252
0.986584067 0.319917470 0.026056252
0.986584067 0.819917440 0.026056252
0.346749187 0.346749246 0.095381320
0.346749187 0.846749246 0.095381320
0.846749187 0.346749246 0.095381320
0.846749187 0.846749246 0.095381320
0.153250769 0.000000000 0.095381320
0.153250769 0.500000000 0.095381320
0.653250754 0.000000000 0.095381320
0.653250754 0.500000000 0.095381320
0.000000000 0.153250784 0.095381320
0.000000000 0.653250813 0.095381320
0.500000000 0.153250784 0.095381320
0.500000000 0.653250813 0.095381320
0.166666657 0.180082574 0.164706394
0.166666657 0.680082560 0.164706394
0.666666627 0.180082574 0.164706394
0.666666627 0.680082560 0.164706394
0.013415871 0.333333373 0.164706394
0.013415871 0.833333373 0.164706394
0.513415873 0.333333373 0.164706394
0.513415873 0.833333373 0.164706394
0.319917411 0.486584157 0.164706394

0.319917411	0.986584187	0.164706394
0.819917440	0.486584157	0.164706394
0.819917440	0.986584187	0.164706394
0.180082545	0.013415892	0.234031439
0.180082545	0.513415873	0.234031439
0.680082560	0.013415892	0.234031439
0.680082560	0.513415873	0.234031439
0.486584067	0.166666687	0.234031439
0.486584067	0.666666687	0.234031439
0.986584067	0.166666687	0.234031439
0.986584067	0.666666687	0.234031439
0.333333313	0.319917470	0.234031439
0.333333313	0.819917440	0.234031439
0.833333313	0.319917470	0.234031439
0.833333313	0.819917440	0.234031439
0.999767959	0.344980180	0.303835541
0.000709909	0.845785975	0.303759426
0.499089926	0.344282418	0.304159671
0.500887811	0.845765769	0.303585261
0.344060183	0.997963965	0.304003567
0.343912452	0.497526497	0.303685546
0.845054746	0.999412060	0.303866148
0.844393194	0.498436868	0.303463280
0.156769067	0.158383369	0.304315001
0.155149519	0.657880664	0.303503931
0.655473650	0.156348199	0.303916335
0.655249357	0.657101512	0.303319842
0.013596703	0.175944149	0.373148382
0.012393733	0.676286459	0.372830749
0.512021422	0.173546135	0.372464627
0.513098419	0.675713897	0.371380955
0.333209783	0.347226560	0.377985090
0.330938160	0.838418841	0.376094490
0.828500867	0.343947202	0.374769360
0.828677416	0.841741681	0.374497324
0.162419528	0.492578149	0.370466709
0.162364841	0.991059840	0.371604264
0.664145172	0.491588771	0.370669514
0.662539661	0.990675628	0.372183472
0.770724297	0.055672299	0.444040328
0.299565613	0.033144739	0.441258788
0.783324540	0.568939865	0.446776718
0.328669220	0.516327202	0.437184811
0.694855809	0.976218104	0.425195396
0.842635930	0.021039909	0.450402737
0.207463473	0.955538750	0.426641017
0.372555166	0.998765647	0.435113966
0.754066288	0.467823535	0.435432702
0.686189473	0.559855163	0.454740882
0.222820997	0.460177571	0.446244657
0.331945837	0.442483932	0.415813506

Pu@Hem(001)-Fe – Fe48O72 • 4H2O Pu(H2O)5

1.0

10.1097135544	0.0000000000	0.0000000000
-5.0548563004	8.7552679372	0.0000000000
0.0000000000	0.0000000000	33.2638816833

