Interaction of Hydrogen with Actinide Dioxide (011) Surfaces (ESI)

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1 Clean Surface

1.1 Fixed Unit Cell Dimensions

Table 1: The fixed unit cell dimensions (Å) for the AnO_2 (011) surface.

Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
5.474	0.000	0.000	5.442	0.000	0.000	5.410	0.000	0.000
0.000	7.742	0.000	0.000	7.697	0.000	0.000	7.651	0.000
0.000	0.000	31.656	0.000	0.000	31.586	0.000	0.000	31.477

1.2 Ionic Positions & Magnetic Structure of the Clean Surface

Table 2: The relaxed ionic direct coordinates for the AnO_2 (011) surface (actinide ions, only).

Actinide Ion	Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
A	0.500	0.750	0.005	0.000	0.500	0.004	0.500	0.750	0.004
B	0.500	0.250	0.005	0.000	0.999	0.004	0.500	0.250	0.004
C	0.000	0.000	0.047	0.500	0.750	0.047	0.000	0.000	0.046
D	0.000	0.500	0.047	0.500	0.250	0.047	0.000	0.500	0.046
E	0.501	0.250	0.100	0.000	0.000	0.099	0.501	0.250	0.098
F	0.500	0.750	0.100	0.000	0.500	0.099	0.499	0.750	0.098
G	0.001	0.500	0.148	0.500	0.250	0.147	0.000	0.500	0.146
H	0.001	0.000	0.148	0.500	0.750	0.147	0.000	0.000	0.146
I	0.500	0.750	0.197	0.000	0.500	0.196	0.500	0.750	0.196
J	0.500	0.250	0.197	0.000	0.000	0.196	0.500	0.250	0.196
K	0.000	0.000	0.246	0.500	0.750	0.245	0.000	1.000	0.244
L	0.000	0.500	0.246	0.500	0.250	0.245	0.000	0.500	0.244
M	0.500	0.250	0.295	0.000	0.000	0.294	0.500	0.250	0.293
N	0.500	0.750	0.295	0.000	0.500	0.294	0.500	0.750	0.293
O	-0.001	0.500	0.345	0.500	0.250	0.344	0.000	0.500	0.343
P	-0.001	0.000	0.345	0.500	0.750	0.344	0.000	0.000	0.343
Q	0.499	0.750	0.393	0.000	0.500	0.392	0.499	0.750	0.391
R	0.500	0.250	0.393	0.000	0.000	0.392	0.501	0.250	0.391
S	0.000	0.000	0.445	0.500	0.750	0.444	0.000	0.000	0.443
T	0.000	0.500	0.445	0.500	0.250	0.444	0.000	0.500	0.443
U	0.500	0.250	0.488	0.000	0.000	0.486	0.500	0.250	0.485
V	0.500	0.750	0.488	0.000	0.501	0.486	0.500	0.750	0.485

Table 3: The relaxed magnetic vectors (μ_B) for the AnO_2 (011) surface (actinide ions, only).

Actinide Ion	Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
A	-0.02	-1.07	1.05	0.00	-2.72	0.08	-3.12	0.00	2.22
B	-0.02	1.08	-1.03	0.02	2.72	-0.08	3.12	0.00	2.22
C	-0.87	-0.01	1.09	0.01	2.06	1.74	0.00	3.21	-2.04
D	1.38	0.00	-0.20	2.18	0.01	-1.60	0.00	-3.21	-2.04
E	0.01	-1.37	0.07	0.00	-2.22	1.53	-3.15	0.00	2.12
F	-0.43	0.61	-1.16	-2.14	0.07	-1.64	3.15	0.00	2.12
G	-0.17	1.31	0.33	-0.02	2.19	1.57	0.00	3.10	-2.19
H	1.37	-0.05	0.03	2.22	-0.01	-1.54	0.00	-3.10	-2.19
I	0.13	-1.36	0.05	0.02	-2.20	1.56	-3.11	0.00	2.17
J	-1.04	0.42	-0.78	-2.18	0.02	-1.59	3.11	0.00	2.17
K	-0.14	1.34	0.21	-0.03	2.21	1.55	0.00	3.10	-2.20
L	1.36	-0.17	0.05	2.20	-0.03	-1.56	0.00	-3.10	-2.19
M	0.13	-1.36	0.05	0.02	-2.20	1.56	-3.11	0.00	2.17
N	-1.04	0.42	-0.78	-2.18	0.02	-1.59	3.11	0.00	2.17
O	-0.17	1.31	0.33	-0.02	2.19	1.57	0.00	3.10	-2.20
P	1.37	-0.05	0.03	2.22	-0.01	-1.54	0.00	-3.10	-2.19
Q	0.01	-1.37	0.07	0.00	-2.22	1.53	-3.15	0.00	2.13
R	-0.43	0.61	-1.16	-2.14	0.07	-1.64	3.15	0.00	2.13
S	-0.87	-0.01	1.09	0.01	2.05	1.74	0.00	3.21	-2.04
T	1.38	0.00	-0.20	2.18	0.01	-1.60	0.00	-3.21	-2.04
U	-0.02	-1.06	1.05	0.00	-2.72	0.09	-3.12	0.00	2.22
V	-0.02	1.08	-1.03	0.02	2.73	-0.08	3.12	0.00	2.22

Note: The magnetic vectors for the low-index AnO_2 (011) surfaces are given for each actinide ion. A diamagnetic (DM) ion (magnetic moment = 0.00), oxygen is not included. An earlier investigation contains a complete analysis of the data.[1]

1.3 K-Point Convergence

The energy of the low-index surfaces has been calculated as function of the number of formula units (**Figure 1**). An earlier investigation contains a complete analysis of the data.[1]

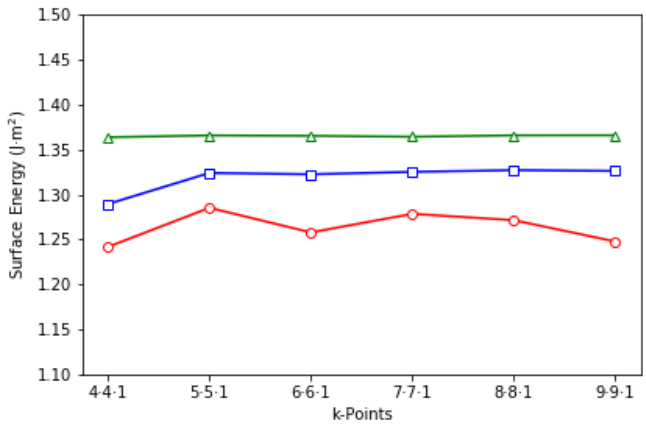

Figure 1: Convergence of the surface energies (J m^{-2}) with respect to the number of formula units (N) employed: (red) uranium dioxide, (blue) neptunium dioxide, and (green) plutonium dioxide.

1.4 Electronic Density of States

The electronic density of states for the clean AnO_2 (An = U, Np, Pu) (011) surface has been calculated (noncollinear relativistic PBEsol+U, **Figure 2**).[1]

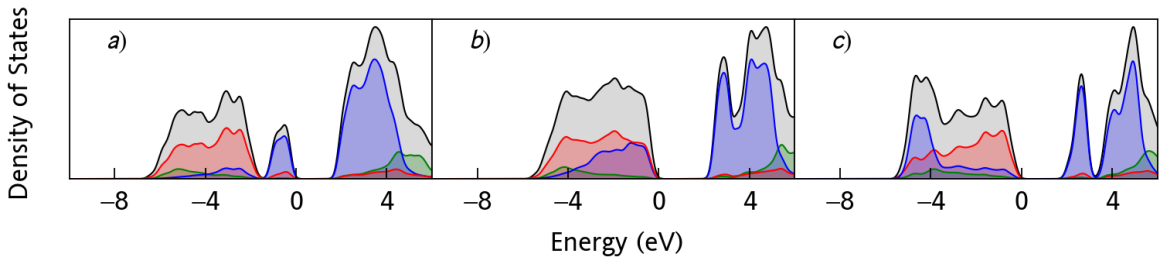

Figure 2: The electronic density of states for the AnO_2 (011) surface, calculated by PBEsol+U: a) UO_2, b) NpO_2, c) PuO_2. The total density of states (black), actinide f- (blue), actinide d- (green), and oxygen p- (red) bands are coloured.[1]

2 Hydrogen Interactions

2.1 Uranium Dioxide

2.1.1 Atomic Hydrogen

Table 4: The ionic positions and magnetic structure of the UO_2 $aH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.495	0.249	0.940	0.00	0.00	0.02
	0.505	0.751	0.429	0.00	0.00	0.02
Actinide Ion	0.499	0.750	0.005	1.00	-0.99	-0.10
	0.499	0.250	0.004	0.03	-0.14	-0.65
	0.999	0.002	0.059	1.01	0.85	-0.35
	0.999	0.497	0.059	-0.84	0.04	1.08
	0.500	0.250	0.124	0.77	-1.36	-0.11
	0.499	0.750	0.124	-0.85	-0.03	-1.31
	0.000	0.500	0.184	0.72	1.12	-0.29
	0.000	0.000	0.184	-0.63	-0.08	1.21
	0.500	0.750	0.245	0.77	-1.36	-0.11
	0.501	0.250	0.245	-0.85	-0.03	-1.31
	0.001	0.998	0.309	1.00	0.85	-0.35
	0.001	0.503	0.309	-0.84	0.04	1.08
	0.501	0.250	0.363	1.01	-0.99	-0.10
	0.501	0.750	0.364	0.03	-0.14	-0.65
Oxygen Ion	0.266	0.492	0.003	0.00	0.01	0.01
	0.728	0.495	0.003	-0.01	0.01	0.01
	0.268	0.005	0.003	-0.02	0.01	0.01
	0.729	0.008	0.003	-0.01	0.01	0.01
	0.250	0.750	0.061	0.00	0.00	0.01
	0.250	0.249	0.063	-0.01	0.00	0.00
	0.747	0.750	0.061	-0.01	-0.01	0.00
	0.747	0.250	0.062	0.00	0.00	0.01
	0.249	0.998	0.123	0.01	0.00	0.00
	0.749	1.000	0.122	0.00	0.01	0.00
	0.251	0.500	0.123	0.00	0.00	0.00
	0.751	0.502	0.122	0.01	0.00	0.00
	0.252	0.249	0.184	0.00	0.00	0.00
	0.248	0.749	0.184	0.00	-0.01	0.00
	0.752	0.251	0.184	-0.01	-0.01	0.00
	0.748	0.751	0.184	0.00	0.00	0.01
	0.249	0.498	0.246	0.01	0.00	0.00
	0.749	0.500	0.245	0.00	0.00	0.00
	0.251	0.000	0.246	0.00	0.01	0.00
	0.751	0.002	0.245	0.01	0.00	0.00
	0.253	0.750	0.306	0.00	0.00	0.01
	0.253	0.250	0.307	-0.01	-0.01	0.00
	0.750	0.751	0.306	-0.01	0.00	0.00
	0.750	0.250	0.307	0.00	0.00	0.01
	0.271	0.992	0.365	-0.01	0.01	0.01
	0.732	0.995	0.365	-0.02	0.01	0.01
	0.272	0.505	0.365	-0.01	0.01	0.01
	0.734	0.508	0.365	0.00	0.01	0.00

Table 5: The ionic positions and magnetic structure of the UO_2 $bH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.503	0.204	0.938	0.00	-0.02	-0.04
	0.497	0.796	0.430	0.00	-0.02	-0.04
Actinide Ion	0.503	0.747	0.007	-0.91	1.09	0.13
	0.502	0.254	0.003	-0.09	1.30	0.05
	0.001	0.001	0.060	0.84	0.50	0.15
	0.003	0.498	0.059	-0.64	-0.03	1.17
	0.501	0.250	0.123	0.70	-1.36	-0.27
	0.501	0.748	0.124	-0.46	-0.48	-1.30
	0.000	0.500	0.184	0.80	1.05	0.26
	0.000	0.000	0.184	-0.22	-0.23	1.29
	0.499	0.750	0.245	0.70	-1.35	-0.27
	0.499	0.252	0.244	-0.46	-0.48	-1.29
	0.999	0.999	0.308	0.83	0.50	0.14
	0.997	0.502	0.309	-0.64	-0.03	1.17
	0.497	0.253	0.362	-0.91	1.10	0.13
	0.498	0.746	0.365	-0.09	1.31	0.05
Oxygen Ion	0.264	0.504	0.004	0.02	-0.02	-0.01
	0.736	0.507	0.004	0.01	-0.03	-0.01
	0.261	0.992	0.008	0.00	-0.03	0.00
	0.748	0.997	0.008	-0.01	-0.03	0.00
	0.254	0.748	0.064	0.01	-0.01	0.00
	0.243	0.245	0.063	-0.01	-0.01	-0.01
	0.759	0.753	0.064	0.00	-0.01	0.00
	0.756	0.249	0.063	-0.01	-0.01	-0.01
	0.244	0.998	0.121	-0.01	0.00	-0.01
	0.753	0.001	0.121	-0.01	0.01	0.00
	0.254	0.497	0.124	-0.01	0.01	0.00
	0.750	0.501	0.124	0.00	0.01	-0.01
	0.251	0.245	0.184	0.00	0.00	0.00
	0.247	0.753	0.184	-0.01	0.00	0.00
	0.753	0.247	0.184	-0.01	0.00	0.00
	0.749	0.755	0.184	0.00	0.00	0.01
	0.250	0.499	0.244	0.00	0.00	-0.01
	0.746	0.503	0.244	-0.01	0.01	0.00
	0.247	0.999	0.247	-0.01	0.00	0.00
	0.756	0.002	0.247	-0.01	0.00	-0.01
	0.244	0.751	0.305	-0.01	-0.01	-0.01
	0.241	0.247	0.305	0.00	-0.01	0.00
	0.757	0.755	0.306	-0.01	-0.01	-0.01
	0.746	0.252	0.304	0.01	-0.01	0.00
	0.252	0.003	0.361	-0.02	-0.03	0.00
	0.739	0.008	0.360	0.00	-0.03	0.00
	0.264	0.493	0.364	0.01	-0.03	-0.01
	0.736	0.496	0.364	0.02	-0.02	-0.01

Table 6: The ionic positions and magnetic structure of the UO_2 $cH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.008	0.268	0.009	0.02	0.01	-0.01
	0.992	0.732	0.360	0.02	0.01	-0.01
Actinide Ion	0.496	0.755	0.007	-0.97	1.17	-0.18
	0.492	0.246	0.007	-1.56	0.07	-0.02
	0.996	0.005	0.059	0.22	0.86	-1.19
	0.997	0.486	0.056	-0.57	-0.26	0.50
	0.500	0.251	0.125	0.10	-1.34	0.23
	0.498	0.748	0.123	-0.96	-0.10	-1.25
	0.000	0.500	0.184	0.25	1.18	-0.71
	0.000	0.000	0.184	-0.18	0.18	1.37
	0.500	0.749	0.243	0.10	-1.34	0.23
	0.502	0.252	0.245	-0.96	-0.10	-1.25
	0.004	0.995	0.310	0.22	0.86	-1.19
	0.003	0.514	0.313	-0.57	-0.25	0.50
	0.504	0.245	0.361	-0.97	1.18	-0.18
	0.508	0.754	0.362	-1.56	0.08	-0.02
Oxygen Ion	0.263	0.506	0.004	0.04	-0.01	-0.02
	0.730	0.506	0.004	0.03	0.00	-0.01
	0.263	0.994	0.003	0.02	-0.01	0.01
	0.725	0.999	0.003	0.03	-0.01	0.01
	0.240	0.747	0.062	0.01	-0.01	0.01
	0.259	0.253	0.065	0.02	0.01	-0.01
	0.751	0.748	0.062	0.01	-0.01	0.01
	0.737	0.254	0.064	0.02	0.01	0.01
	0.249	0.999	0.123	0.01	0.00	0.00
	0.750	0.001	0.123	-0.01	0.01	0.00
	0.247	0.499	0.122	0.00	0.01	0.01
	0.755	0.500	0.121	0.01	0.00	0.00
	0.250	0.252	0.185	0.01	0.00	0.00
	0.248	0.747	0.184	0.00	-0.01	0.00
	0.752	0.253	0.185	0.00	-0.01	0.00
	0.750	0.748	0.183	0.01	0.00	0.00
	0.245	0.500	0.247	0.01	0.00	0.00
	0.753	0.501	0.246	0.00	0.01	0.00
	0.250	0.999	0.246	-0.01	0.01	0.01
	0.751	0.001	0.245	0.01	0.00	0.00
	0.263	0.746	0.304	0.02	0.01	0.00
	0.249	0.252	0.306	0.01	-0.01	0.01
	0.741	0.747	0.303	0.02	0.01	-0.01
	0.760	0.253	0.306	0.01	-0.01	0.01
	0.275	0.001	0.365	0.02	-0.02	0.01
	0.737	0.006	0.365	0.02	-0.01	0.01
	0.270	0.494	0.364	0.03	0.00	-0.01
	0.737	0.494	0.364	0.04	-0.01	-0.02

Table 7: The ionic positions and magnetic structure of the UO_2 $dH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.084	0.985	0.980	0.00	0.00	0.00
	0.916	0.015	0.388	0.00	0.00	0.00
Actinide Ion	0.520	0.742	0.005	-0.02	-1.62	-0.10
	0.518	0.257	0.003	0.09	0.08	-0.10
	0.999	0.000	0.062	0.56	1.28	0.05
	0.012	0.501	0.058	0.06	-0.05	1.39
	0.503	0.252	0.123	0.52	-1.25	0.01
	0.503	0.748	0.124	-0.93	-0.61	-0.82
	0.000	0.500	0.184	0.65	1.41	0.16
	0.000	0.000	0.184	-0.90	0.07	1.32
	0.497	0.748	0.245	0.52	-1.25	0.00
	0.497	0.252	0.244	-0.93	-0.61	-0.82
	0.001	1.000	0.306	0.56	1.28	0.05
	0.988	0.499	0.310	0.06	-0.05	1.39
	0.480	0.258	0.363	-0.02	-1.62	-0.09
	0.482	0.743	0.365	0.09	0.07	-0.09
Oxygen Ion	0.278	0.514	0.002	0.01	0.02	0.00
	0.763	0.512	0.001	-0.01	0.02	0.00
	0.256	0.989	0.990	0.00	0.00	0.00
	0.761	0.986	0.001	0.00	0.01	0.00
	0.264	0.762	0.061	0.01	0.01	0.00
	0.258	0.242	0.060	-0.01	0.00	0.00
	0.760	0.747	0.064	0.00	0.00	0.00
	0.760	0.252	0.062	-0.01	-0.01	-0.01
	0.249	0.002	0.124	0.00	0.00	0.00
	0.751	0.001	0.123	0.00	0.01	0.00
	0.252	0.501	0.121	0.00	0.01	-0.01
	0.750	0.498	0.123	0.00	0.00	0.00
	0.252	0.252	0.184	0.01	0.00	0.00
	0.248	0.748	0.184	0.00	0.00	0.00
	0.752	0.252	0.184	0.00	0.00	0.00
	0.748	0.748	0.184	0.01	0.00	0.01
	0.250	0.502	0.245	0.00	0.00	0.00
	0.748	0.499	0.247	0.00	0.01	-0.01
	0.249	0.999	0.245	0.00	0.01	0.00
	0.751	0.998	0.245	0.00	0.00	-0.01
	0.240	0.748	0.306	-0.01	-0.01	-0.01
	0.240	0.253	0.305	0.00	0.00	0.00
	0.742	0.758	0.308	-0.01	0.00	0.01
	0.736	0.238	0.307	0.01	0.01	0.00
	0.239	0.014	0.367	0.00	0.01	0.00
	0.744	0.011	0.378	0.00	0.00	0.00
	0.237	0.488	0.368	-0.01	0.02	-0.01
	0.722	0.486	0.366	0.00	0.02	-0.01