Fe	O	H	Pu
48	81	18	1

Direct

0.166666642	0.333333373	0.999995291
0.166666642	0.833333373	0.999995291
0.666666627	0.333333373	0.999995291
0.666666627	0.833333373	0.999995291
0.000000000	0.000000000	0.052117266
0.000000000	0.500000000	0.052117266
0.500000000	0.000000000	0.052117266
0.500000000	0.500000000	0.052117266
0.333333313	0.166666687	0.069320321
0.333333313	0.666666687	0.069320321
0.833333313	0.166666687	0.069320321
0.833333313	0.666666687	0.069320321
0.166666642	0.333333373	0.121442333
0.166666642	0.833333373	0.121442333
0.666666627	0.333333373	0.121442333
0.666666627	0.833333373	0.121442333
0.000000000	0.000000000	0.138645381
0.000000000	0.500000000	0.138645381
0.500000000	0.000000000	0.138645381
0.500000000	0.500000000	0.138645381
0.333333313	0.166666687	0.190767378
0.333333313	0.666666687	0.190767378
0.833333313	0.166666687	0.190767378
0.833333313	0.666666687	0.190767378
0.166666642	0.333333373	0.207970440
0.166666642	0.833333373	0.207970440
0.666666627	0.333333373	0.207970440
0.666666627	0.833333373	0.207970440
0.000000000	0.000000000	0.260092437
0.000000000	0.500000000	0.260092437
0.500000000	0.000000000	0.260092437
0.500000000	0.500000000	0.260092437
0.333333313	0.166666687	0.277295470
0.333333313	0.666666687	0.277295470
0.833333313	0.166666687	0.277295470
0.833333313	0.666666687	0.277295470
0.161128163	0.336184591	0.329200208
0.166491061	0.831472754	0.334712684
0.664950132	0.335427612	0.330939859
0.669622004	0.827364147	0.329916656
0.999400437	0.997673869	0.343148351
0.995255768	0.493881077	0.347089201
0.500914991	0.005818421	0.345543772
0.489301503	0.488164037	0.348264366
0.317388028	0.160101295	0.385172427
0.313490748	0.662599385	0.382703036
0.875099659	0.182077229	0.394852221
0.845974207	0.680743277	0.387430638
0.333333313	0.013415892	0.026056252
0.333333313	0.513415873	0.026056252
0.833333313	0.013415892	0.026056252
0.833333313	0.513415873	0.026056252
0.180082545	0.166666687	0.026056252
0.180082545	0.666666687	0.026056252
0.680082560	0.166666687	0.026056252
0.680082560	0.666666687	0.026056252
0.486584067	0.319917470	0.026056252
0.486584067	0.819917440	0.026056252
0.986584067	0.319917470	0.026056252
0.986584067	0.819917440	0.026056252
0.346749187	0.346749246	0.095381320
0.346749187	0.846749246	0.095381320
0.846749187	0.346749246	0.095381320
0.846749187	0.846749246	0.095381320
0.153250769	0.000000000	0.095381320
0.153250769	0.500000000	0.095381320
0.653250754	0.000000000	0.095381320
0.653250754	0.500000000	0.095381320
0.000000000	0.153250784	0.095381320
0.000000000	0.653250813	0.095381320
0.500000000	0.153250784	0.095381320
0.500000000	0.653250813	0.095381320
0.166666657	0.180082574	0.164706394
0.166666657	0.680082560	0.164706394