2.1.2 Molecular Hydrogen

Table 8: The ionic positions and magnetic structure of the UO_2 $aH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.488	0.313	0.917	0.00	0.00	0.00
	0.504	0.215	0.915	0.00	0.00	0.00
	0.496	0.785	0.453	0.00	0.00	0.00
	0.512	0.687	0.451	0.00	0.00	0.00
Actinide Ion	0.504	0.747	0.006	-0.43	-1.51	-0.09
	0.504	0.247	0.006	0.83	-1.14	0.12
	0.003	0.998	0.059	1.26	0.43	-0.41
	0.003	0.498	0.059	-0.81	0.05	1.11
	0.501	0.249	0.124	1.01	-1.00	-0.27
	0.501	0.749	0.124	-0.47	-0.10	-1.31
	0.000	0.500	0.184	0.61	1.37	0.41
	0.000	0.000	0.184	-0.97	0.16	1.23
	0.499	0.751	0.245	1.02	-1.00	-0.27
	0.499	0.251	0.244	-0.47	-0.10	-1.31
	0.997	0.002	0.309	1.26	0.43	-0.41
	0.997	0.502	0.309	-0.81	0.05	1.11
	0.496	0.253	0.362	-0.42	-1.51	-0.09
	0.496	0.753	0.362	0.83	-1.14	0.12
Oxygen Ion	0.266	0.500	0.002	0.01	0.03	-0.01
	0.737	0.494	0.002	0.00	0.02	-0.01
	0.268	0.000	0.002	-0.01	0.02	0.01
	0.740	0.994	0.002	-0.01	0.02	0.00
	0.255	0.748	0.062	0.01	0.01	0.01
	0.255	0.248	0.062	-0.01	0.00	0.00
	0.752	0.747	0.062	0.00	0.00	0.01
	0.753	0.247	0.062	-0.01	0.01	0.00
	0.252	0.999	0.123	0.00	0.00	0.00
	0.752	0.998	0.123	-0.01	0.01	0.00
	0.251	0.500	0.123	0.00	0.00	0.00
	0.750	0.499	0.123	0.00	0.00	-0.01
	0.251	0.250	0.184	0.00	0.00	0.01
	0.248	0.750	0.184	0.00	0.00	0.00
	0.752	0.250	0.184	0.00	0.00	0.00
	0.749	0.750	0.184	0.00	0.00	0.01
	0.250	0.501	0.246	0.00	0.00	-0.01
	0.749	0.500	0.246	0.00	0.00	0.00
	0.248	0.002	0.245	-0.01	0.01	0.00
	0.748	0.001	0.246	0.00	0.00	0.00
	0.247	0.753	0.306	-0.01	0.01	0.00
	0.248	0.253	0.306	0.00	0.00	0.01
	0.745	0.752	0.306	-0.01	0.00	0.00
	0.745	0.252	0.306	0.01	0.01	0.01
	0.260	0.006	0.366	-0.01	0.02	0.00
	0.732	1.000	0.366	-0.01	0.02	0.01
	0.263	0.506	0.366	0.00	0.02	-0.01
	0.734	0.500	0.366	0.00	0.03	-0.01

Table 9: The ionic positions and magnetic structure of the UO_2 $bH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.460	0.209	0.916	0.00	0.00	0.00
	0.538	0.291	0.917	0.00	0.00	0.00
	0.540	0.791	0.452	0.00	0.00	0.00
	0.462	0.709	0.452	0.00	0.00	0.00
Actinide Ion	0.495	0.748	0.006	0.21	-1.56	-0.12
	0.495	0.248	0.006	0.71	-1.20	0.07
	0.996	0.999	0.059	1.11	0.77	-0.20
	0.995	0.498	0.059	-0.82	0.05	1.10
	0.498	0.249	0.124	1.06	-1.13	-0.18
	0.498	0.749	0.124	-0.67	0.01	-1.38
	0.000	0.500	0.184	0.74	1.35	0.22
	0.000	0.000	0.184	-0.80	0.33	1.30
	0.502	0.751	0.244	1.06	-1.13	-0.18
	0.502	0.251	0.244	-0.67	0.01	-1.38
	0.004	0.001	0.309	1.11	0.77	-0.20
	0.005	0.502	0.309	-0.82	0.05	1.10
	0.505	0.252	0.362	0.21	-1.55	-0.12
	0.505	0.752	0.362	0.72	-1.20	0.07
Oxygen Ion	0.258	0.495	0.003	0.00	0.03	-0.01
	0.730	0.501	0.002	0.00	0.02	-0.01
	0.257	0.995	0.002	-0.01	0.02	0.01
	0.728	0.001	0.002	-0.02	0.02	0.00
	0.246	0.748	0.062	0.00	0.01	0.01
	0.246	0.247	0.062	-0.01	0.00	0.00
	0.744	0.749	0.062	0.00	0.00	0.01
	0.744	0.249	0.062	-0.01	0.01	0.00
	0.250	0.998	0.123	0.00	0.00	0.00
	0.751	1.000	0.122	-0.01	0.00	0.00
	0.248	0.499	0.123	0.00	0.00	0.00
	0.748	0.500	0.122	0.00	0.00	-0.01
	0.249	0.250	0.184	0.00	0.00	0.00
	0.251	0.749	0.185	0.00	0.00	0.00
	0.749	0.251	0.184	0.00	0.00	0.00
	0.751	0.750	0.184	0.00	0.00	0.00
	0.252	0.500	0.246	0.00	0.00	-0.01
	0.752	0.501	0.245	0.00	0.00	0.00
	0.249	0.000	0.246	0.00	0.00	0.00
	0.750	0.002	0.245	0.00	0.00	0.00
	0.256	0.751	0.306	-0.01	0.01	0.00
	0.256	0.251	0.306	0.00	0.00	0.00
	0.754	0.753	0.306	-0.01	0.00	0.00
	0.754	0.252	0.306	0.00	0.01	0.01
	0.272	0.999	0.366	-0.02	0.02	0.00
	0.743	0.005	0.366	-0.01	0.02	0.01
	0.270	0.499	0.366	0.00	0.02	-0.01
	0.742	0.505	0.366	0.00	0.03	-0.01

Table 10: The ionic positions and magnetic structure of the UO_2 $cH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.427	0.250	0.916	0.00	0.00	0.00
	0.567	0.248	0.916	0.00	0.00	0.00
	0.573	0.750	0.453	0.00	0.00	0.00
	0.433	0.752	0.453	0.00	0.00	0.00
Actinide Ion	0.496	0.748	0.006	0.15	-1.57	-0.11
	0.496	0.248	0.006	-0.46	-1.33	0.14
	0.996	0.998	0.059	1.21	0.63	-0.17
	0.996	0.498	0.059	-0.82	0.10	1.10
	0.498	0.249	0.124	1.03	-1.15	-0.18
	0.498	0.749	0.124	-0.45	-0.11	-1.34
	0.000	0.500	0.184	0.73	1.35	0.16
	0.000	0.000	0.184	-0.89	0.13	1.29
	0.502	0.751	0.244	1.03	-1.16	-0.18
	0.502	0.251	0.244	-0.45	-0.11	-1.34
	0.004	0.002	0.309	1.21	0.63	-0.17
	0.004	0.502	0.309	-0.82	0.10	1.10
	0.504	0.252	0.362	0.15	-1.56	-0.11
	0.504	0.752	0.362	-0.45	-1.33	0.14
Oxygen Ion	0.258	0.497	0.002	0.01	0.02	-0.01
	0.730	0.500	0.002	0.01	0.03	-0.01
	0.259	0.996	0.002	-0.01	0.02	0.01
	0.731	1.000	0.002	-0.01	0.02	0.00
	0.247	0.747	0.062	0.00	0.01	0.01
	0.247	0.247	0.062	0.00	0.00	-0.01
	0.744	0.749	0.062	0.00	0.00	0.01
	0.744	0.249	0.062	0.00	0.01	0.00
	0.249	0.998	0.123	0.00	0.00	0.00
	0.749	0.000	0.122	-0.01	0.01	0.00
	0.249	0.498	0.123	0.00	0.00	0.00
	0.749	0.500	0.122	0.00	0.00	-0.01
	0.251	0.249	0.184	0.00	0.00	0.00
	0.249	0.749	0.184	-0.01	0.00	0.00
	0.751	0.251	0.184	-0.01	0.00	0.00
	0.749	0.751	0.184	0.00	0.00	0.01
	0.251	0.500	0.246	0.00	0.00	-0.01
	0.751	0.502	0.245	0.00	0.00	0.00
	0.251	1.000	0.246	-0.01	0.01	0.00
	0.751	0.002	0.245	0.00	0.00	0.00
	0.256	0.751	0.306	0.00	0.01	0.00
	0.256	0.251	0.306	0.00	0.00	0.01
	0.753	0.753	0.306	0.00	0.00	-0.01
	0.753	0.253	0.306	0.00	0.01	0.01
	0.269	0.000	0.366	-0.01	0.02	0.00
	0.741	0.004	0.366	-0.01	0.02	0.01
	0.270	0.500	0.366	0.01	0.03	-0.01
	0.742	0.503	0.366	0.01	0.02	-0.01

Table 11: The ionic positions and magnetic structure of the UO_2 $dH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.023	0.998	0.908	0.00	0.00	0.00
	0.024	0.999	0.932	0.00	0.00	0.00
	0.977	0.002	0.461	0.00	0.00	0.00
	0.976	0.001	0.436	0.00	0.00	0.00
Actinide Ion	0.501	0.751	0.006	-1.02	1.09	-0.04
	0.501	0.252	0.006	1.06	-1.04	-0.01
	0.001	0.001	0.059	1.20	0.21	-0.69
	0.000	0.501	0.059	-0.71	-0.07	1.18
	0.500	0.251	0.124	1.04	-0.91	0.04
	0.501	0.751	0.124	-0.47	-0.29	-1.24
	0.000	0.500	0.184	0.17	0.90	1.10
	0.000	0.000	0.184	-1.18	0.29	0.71
	0.500	0.749	0.244	1.04	-0.91	0.04
	0.499	0.249	0.244	-0.47	-0.29	-1.24
	0.999	0.999	0.309	1.20	0.21	-0.69
	1.000	0.499	0.309	-0.71	-0.07	1.18
	0.499	0.249	0.362	-1.01	1.09	-0.04
	0.499	0.748	0.362	1.06	-1.04	-0.01
Oxygen Ion	0.264	0.498	0.003	0.00	0.01	-0.01
	0.735	0.505	0.002	0.01	-0.01	-0.01
	0.263	0.998	0.003	-0.01	-0.01	0.01
	0.735	0.005	0.002	-0.01	0.01	0.00
	0.253	0.750	0.062	0.01	0.00	0.00
	0.253	0.251	0.062	-0.01	0.00	0.00
	0.750	0.753	0.062	0.00	-0.01	0.01
	0.750	0.252	0.062	-0.01	0.01	0.00
	0.251	0.999	0.123	0.00	0.00	0.00
	0.751	0.002	0.123	-0.01	0.01	0.01
	0.250	0.499	0.123	0.00	0.01	-0.01
	0.750	0.502	0.122	0.00	0.00	-0.01
	0.249	0.249	0.184	0.01	0.00	0.01
	0.250	0.749	0.184	0.00	-0.01	0.00
	0.750	0.251	0.184	0.00	-0.01	0.00
	0.751	0.751	0.184	0.01	0.00	0.01
	0.250	0.498	0.246	0.00	0.00	-0.01
	0.750	0.501	0.245	0.00	0.01	-0.01
	0.249	0.998	0.246	-0.01	0.01	0.01
	0.749	0.001	0.245	0.00	0.00	0.00
	0.250	0.748	0.306	-0.01	0.01	0.00
	0.250	0.247	0.306	0.00	-0.01	0.01
	0.747	0.749	0.306	-0.01	0.00	0.00
	0.747	0.250	0.306	0.01	0.00	0.01
	0.265	0.995	0.366	-0.01	0.01	0.01
	0.737	0.002	0.366	-0.01	-0.01	0.01
	0.265	0.495	0.366	0.01	-0.01	-0.01
	0.736	0.502	0.366	0.00	0.01	-0.01

Table 12: The ionic positions and magnetic structure of the UO_2 $eH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.076	0.998	0.933	0.00	0.00	0.00
	0.070	0.997	0.909	0.00	0.00	0.00
	0.930	0.003	0.459	0.00	0.00	0.00
	0.924	0.002	0.435	0.00	0.00	0.00
Actinide Ion	0.506	0.750	0.006	-1.02	1.09	-0.06
	0.506	0.250	0.006	1.45	-0.43	-0.12
	0.005	0.000	0.059	1.23	0.34	-0.55
	0.005	0.500	0.059	-0.73	-0.04	1.17
	0.503	0.250	0.124	1.22	-0.72	0.01
	0.502	0.750	0.124	-0.45	-0.56	-1.21
	0.000	0.500	0.184	0.40	1.28	0.76
	0.000	0.000	0.184	-1.24	0.06	0.94
	0.497	0.750	0.244	1.22	-0.72	0.01
	0.498	0.250	0.244	-0.45	-0.56	-1.21
	0.995	1.000	0.309	1.23	0.34	-0.55
	0.995	0.500	0.309	-0.74	-0.04	1.17
	0.494	0.250	0.362	-1.02	1.09	-0.06
	0.494	0.750	0.362	1.45	-0.43	-0.12
Oxygen Ion	0.270	0.497	0.003	0.00	0.00	-0.01
	0.741	0.503	0.002	0.00	-0.01	-0.01
	0.270	0.997	0.002	-0.01	-0.01	0.01
	0.742	0.003	0.002	-0.01	0.00	0.00
	0.257	0.749	0.062	0.01	0.00	0.00
	0.257	0.249	0.062	-0.02	0.00	0.00
	0.755	0.751	0.062	0.00	-0.01	0.01
	0.755	0.251	0.062	-0.01	0.01	0.00
	0.252	0.999	0.123	0.00	0.00	0.00
	0.752	0.002	0.123	0.00	0.01	0.00
	0.252	0.499	0.123	0.00	0.01	-0.01
	0.751	0.501	0.122	0.00	0.00	-0.01
	0.250	0.249	0.184	0.01	0.00	0.01
	0.249	0.748	0.184	-0.01	-0.01	0.00
	0.751	0.252	0.184	-0.01	-0.01	0.00
	0.750	0.751	0.184	0.01	0.00	0.01
	0.249	0.499	0.246	0.00	0.00	-0.01
	0.748	0.501	0.245	0.00	0.01	-0.01
	0.248	0.998	0.245	0.00	0.01	0.01
	0.748	0.001	0.245	0.00	0.00	0.00
	0.245	0.749	0.306	-0.01	0.01	0.00
	0.245	0.249	0.306	0.00	-0.01	0.01
	0.743	0.751	0.306	-0.02	0.00	0.00
	0.743	0.251	0.306	0.01	0.00	0.01
	0.258	0.997	0.366	-0.02	0.00	0.00
	0.730	0.003	0.366	-0.01	-0.01	0.01
	0.259	0.497	0.366	0.00	-0.01	-0.01
	0.730	0.503	0.366	0.00	0.00	-0.01

Table 13: The ionic positions and magnetic structure of the UO_2 $fH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.243	0.993	0.928	0.00	0.00	0.00
	0.279	0.990	0.905	0.00	0.00	0.00
	0.721	0.010	0.464	0.00	0.00	0.00
	0.757	0.007	0.440	0.00	0.00	0.00
Actinide Ion	0.499	0.749	0.006	-1.06	1.03	-0.13
	0.498	0.249	0.006	1.49	-0.15	-0.12
	0.999	0.999	0.059	1.26	0.46	-0.39
	0.998	0.499	0.059	-0.77	-0.07	1.13
	0.500	0.250	0.124	1.10	-0.93	-0.14
	0.499	0.750	0.124	-0.49	0.06	-1.33
	0.000	0.500	0.184	0.65	1.36	0.38
	0.000	0.000	0.184	-0.85	-0.14	1.33
	0.500	0.750	0.244	1.10	-0.93	-0.14
	0.501	0.250	0.244	-0.49	0.06	-1.33
	0.001	0.001	0.309	1.26	0.46	-0.39
	0.002	0.501	0.309	-0.78	-0.07	1.13
	0.501	0.251	0.362	-1.06	1.03	-0.13
	0.502	0.751	0.362	1.50	-0.15	-0.12
Oxygen Ion	0.263	0.498	0.003	0.00	0.00	-0.01
	0.734	0.500	0.002	0.00	-0.01	-0.01
	0.259	0.999	0.003	-0.01	-0.01	0.01
	0.731	0.999	0.002	-0.01	0.00	0.00
	0.250	0.747	0.062	0.01	0.00	0.00
	0.250	0.250	0.062	-0.02	0.00	0.00
	0.747	0.750	0.062	0.01	-0.01	0.01
	0.747	0.248	0.062	-0.01	0.01	0.00
	0.251	0.999	0.123	0.00	0.00	0.00
	0.750	0.001	0.123	-0.01	0.01	0.00
	0.250	0.499	0.123	-0.01	0.00	0.00
	0.749	0.500	0.122	0.00	0.00	-0.01
	0.250	0.249	0.185	0.00	0.00	0.01
	0.249	0.749	0.184	-0.01	0.00	0.00
	0.751	0.251	0.184	-0.01	0.00	0.00
	0.750	0.751	0.184	0.00	0.00	0.01
	0.251	0.500	0.246	0.00	0.00	-0.01
	0.750	0.501	0.245	-0.01	0.00	0.00
	0.250	0.999	0.246	-0.01	0.01	0.00
	0.749	0.001	0.245	0.00	0.00	0.00
	0.253	0.752	0.306	-0.01	0.00	0.00
	0.253	0.250	0.306	0.01	-0.01	0.01
	0.750	0.750	0.306	-0.02	0.00	0.00
	0.750	0.253	0.306	0.01	0.00	0.00
	0.269	0.001	0.366	-0.01	0.00	0.00
	0.741	0.001	0.365	-0.01	-0.01	0.01
	0.266	0.500	0.366	0.00	-0.01	-0.01
	0.737	0.502	0.366	0.00	0.00	-0.01

Table 14: The ionic positions and magnetic structure of the UO_2 $gH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.364	0.003	0.926	0.00	0.00	0.00
	0.446	0.007	0.906	0.00	0.00	0.00
	0.554	0.993	0.462	0.00	0.00	0.00
	0.636	0.997	0.442	0.00	0.00	0.00
Actinide Ion	0.497	0.747	0.006	-1.04	1.07	-0.11
	0.497	0.247	0.006	1.29	0.71	-0.27
	0.997	0.998	0.059	1.26	0.53	-0.26
	0.997	0.498	0.059	-0.76	-0.06	1.14
	0.499	0.249	0.124	1.03	-0.95	-0.16
	0.499	0.749	0.124	-0.46	-0.23	-1.36
	0.000	0.500	0.184	0.76	1.36	0.05
	0.000	0.000	0.184	-0.98	0.12	1.21
	0.501	0.751	0.244	1.03	-0.95	-0.16
	0.501	0.251	0.244	-0.47	-0.23	-1.36
	0.003	0.002	0.309	1.26	0.53	-0.26
	0.003	0.502	0.309	-0.76	-0.06	1.14
	0.503	0.253	0.362	-1.03	1.07	-0.11
	0.503	0.753	0.362	1.30	0.71	-0.27
Oxygen Ion	0.262	0.494	0.002	0.01	-0.01	-0.01
	0.733	0.500	0.002	0.00	-0.02	0.00
	0.262	0.994	0.002	-0.01	-0.02	0.01
	0.733	0.000	0.003	-0.01	-0.01	0.00
	0.248	0.747	0.062	0.01	0.00	0.00
	0.248	0.247	0.062	-0.02	-0.01	0.00
	0.745	0.748	0.062	0.00	-0.01	0.01
	0.745	0.248	0.062	-0.01	0.00	0.00
	0.248	0.998	0.123	0.00	0.00	0.00
	0.749	0.001	0.123	-0.01	0.01	0.00
	0.248	0.498	0.123	-0.01	0.00	0.00
	0.748	0.500	0.123	0.00	0.00	-0.01
	0.250	0.249	0.184	0.00	0.00	0.01
	0.250	0.748	0.184	0.00	0.00	0.00
	0.750	0.252	0.184	0.00	0.00	0.00
	0.750	0.751	0.184	0.00	0.00	0.01
	0.252	0.500	0.246	0.00	0.00	0.00
	0.752	0.502	0.245	-0.01	0.01	0.00
	0.251	0.999	0.245	-0.01	0.01	0.00
	0.752	0.002	0.246	0.00	0.00	0.00
	0.255	0.752	0.306	-0.01	0.00	0.00
	0.255	0.252	0.306	0.01	-0.01	0.01
	0.752	0.753	0.306	-0.02	-0.01	0.00
	0.752	0.253	0.306	0.01	0.00	0.00
	0.267	1.000	0.366	-0.01	-0.01	0.00
	0.738	0.006	0.366	-0.01	-0.02	0.01
	0.267	0.500	0.366	0.00	-0.02	0.00
	0.738	0.506	0.366	0.00	-0.01	-0.01