0.666666627 0.180082574 0.164706394
0.666666627 0.680082560 0.164706394
0.013415871 0.333333373 0.164706394
0.013415871 0.833333373 0.164706394
0.513415873 0.333333373 0.164706394
0.513415873 0.833333373 0.164706394
0.319917411 0.486584157 0.164706394
0.319917411 0.986584187 0.164706394
0.819917440 0.486584157 0.164706394
0.819917440 0.986584187 0.164706394
0.180082545 0.013415892 0.234031439
0.180082545 0.513415873 0.234031439
0.680082560 0.013415892 0.234031439
0.680082560 0.513415873 0.234031439
0.486584067 0.166666687 0.234031439
0.486584067 0.666666687 0.234031439
0.986584067 0.166666687 0.234031439
0.986584067 0.666666687 0.234031439
0.333333313 0.319917470 0.234031439
0.333333313 0.819917440 0.234031439
0.833333313 0.319917470 0.234031439
0.833333313 0.819917440 0.234031439
0.995195985 0.344352424 0.303263932
0.002124848 0.844870090 0.302840799
0.496643484 0.343231410 0.304655224
0.502878308 0.846822500 0.304872751
0.346878052 0.001136722 0.304485887
0.342997521 0.498524636 0.304062426
0.843931794 0.999865592 0.303004414
0.845310867 0.496323109 0.303380072
0.156750664 0.157383353 0.302965045
0.155843496 0.654541016 0.304343939
0.657454610 0.155741662 0.305044293
0.653956532 0.655344665 0.301907390
0.034339659 0.177731112 0.370974302
0.016383471 0.671315312 0.372785658
0.518746197 0.183056474 0.374318361
0.514517009 0.681053758 0.375263512
0.409571081 0.365757793 0.404082388
0.333158940 0.854902864 0.375618219
0.831938624 0.336543798 0.382110387
0.822077692 0.839898407 0.370475888
0.153492033 0.468646556 0.372114569
0.145139277 0.974581480 0.374122590
0.683226109 0.493664026 0.370556563
0.674857140 0.002925822 0.377688557
0.876804829 0.138179526 0.450712383
0.039096393 0.933452666 0.453639567
0.786095381 0.626683056 0.443698794
0.360313535 0.465720057 0.469085991
0.634350896 0.115107894 0.473887473
0.839545906 0.432682604 0.493786544
0.330181897 0.967099428 0.449362099
0.589217722 0.741356611 0.451217920
0.474890262 0.311234683 0.487843752
0.731477082 0.104501188 0.467068672
0.062244307 0.945873618 0.424328804
0.134633169 0.942109466 0.463726491
0.921779692 0.073850796 0.456466615
0.874926567 0.698604703 0.459621191
0.671646476 0.715487957 0.452961355
0.257407606 0.432873040 0.478336573
0.366773039 0.401770979 0.427042067
0.601476431 0.078168310 0.501066864
0.825754821 0.334045470 0.502154469
0.782835782 0.456825405 0.513283908
0.316177249 0.916662514 0.422457218
0.435355574 0.995782793 0.456851572
0.559549510 0.702339590 0.403490156
0.496866614 0.645730913 0.461735934
0.393079638 0.204843327 0.488339394
0.414018869 0.381172627 0.482542425
0.639917254 0.931431830 0.400376499
0.644848347 0.349104553 0.429820299

Pu@Hem(001)-O_3 – Fe48O72 • Pu(H2O)5

1.0

10.1097135544 0.0000000000 0.0000000000
-5.0548563004 8.7552679372 0.0000000000
0.0000000000 0.0000000000 32.9692344666

Fe O H Pu
48 77 10 1

Direct

0.005999479 0.007984923 0.367631495
0.995532334 0.497777373 0.363742322
0.483849406 0.985177875 0.363481224
0.504640162 0.502094924 0.364396840
0.333744526 0.168200359 0.354392737
0.327217758 0.655527771 0.359431565
0.829909742 0.160966530 0.354407310
0.836163640 0.680415213 0.353426456
0.167351887 0.333413839 0.298474729
0.165719941 0.834774554 0.298322856
0.664922178 0.333223939 0.297857016
0.664099514 0.831349134 0.298246950
0.000000000 0.000000000 0.279781997
0.000000000 0.500000000 0.279781997
0.500000000 0.000000000 0.279781997
0.500000000 0.500000000 0.279781997
0.333333313 0.166666687 0.227194265
0.333333313 0.666666687 0.227194265
0.833333313 0.166666687 0.227194265
0.833333313 0.666666687 0.227194265
0.166666642 0.333333373 0.209837452
0.166666642 0.833333373 0.209837452
0.666666627 0.333333373 0.209837452
0.666666627 0.833333373 0.209837452
0.000000000 0.000000000 0.157249644
0.000000000 0.500000000 0.157249644
0.500000000 0.000000000 0.157249644
0.500000000 0.500000000 0.157249644
0.333333313 0.166666687 0.139892772
0.333333313 0.666666687 0.139892772
0.833333313 0.166666687 0.139892772
0.833333313 0.666666687 0.139892772
0.166666642 0.333333373 0.087305017
0.166666642 0.833333373 0.087305017
0.666666627 0.333333373 0.087305017
0.666666627 0.833333373 0.087305017
0.000000000 0.000000000 0.069948144
0.000000000 0.500000000 0.069948144
0.500000000 0.000000000 0.069948144
0.500000000 0.500000000 0.069948144
0.333333313 0.166666687 0.017360399
0.333333313 0.666666687 0.017360399
0.833333313 0.166666687 0.017360399
0.833333313 0.666666687 0.017360399
0.166666642 0.333333373 0.000003526
0.166666642 0.833333373 0.000003526
0.666666627 0.333333373 0.000003526
0.666666627 0.833333373 0.000003526
0.349645585 0.016194647 0.389395148
0.366150230 0.515641570 0.391968817
0.869216263 0.036839094 0.392587155