Table 15: The ionic positions and magnetic structure of the UO_2 $hH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.134	0.166	0.945	0.00	0.00	0.00
	0.143	0.256	0.935	0.00	0.00	0.00
	0.857	0.744	0.433	0.00	0.00	0.00
	0.866	0.834	0.423	0.00	0.00	0.00
Actinide Ion	0.493	0.749	0.006	0.07	-1.55	-0.24
	0.492	0.250	0.006	1.19	-0.89	-0.09
	0.993	1.000	0.059	1.27	0.55	-0.18
	0.994	0.499	0.059	-0.87	-0.05	1.06
	0.497	0.250	0.124	0.38	-1.24	-0.53
	0.497	0.750	0.124	-0.41	0.19	-1.34
	0.000	0.500	0.184	0.51	1.38	0.28
	0.000	0.000	0.184	-0.90	0.35	1.18
	0.503	0.750	0.244	0.38	-1.24	-0.53
	0.503	0.250	0.244	-0.41	0.19	-1.34
	0.007	0.000	0.309	1.27	0.55	-0.18
	0.006	0.501	0.309	-0.87	-0.05	1.06
	0.507	0.251	0.362	0.08	-1.54	-0.24
	0.508	0.750	0.363	1.19	-0.88	-0.09
Oxygen Ion	0.256	0.497	0.002	0.00	0.02	-0.01
	0.727	0.502	0.002	-0.01	0.02	0.00
	0.255	0.994	0.002	-0.02	0.02	0.01
	0.726	0.003	0.002	-0.02	0.02	0.00
	0.245	0.748	0.062	0.00	0.01	0.01
	0.245	0.248	0.062	-0.01	0.00	0.00
	0.742	0.751	0.062	0.00	0.00	0.01
	0.742	0.250	0.062	-0.01	0.01	0.00
	0.249	0.999	0.123	0.01	0.00	0.00
	0.749	0.001	0.123	-0.01	0.01	0.00
	0.248	0.498	0.123	0.00	0.00	0.00
	0.748	0.500	0.122	0.01	0.00	-0.01
	0.250	0.250	0.185	0.01	0.00	0.01
	0.249	0.748	0.184	0.00	-0.01	0.01
	0.751	0.252	0.184	0.00	-0.01	0.01
	0.750	0.750	0.184	0.01	0.00	0.01
	0.252	0.500	0.246	0.01	0.00	-0.01
	0.752	0.502	0.245	0.00	0.00	0.00
	0.251	0.999	0.246	-0.01	0.01	0.00
	0.751	0.001	0.245	0.00	0.00	0.00
	0.258	0.750	0.306	-0.01	0.01	0.00
	0.258	0.249	0.306	0.00	0.00	0.01
	0.755	0.752	0.306	-0.01	0.00	0.00
	0.755	0.252	0.306	0.00	0.01	0.01
	0.274	0.997	0.366	-0.02	0.02	0.00
	0.745	0.006	0.366	-0.02	0.02	0.01
	0.273	0.498	0.366	-0.01	0.02	0.00
	0.744	0.503	0.366	0.00	0.02	-0.01

Table 16: The ionic positions and magnetic structure of the UO_2 $iH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.124	0.289	0.944	0.00	0.00	0.00
	0.123	0.190	0.946	0.00	0.00	0.00
	0.876	0.711	0.424	0.00	0.00	0.00
	0.877	0.810	0.422	0.00	0.00	0.00
Actinide Ion	0.507	0.750	0.006	0.21	-1.56	-0.16
	0.506	0.250	0.006	1.04	-1.03	-0.05
	0.005	0.000	0.059	1.16	0.67	-0.31
	0.005	0.500	0.059	-0.79	-0.01	1.11
	0.503	0.250	0.124	0.82	-1.09	-0.09
	0.502	0.750	0.124	-0.44	0.27	-1.30
	0.000	0.500	0.184	0.79	1.34	-0.06
	0.000	0.000	0.184	-0.95	0.34	1.06
	0.497	0.750	0.244	0.82	-1.09	-0.09
	0.498	0.250	0.244	-0.44	0.27	-1.29
	0.995	1.000	0.309	1.16	0.67	-0.31
	0.995	0.500	0.309	-0.79	-0.01	1.11
	0.493	0.250	0.362	0.22	-1.55	-0.16
	0.494	0.750	0.363	1.05	-1.02	-0.05
Oxygen Ion	0.274	0.498	0.002	0.00	0.03	-0.01
	0.745	0.503	0.002	-0.01	0.02	-0.01
	0.271	0.995	0.002	-0.02	0.02	0.01
	0.743	0.004	0.002	-0.02	0.02	0.00
	0.257	0.749	0.062	0.00	0.01	0.01
	0.258	0.249	0.062	-0.01	0.00	0.00
	0.755	0.751	0.062	-0.01	0.00	0.01
	0.756	0.251	0.062	-0.01	0.01	0.00
	0.251	0.999	0.123	0.00	0.00	0.00
	0.752	0.002	0.123	-0.01	0.01	0.00
	0.251	0.498	0.123	-0.01	0.00	0.00
	0.752	0.502	0.123	0.00	0.00	-0.01
	0.251	0.249	0.184	0.00	0.00	0.01
	0.249	0.749	0.184	0.00	-0.01	0.00
	0.751	0.251	0.184	0.00	-0.01	0.00
	0.749	0.751	0.184	0.00	0.00	0.01
	0.248	0.498	0.245	0.00	0.00	0.00
	0.749	0.502	0.246	-0.01	0.00	0.00
	0.248	0.998	0.245	-0.01	0.01	0.01
	0.749	0.001	0.246	0.00	0.00	0.00
	0.244	0.749	0.306	-0.01	0.01	0.00
	0.245	0.249	0.306	-0.01	0.00	0.01
	0.742	0.751	0.306	-0.01	0.00	0.00
	0.743	0.251	0.306	0.00	0.01	0.01
	0.257	0.996	0.366	-0.02	0.02	0.00
	0.729	0.005	0.366	-0.02	0.02	0.01
	0.255	0.497	0.366	-0.01	0.02	0.00
	0.726	0.502	0.366	0.00	0.03	-0.01

Table 17: The ionic positions and magnetic structure of the UO_2 $jH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.215	0.140	0.939	0.00	0.00	0.00
	0.243	0.218	0.925	0.00	0.00	0.00
	0.757	0.782	0.443	0.00	0.00	0.00
	0.785	0.860	0.429	0.00	0.00	0.00
Actinide Ion	0.496	0.747	0.006	0.15	-1.56	-0.11
	0.496	0.248	0.006	1.02	-1.02	0.07
	0.996	0.998	0.059	1.07	0.84	-0.09
	0.997	0.498	0.059	-0.87	0.04	1.07
	0.499	0.249	0.124	0.70	-1.14	-0.26
	0.498	0.749	0.124	-0.52	0.14	-1.35
	0.000	0.500	0.184	0.68	1.37	0.03
	0.000	0.000	0.184	-0.82	0.37	1.27
	0.501	0.751	0.244	0.70	-1.14	-0.26
	0.502	0.251	0.244	-0.52	0.14	-1.35
	0.004	0.002	0.309	1.07	0.84	-0.09
	0.003	0.502	0.309	-0.87	0.04	1.07
	0.504	0.253	0.362	0.16	-1.56	-0.11
	0.504	0.752	0.363	1.02	-1.02	0.07
Oxygen Ion	0.260	0.495	0.003	0.00	0.03	-0.01
	0.731	0.500	0.002	-0.01	0.02	-0.01
	0.258	0.993	0.002	-0.01	0.02	0.01
	0.730	0.001	0.002	-0.02	0.02	0.00
	0.247	0.747	0.062	0.00	0.01	0.01
	0.248	0.247	0.062	-0.01	0.00	0.00
	0.744	0.749	0.062	0.00	0.00	0.01
	0.745	0.248	0.062	-0.01	0.01	0.00
	0.249	0.998	0.123	0.00	0.00	0.00
	0.749	0.000	0.122	-0.01	0.01	0.00
	0.249	0.497	0.123	-0.01	0.00	0.00
	0.749	0.500	0.122	0.01	0.00	-0.01
	0.251	0.249	0.184	0.00	0.00	0.01
	0.248	0.749	0.184	0.00	-0.01	0.00
	0.752	0.251	0.184	0.00	-0.01	0.00
	0.749	0.751	0.184	0.00	0.00	0.01
	0.251	0.500	0.246	0.01	0.00	0.00
	0.751	0.503	0.245	-0.01	0.00	0.00
	0.251	1.000	0.246	-0.01	0.01	0.00
	0.751	0.002	0.245	0.00	0.00	0.00
	0.255	0.752	0.306	-0.01	0.01	0.00
	0.256	0.251	0.306	0.00	0.00	0.01
	0.752	0.753	0.306	-0.01	0.00	0.00
	0.753	0.253	0.306	0.00	0.01	0.01
	0.270	0.999	0.366	-0.02	0.02	0.00
	0.742	0.007	0.366	-0.01	0.02	0.00
	0.269	0.500	0.366	-0.01	0.02	-0.01
	0.740	0.505	0.366	0.00	0.03	-0.01

Table 18: The ionic positions and magnetic structure of the UO_2 $kH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.290	0.121	0.934	0.00	0.00	0.00
	0.342	0.191	0.920	0.00	0.00	0.00
	0.710	0.879	0.434	0.00	0.00	0.00
	0.658	0.809	0.449	0.00	0.00	0.00
Actinide Ion	0.495	0.748	0.006	0.08	-1.57	-0.11
	0.496	0.249	0.006	0.70	-1.27	0.21
	0.996	0.998	0.059	0.85	1.04	0.04
	0.996	0.498	0.059	-0.85	0.11	1.07
	0.498	0.249	0.124	0.68	-1.18	-0.01
	0.498	0.749	0.124	-0.81	-0.18	-1.32
	0.000	0.500	0.184	1.08	1.15	-0.11
	0.000	0.000	0.184	-0.96	-0.09	1.26
	0.502	0.751	0.244	0.68	-1.18	-0.01
	0.502	0.251	0.244	-0.81	-0.18	-1.32
	0.004	0.002	0.309	0.85	1.04	0.04
	0.004	0.502	0.309	-0.85	0.11	1.07
	0.505	0.252	0.362	0.08	-1.56	-0.11
	0.504	0.751	0.363	0.71	-1.26	0.20
Oxygen Ion	0.259	0.495	0.002	0.00	0.03	-0.01
	0.731	0.501	0.002	0.00	0.03	-0.01
	0.257	0.993	0.002	-0.01	0.02	0.00
	0.729	0.001	0.002	-0.01	0.02	0.00
	0.247	0.747	0.062	0.00	0.01	0.00
	0.247	0.247	0.062	-0.01	0.00	-0.01
	0.744	0.749	0.062	0.00	0.00	0.00
	0.744	0.249	0.062	-0.01	0.01	0.00
	0.249	0.998	0.123	0.00	0.00	0.00
	0.749	0.000	0.122	0.00	0.01	0.00
	0.249	0.498	0.123	-0.01	0.01	0.00
	0.749	0.500	0.122	0.01	0.00	0.00
	0.250	0.249	0.184	0.00	0.00	0.00
	0.249	0.749	0.184	0.00	0.00	0.00
	0.751	0.251	0.184	0.00	0.00	0.00
	0.750	0.751	0.184	0.00	0.00	0.00
	0.251	0.500	0.246	0.00	0.00	0.00
	0.751	0.502	0.245	-0.01	0.01	0.00
	0.251	1.000	0.246	0.00	0.01	0.00
	0.751	0.002	0.245	0.01	0.00	0.00
	0.256	0.751	0.306	-0.01	0.01	0.00
	0.256	0.251	0.306	0.00	0.00	0.00
	0.753	0.753	0.306	-0.01	0.00	0.00
	0.753	0.253	0.306	0.00	0.01	0.01
	0.271	0.999	0.366	-0.01	0.02	0.00
	0.743	0.007	0.366	-0.01	0.02	0.00
	0.269	0.499	0.366	0.00	0.03	-0.01
	0.741	0.505	0.366	0.00	0.03	-0.01

Table 19: The ionic positions and magnetic structure of the UO_2 $lH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.999	0.297	0.948	0.00	0.00	0.00
	0.995	0.198	0.949	0.00	0.00	0.00
	0.001	0.703	0.420	0.00	0.00	0.00
	0.005	0.802	0.419	0.00	0.00	0.00
Actinide Ion	0.492	0.749	0.006	-1.03	1.10	-0.14
	0.492	0.249	0.006	1.18	0.86	-0.35
	0.994	1.000	0.059	1.15	0.74	-0.13
	0.994	0.499	0.059	-0.79	-0.10	1.13
	0.497	0.250	0.124	1.10	-1.08	-0.13
	0.497	0.750	0.124	-0.65	-0.04	-1.39
	0.000	0.500	0.184	0.86	1.30	0.07
	0.000	0.000	0.184	-0.91	-0.06	1.29
	0.503	0.750	0.244	1.10	-1.08	-0.13
	0.503	0.250	0.244	-0.65	-0.04	-1.38
	0.006	0.000	0.309	1.15	0.74	-0.13
	0.006	0.501	0.309	-0.79	-0.10	1.13
	0.508	0.251	0.362	-1.03	1.10	-0.14
	0.508	0.751	0.363	1.18	0.86	-0.35
Oxygen Ion	0.256	0.497	0.002	0.01	-0.01	-0.01
	0.726	0.503	0.002	0.00	-0.02	0.00
	0.255	0.996	0.002	-0.01	-0.02	0.01
	0.726	0.002	0.002	-0.01	-0.01	0.00
	0.244	0.749	0.062	0.01	0.00	0.00
	0.245	0.248	0.062	-0.02	-0.01	0.00
	0.742	0.750	0.062	0.01	-0.01	0.01
	0.741	0.250	0.062	-0.01	0.00	0.00
	0.249	0.999	0.123	0.00	0.00	0.00
	0.749	0.001	0.123	0.00	0.01	0.00
	0.248	0.498	0.123	-0.01	0.00	0.00
	0.748	0.500	0.122	0.00	0.00	-0.01
	0.250	0.250	0.185	0.00	0.00	0.00
	0.250	0.748	0.184	0.00	0.00	0.00
	0.750	0.252	0.184	0.00	0.00	0.00
	0.750	0.750	0.184	0.00	0.00	0.01
	0.252	0.500	0.246	0.00	0.00	0.00
	0.752	0.502	0.245	-0.01	0.00	0.00
	0.251	0.999	0.246	0.00	0.01	0.00
	0.751	0.001	0.245	0.00	0.00	0.00
	0.259	0.750	0.307	-0.01	0.00	0.00
	0.258	0.250	0.306	0.01	-0.01	0.01
	0.755	0.752	0.306	-0.02	-0.01	0.00
	0.756	0.251	0.306	0.01	0.00	0.00
	0.274	0.998	0.366	-0.01	-0.02	0.00
	0.745	0.004	0.366	-0.01	-0.02	0.01
	0.274	0.497	0.366	0.00	-0.02	0.00
	0.744	0.503	0.366	0.01	-0.01	-0.01

2.2 Neptunium Dioxide

2.2.1 Atomic Hydrogen

Table 20: The ionic positions and magnetic structure of the NpO_2 $aH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.051	0.998	0.938	0.12	0.00	0.16
	0.968	1.000	0.429	0.00	0.20	0.01
Actinide Ion	0.998	0.500	0.006	-1.54	-2.24	0.00
	0.997	0.000	0.005	-1.21	-0.04	-2.06
	0.498	0.751	0.059	1.67	2.10	-0.09
	0.499	0.249	0.059	-1.74	-0.04	2.06
	1.000	0.000	0.123	1.52	-2.24	-0.05
	0.999	0.500	0.123	-1.57	-0.05	-2.19
	0.499	0.250	0.183	1.54	2.21	0.01
	0.499	0.750	0.183	-1.53	-0.02	2.23
	0.999	0.500	0.244	1.49	-2.25	0.00
	0.999	0.000	0.244	-1.53	-0.10	-2.22
	0.501	0.751	0.308	1.80	2.00	-0.08
	0.500	0.249	0.308	-1.61	-0.08	2.16
	0.002	1.000	0.362	0.04	-2.48	0.00
	0.002	0.500	0.361	2.50	-0.93	0.16
Oxygen Ion	0.229	0.248	0.003	0.05	0.01	0.02
	0.232	0.752	0.003	0.03	0.02	0.02
	0.761	0.248	0.002	0.05	0.02	0.00
	0.764	0.752	0.002	0.02	0.01	0.02
	0.249	0.500	0.061	0.01	0.00	0.00
	0.752	0.500	0.062	0.02	0.00	0.01
	0.250	0.000	0.062	0.02	0.00	0.02
	0.753	1.000	0.062	0.02	0.00	0.04
	0.246	0.752	0.122	0.00	0.01	0.00
	0.252	0.251	0.122	0.01	0.00	-0.01
	0.746	0.750	0.122	0.01	0.00	-0.01
	0.752	0.248	0.122	0.00	0.01	0.00
	0.251	0.002	0.183	-0.01	-0.01	0.00
	0.751	0.999	0.184	0.01	0.00	0.01
	0.248	0.500	0.183	0.01	0.00	0.01
	0.748	0.499	0.183	0.00	-0.01	0.00
	0.246	0.252	0.245	-0.01	0.01	0.00
	0.251	0.750	0.244	0.01	0.00	-0.01
	0.746	0.250	0.245	0.00	0.00	-0.01
	0.750	0.748	0.245	-0.01	0.01	0.00
	0.249	0.501	0.305	-0.02	0.00	-0.01
	0.751	0.500	0.306	-0.01	0.01	-0.01
	0.246	0.000	0.305	0.01	0.05	0.01
	0.750	0.999	0.305	0.00	0.03	0.00
	0.238	0.753	0.364	-0.03	0.03	0.00
	0.237	0.248	0.364	-0.01	0.04	-0.02
	0.770	0.752	0.364	-0.03	0.04	-0.01
	0.770	0.248	0.364	-0.01	0.04	-0.01