0.838515580	0.522913873	0.387513012
0.170959324	0.144650206	0.391382843
0.150320023	0.620446503	0.394186735
0.648993194	0.137228698	0.388499707
0.665520132	0.649712801	0.389388740
0.504759192	0.342713267	0.389559954
0.468890011	0.835300744	0.392040282
0.925983250	0.330497295	0.396803707
0.976288795	0.842661738	0.390859663
0.350476205	0.347260535	0.323809713
0.345163912	0.841792285	0.324282020
0.848451078	0.346563548	0.322646976
0.847844541	0.852467537	0.322821110
0.152164266	0.002675155	0.323194534
0.151512563	0.498046398	0.324502766
0.648740709	0.997148335	0.323679715
0.653856039	0.505639255	0.321865737
0.999789715	0.155608132	0.323974222
0.999823809	0.654036343	0.323439032
0.494617015	0.147609711	0.322173089
0.495343655	0.648347974	0.324337363
0.166666657	0.180082574	0.253488123
0.166666657	0.680082560	0.253488123
0.666666627	0.180082574	0.253488123
0.666666627	0.680082560	0.253488123
0.013415871	0.333333373	0.253488123
0.013415871	0.833333373	0.253488123
0.513415873	0.333333373	0.253488123
0.513415873	0.833333373	0.253488123
0.319917411	0.486584157	0.253488123
0.319917411	0.986584187	0.253488123
0.819917440	0.486584157	0.253488123
0.819917440	0.986584187	0.253488123
0.180082545	0.013415892	0.183543518
0.180082545	0.513415873	0.183543518
0.680082560	0.013415892	0.183543518
0.680082560	0.513415873	0.183543518
0.486584067	0.166666687	0.183543518
0.486584067	0.666666687	0.183543518
0.986584067	0.166666687	0.183543518
0.986584067	0.666666687	0.183543518
0.333333313	0.319917470	0.183543518
0.333333313	0.819917440	0.183543518
0.833333313	0.319917470	0.183543518
0.833333313	0.819917440	0.183543518
0.000000000	0.346749246	0.113598891
0.000000000	0.846749246	0.113598891
0.500000000	0.346749246	0.113598891
0.500000000	0.846749246	0.113598891
0.346749216	0.000000000	0.113598891
0.346749216	0.500000000	0.113598891
0.846749187	0.000000000	0.113598891
0.846749187	0.500000000	0.113598891
0.153250754	0.153250784	0.113598891
0.153250754	0.653250813	0.113598891
0.653250754	0.153250784	0.113598891
0.653250754	0.653250813	0.113598891
0.013415889	0.180082574	0.043654270
0.013415889	0.680082560	0.043654270
0.513415873	0.180082574	0.043654270
0.513415873	0.680082560	0.043654270
0.319917411	0.333333373	0.043654270
0.319917411	0.833333373	0.043654270
0.819917440	0.333333373	0.043654270
0.819917440	0.833333373	0.043654270
0.166666657	0.486584157	0.043654270
0.166666657	0.986584187	0.043654270
0.666666627	0.486584157	0.043654270
0.666666627	0.986584187	0.043654270
0.677208304	0.289241135	0.505711019
0.685878336	0.547306836	0.457563430
0.958814979	0.521836817	0.463948965
0.767538965	0.115612783	0.461467594
0.435769826	0.157266587	0.455761313
0.568166912	0.211098447	0.504827917
0.678189456	0.601215959	0.431289256
0.597170472	0.526174128	0.473905534
0.944134891	0.607322335	0.471158445
0.041699741	0.563556135	0.443048745
0.846386254	0.116817497	0.443138242
0.677598953	0.020832637	0.452537596
0.393064559	0.080482677	0.431367695
0.379251033	0.211295381	0.451578140
0.731601119	0.233385369	0.510560691
0.712070107	0.333904952	0.428390205