Table 21: The ionic positions and magnetic structure of the NpO_2 $bH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.566	0.236	0.981	0.00	0.00	0.00
	0.565	0.765	0.386	0.00	0.00	0.00
Actinide Ion	0.006	0.509	0.003	1.36	-3.42	-0.35
	0.009	0.994	0.005	-1.59	-0.63	-2.05
	0.501	0.751	0.058	1.57	2.17	0.14
	0.489	0.251	0.062	-1.21	0.06	2.39
	0.993	0.000	0.123	1.56	-2.20	-0.03
	0.994	0.501	0.122	-1.52	0.01	-2.23
	0.492	0.251	0.184	1.52	2.22	-0.05
	0.492	0.749	0.183	-1.46	0.01	2.26
	0.993	0.499	0.244	1.41	-2.30	0.02
	0.994	0.000	0.243	-1.34	0.02	-2.34
	0.489	0.748	0.305	1.48	2.26	-0.19
	0.500	0.249	0.309	-1.56	-0.08	2.20
	0.008	0.006	0.361	1.50	-2.28	-0.01
	0.005	0.492	0.364	-2.22	-0.41	-2.92
Oxygen Ion	0.247	0.235	0.001	0.01	0.01	0.01
	0.253	0.761	0.001	0.00	0.01	0.01
	0.738	0.242	0.991	0.01	0.00	0.00
	0.767	0.765	0.002	0.01	0.01	0.02
	0.252	0.502	0.062	-0.01	0.00	0.00
	0.749	0.493	0.060	0.00	0.01	0.01
	0.248	0.999	0.063	0.00	0.00	0.00
	0.752	0.011	0.061	0.00	0.00	0.00
	0.238	0.751	0.123	0.00	0.01	0.00
	0.240	0.251	0.122	0.00	0.00	-0.01
	0.739	0.750	0.121	0.00	0.00	-0.01
	0.738	0.249	0.123	-0.01	0.01	0.00
	0.248	0.002	0.183	-0.01	-0.01	0.00
	0.747	0.000	0.184	0.00	0.00	0.01
	0.243	0.500	0.183	0.01	0.00	0.01
	0.744	0.498	0.183	-0.01	-0.01	0.00
	0.239	0.253	0.244	-0.01	0.01	0.00
	0.243	0.749	0.244	0.01	0.00	-0.01
	0.740	0.249	0.246	0.01	0.00	-0.01
	0.742	0.747	0.244	-0.01	0.01	0.00
	0.251	0.501	0.305	0.00	-0.01	0.01
	0.747	0.507	0.307	0.01	0.00	0.01
	0.246	0.001	0.303	0.00	0.00	0.01
	0.750	0.987	0.306	-0.01	-0.01	0.00
	0.247	0.766	0.366	-0.02	0.02	0.01
	0.253	0.239	0.366	0.01	0.02	0.00
	0.738	0.759	0.376	0.00	0.00	0.00
	0.767	0.235	0.365	-0.01	0.03	0.00

2.2.2 Molecular Hydrogen

Table 22: The ionic positions and magnetic structure of the NpO_2 $aH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.070	0.001	0.915	0.00	0.00	0.00
	0.930	0.997	0.915	0.00	0.00	0.00
	0.930	0.999	0.452	0.00	0.00	0.00
	0.070	0.998	0.452	0.00	0.00	0.00
Actinide Ion	0.000	0.501	0.006	0.31	-2.71	0.00
	0.000	0.001	0.006	-2.15	0.00	-1.59
	0.500	0.751	0.059	1.72	2.07	0.08
	0.500	0.250	0.059	-1.61	-0.02	2.17
	1.000	0.000	0.123	1.56	-2.20	-0.02
	1.000	0.500	0.123	-1.58	0.00	-2.18
	0.499	0.250	0.183	1.57	2.19	0.01
	0.499	0.750	0.183	-1.51	-0.01	2.23
	0.999	0.500	0.244	1.55	-2.21	-0.02
	0.999	1.000	0.244	-1.58	0.00	-2.18
	0.501	0.750	0.308	1.73	2.06	-0.09
	0.500	0.250	0.308	-1.60	-0.02	2.17
	0.000	1.000	0.361	0.15	-2.71	0.00
	0.001	0.500	0.361	-2.20	0.08	-1.53
Oxygen Ion	0.234	0.250	0.001	0.01	0.02	0.00
	0.238	0.750	0.002	0.01	0.01	0.01
	0.762	0.251	0.002	0.03	0.02	-0.01
	0.767	0.750	0.002	0.00	0.02	0.01
	0.250	0.501	0.061	0.00	0.00	0.00
	0.752	0.500	0.062	0.01	0.01	0.01
	0.250	0.001	0.061	0.01	0.00	0.00
	0.751	1.000	0.061	0.00	0.00	0.00
	0.246	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.746	0.750	0.122	0.01	0.00	-0.01
	0.752	0.248	0.122	-0.01	0.01	0.00
	0.251	0.002	0.183	-0.01	-0.01	0.00
	0.751	0.999	0.184	0.01	0.00	0.01
	0.249	0.500	0.183	0.01	0.00	0.01
	0.749	0.499	0.183	-0.01	-0.01	0.00
	0.246	0.252	0.244	-0.01	0.01	0.00
	0.251	0.750	0.244	0.01	0.00	-0.01
	0.746	0.249	0.245	0.01	0.00	-0.01
	0.751	0.748	0.245	-0.01	0.01	0.00
	0.250	0.501	0.305	0.00	-0.01	0.00
	0.752	0.500	0.305	0.01	0.00	0.00
	0.248	1.000	0.305	0.01	0.01	0.01
	0.750	0.999	0.305	0.00	0.00	0.00
	0.238	0.751	0.365	0.00	0.02	0.01
	0.238	0.250	0.365	0.03	0.02	-0.01
	0.766	0.749	0.365	0.01	0.01	0.01
	0.767	0.250	0.365	0.02	0.02	0.00

Table 23: The ionic positions and magnetic structure of the NpO_2 $bH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.029	0.046	0.916	0.00	0.00	0.00
	0.974	0.954	0.916	0.00	0.00	0.00
	0.970	0.953	0.451	0.00	0.00	0.00
	0.028	0.043	0.451	0.00	0.00	0.00
Actinide Ion	0.999	0.500	0.006	0.05	-2.73	0.01
	0.999	1.000	0.006	-2.23	0.15	-1.46
	0.499	0.750	0.059	1.74	2.06	0.00
	0.500	0.250	0.059	-1.60	-0.03	2.17
	1.000	0.000	0.123	1.56	-2.20	-0.02
	0.000	0.500	0.123	-1.63	0.01	-2.15
	0.500	0.250	0.183	1.57	2.19	0.01
	0.500	0.750	0.183	-1.51	-0.01	2.24
	1.000	0.500	0.244	1.55	-2.21	-0.02
	1.000	1.000	0.244	-1.62	-0.01	-2.15
	0.501	0.750	0.308	1.75	2.05	-0.04
	0.500	0.250	0.308	-1.61	-0.02	2.17
	0.001	1.000	0.361	0.07	-2.72	0.00
	0.001	0.501	0.361	-2.47	-0.05	-1.01
Oxygen Ion	0.233	0.251	0.001	0.02	0.02	0.00
	0.235	0.751	0.001	0.01	0.01	0.01
	0.762	0.250	0.002	0.03	0.02	-0.01
	0.763	0.748	0.001	0.00	0.02	0.01
	0.250	0.501	0.061	0.00	0.00	0.00
	0.753	0.500	0.062	0.01	0.01	0.01
	0.249	0.001	0.061	0.01	0.00	0.00
	0.749	0.998	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.747	0.750	0.122	0.01	0.00	-0.01
	0.753	0.248	0.122	-0.01	0.01	0.00
	0.251	0.001	0.183	-0.01	-0.01	0.00
	0.751	1.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.498	0.183	-0.01	-0.01	0.00
	0.247	0.252	0.244	-0.01	0.01	0.00
	0.253	0.750	0.244	0.01	0.00	-0.01
	0.746	0.249	0.245	0.01	0.00	-0.01
	0.753	0.748	0.245	-0.01	0.01	0.00
	0.250	0.501	0.305	0.00	-0.01	0.00
	0.752	0.500	0.305	0.01	0.00	0.00
	0.248	0.000	0.305	0.01	0.01	0.01
	0.750	0.998	0.305	0.00	0.00	0.00
	0.237	0.751	0.365	0.00	0.02	0.01
	0.239	0.250	0.365	0.03	0.02	-0.01
	0.766	0.750	0.366	0.01	0.01	0.01
	0.767	0.250	0.365	0.02	0.02	0.00

Table 24: The ionic positions and magnetic structure of the NpO_2 $cH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.499	0.249	0.933	0.00	0.00	0.00
	0.500	0.248	0.909	0.00	0.00	0.00
	0.499	0.748	0.458	0.00	0.00	0.00
	0.500	0.749	0.434	0.00	0.00	0.00
Actinide Ion	0.999	0.501	0.006	0.96	-2.55	0.00
	0.999	1.000	0.006	-1.54	0.30	-1.99
	0.499	0.750	0.059	1.59	2.18	0.01
	0.500	0.250	0.059	-1.61	-0.01	2.17
	0.000	0.000	0.123	1.54	-2.22	-0.01
	0.000	0.500	0.123	-1.53	-0.01	-2.22
	0.500	0.250	0.183	1.54	2.21	0.01
	0.500	0.750	0.183	-1.52	-0.01	2.23
	0.000	0.500	0.244	1.53	-2.23	-0.02
	0.000	0.000	0.244	-1.53	-0.01	-2.22
	0.501	0.750	0.308	1.59	2.17	0.00
	0.500	0.250	0.308	-1.61	-0.01	2.17
	0.001	1.000	0.361	0.85	-2.59	0.02
	0.001	0.500	0.361	-1.77	0.01	-2.00
Oxygen Ion	0.233	0.250	0.002	0.00	0.02	0.00
	0.234	0.751	0.001	0.00	0.01	0.00
	0.762	0.250	0.002	0.02	0.02	-0.01
	0.763	0.748	0.002	-0.01	0.01	0.01
	0.250	0.502	0.061	-0.01	0.00	0.00
	0.753	0.500	0.062	0.00	0.01	0.01
	0.248	0.000	0.061	0.01	0.00	0.01
	0.750	0.998	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.747	0.750	0.122	0.01	0.00	-0.01
	0.753	0.248	0.122	-0.01	0.01	0.00
	0.252	0.002	0.183	-0.01	-0.01	0.00
	0.752	0.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.499	0.183	-0.01	-0.01	0.00
	0.247	0.252	0.245	-0.01	0.01	0.00
	0.254	0.750	0.244	0.01	0.00	-0.01
	0.747	0.250	0.245	0.01	0.00	-0.01
	0.753	0.748	0.245	-0.01	0.01	0.00
	0.250	0.502	0.305	0.00	-0.01	0.00
	0.752	0.500	0.305	0.01	0.00	0.01
	0.248	0.000	0.305	0.00	0.01	0.01
	0.750	0.999	0.305	-0.01	0.00	0.00
	0.236	0.752	0.365	-0.01	0.02	0.01
	0.238	0.250	0.365	0.02	0.02	0.00
	0.765	0.749	0.365	0.00	0.01	0.01
	0.767	0.250	0.365	0.01	0.02	0.01

Table 25: The ionic positions and magnetic structure of the NpO_2 $dH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.424	0.248	0.932	0.00	0.00	0.00
	0.434	0.247	0.908	0.00	0.00	0.00
	0.570	0.747	0.459	0.00	0.00	0.00
	0.577	0.748	0.435	0.00	0.00	0.00
Actinide Ion	0.999	0.501	0.006	1.10	-2.49	-0.01
	0.999	1.000	0.006	-1.70	-0.05	-2.04
	0.499	0.751	0.059	1.55	2.20	-0.02
	0.500	0.250	0.059	-1.60	-0.01	2.17
	0.000	0.000	0.123	1.52	-2.23	-0.02
	0.000	0.500	0.123	-1.51	-0.01	-2.23
	0.500	0.250	0.183	1.53	2.22	0.01
	0.501	0.750	0.183	-1.52	0.00	2.23
	0.000	0.500	0.244	1.52	-2.23	-0.01
	0.000	0.000	0.244	-1.51	-0.01	-2.23
	0.500	0.750	0.308	1.56	2.19	0.02
	0.500	0.250	0.308	-1.60	-0.01	2.17
	0.000	1.000	0.361	1.08	-2.50	0.00
	0.000	0.499	0.361	-1.71	-0.05	-2.04
Oxygen Ion	0.233	0.250	0.002	0.00	0.02	0.01
	0.234	0.752	0.002	0.00	0.01	0.01
	0.762	0.251	0.002	0.02	0.01	0.00
	0.763	0.749	0.002	-0.01	0.02	0.01
	0.250	0.502	0.061	-0.01	0.00	0.00
	0.752	0.500	0.062	0.00	0.01	0.01
	0.248	0.001	0.061	0.01	0.00	0.01
	0.750	0.999	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.747	0.751	0.122	0.01	0.00	-0.01
	0.753	0.248	0.122	-0.01	0.01	0.00
	0.251	0.002	0.183	-0.01	-0.01	0.00
	0.752	0.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.499	0.183	-0.01	-0.01	0.00
	0.248	0.252	0.245	-0.01	0.01	0.00
	0.254	0.750	0.245	0.01	0.00	-0.01
	0.748	0.250	0.245	0.01	0.00	-0.01
	0.754	0.748	0.245	-0.01	0.01	0.00
	0.249	0.500	0.305	0.00	-0.01	0.00
	0.751	0.499	0.305	0.01	0.00	0.01
	0.248	0.000	0.305	0.00	0.01	0.01
	0.751	1.000	0.305	-0.01	0.00	0.00
	0.233	0.750	0.365	-0.01	0.02	0.01
	0.238	0.249	0.365	0.02	0.01	0.00
	0.762	0.750	0.365	0.00	0.01	0.01
	0.767	0.250	0.365	0.00	0.02	0.01

Table 26: The ionic positions and magnetic structure of the NpO_2 $eH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.253	0.247	0.927	0.00	0.00	0.00
	0.218	0.246	0.903	0.00	0.00	0.00
	0.782	0.746	0.464	0.00	0.00	0.00
	0.747	0.747	0.440	0.00	0.00	0.00
Actinide Ion	0.999	0.501	0.006	1.10	-2.50	0.00
	0.999	1.000	0.006	-1.04	0.02	-2.32
	0.499	0.751	0.059	1.53	2.22	0.00
	0.500	0.250	0.059	-1.60	0.00	2.17
	0.000	0.000	0.123	1.53	-2.23	-0.01
	0.000	0.500	0.123	-1.51	-0.01	-2.23
	0.500	0.250	0.183	1.53	2.22	0.01
	0.500	0.750	0.183	-1.52	0.00	2.23
	0.000	0.500	0.244	1.53	-2.23	-0.01
	0.000	0.000	0.244	-1.51	0.00	-2.23
	0.500	0.750	0.308	1.54	2.21	0.00
	0.500	0.250	0.308	-1.61	-0.01	2.17
	0.000	1.000	0.361	1.13	-2.48	0.01
	0.000	0.500	0.361	-1.69	-0.06	-2.05
Oxygen Ion	0.234	0.250	0.002	0.00	0.02	0.00
	0.233	0.751	0.001	-0.01	0.01	0.01
	0.762	0.251	0.002	0.01	0.02	0.00
	0.763	0.749	0.002	-0.02	0.01	0.01
	0.250	0.502	0.061	-0.01	0.00	0.00
	0.753	0.501	0.062	0.00	0.01	0.01
	0.248	0.000	0.061	0.01	0.00	0.01
	0.750	0.999	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.747	0.751	0.122	0.01	0.00	-0.01
	0.753	0.248	0.122	-0.01	0.01	0.00
	0.252	0.002	0.183	-0.01	-0.01	0.00
	0.752	0.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.499	0.183	-0.01	-0.01	0.00
	0.247	0.252	0.245	-0.01	0.01	0.00
	0.253	0.751	0.244	0.01	0.00	-0.01
	0.748	0.250	0.245	0.00	0.00	-0.01
	0.753	0.748	0.245	-0.01	0.01	0.00
	0.250	0.502	0.305	0.00	-0.01	0.00
	0.752	0.500	0.305	0.01	0.00	0.01
	0.248	0.000	0.305	0.00	0.01	0.01
	0.750	0.999	0.305	-0.01	0.00	0.00
	0.234	0.751	0.365	-0.01	0.02	0.01
	0.238	0.250	0.365	0.02	0.01	0.00
	0.763	0.749	0.365	0.00	0.01	0.01
	0.767	0.250	0.365	0.00	0.02	0.01

Table 27: The ionic positions and magnetic structure of the NpO_2 $fH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.291	0.920	0.938	0.00	0.00	0.00
	0.267	0.007	0.927	0.00	0.00	0.00
	0.727	0.004	0.439	0.00	0.00	0.00
	0.703	0.916	0.428	0.00	0.00	0.00
Actinide Ion	0.001	0.504	0.006	1.48	-2.26	0.34
	0.001	0.004	0.006	-2.18	-0.20	-1.55
	0.500	0.754	0.059	1.66	2.12	-0.01
	0.501	0.253	0.059	-1.60	-0.01	2.17
	0.000	0.004	0.123	1.55	-2.21	-0.03
	0.001	0.504	0.123	-1.57	-0.01	-2.19
	0.500	0.254	0.183	1.55	2.21	0.00
	0.500	0.754	0.183	-1.51	0.01	2.23
	1.000	0.503	0.244	1.56	-2.21	-0.01
	0.000	0.003	0.244	-1.58	0.00	-2.18
	0.500	0.753	0.308	1.68	2.10	0.03
	0.500	0.253	0.308	-1.59	-0.01	2.19
	1.000	0.003	0.361	0.13	-2.71	0.03
	1.000	0.503	0.361	-1.20	-0.02	-2.26
Oxygen Ion	0.234	0.255	0.002	0.01	0.02	0.00
	0.238	0.753	0.002	0.00	0.01	0.00
	0.762	0.254	0.002	0.02	0.01	-0.01
	0.767	0.754	0.002	-0.01	0.02	0.01
	0.251	0.505	0.062	-0.01	0.00	0.00
	0.754	0.504	0.062	0.00	0.00	0.01
	0.249	0.003	0.061	0.01	0.00	0.00
	0.750	0.003	0.062	0.00	-0.01	0.00
	0.247	0.756	0.122	-0.01	0.01	0.00
	0.254	0.254	0.122	0.01	0.00	-0.01
	0.746	0.754	0.123	0.01	0.00	-0.01
	0.753	0.252	0.122	-0.01	0.01	0.00
	0.253	0.005	0.184	-0.01	-0.01	0.00
	0.752	0.003	0.184	0.01	0.00	0.01
	0.249	0.503	0.183	0.01	0.00	0.01
	0.749	0.502	0.183	-0.01	-0.01	0.00
	0.246	0.256	0.245	-0.01	0.01	0.00
	0.253	0.753	0.244	0.01	0.00	-0.01
	0.746	0.253	0.245	0.01	0.00	-0.01
	0.752	0.752	0.245	-0.01	0.01	0.00
	0.250	0.504	0.305	0.00	0.00	0.00
	0.751	0.503	0.305	0.01	0.00	0.01
	0.247	0.003	0.305	0.01	0.01	0.01
	0.750	0.001	0.305	0.00	0.00	0.00
	0.235	0.755	0.365	-0.01	0.02	0.01
	0.238	0.252	0.365	0.02	0.02	-0.01
	0.763	0.751	0.366	0.00	0.01	0.01
	0.767	0.254	0.365	0.01	0.02	0.00

Table 28: The ionic positions and magnetic structure of the NpO_2 $gH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.279	0.108	0.938	0.00	0.00	0.00
	0.250	0.029	0.924	0.00	0.00	0.00
	0.757	0.969	0.443	0.00	0.00	0.00
	0.726	0.891	0.429	0.00	0.00	0.00
Actinide Ion	0.999	0.502	0.006	0.89	-2.58	-0.01
	0.999	1.000	0.005	-1.90	0.04	-1.88
	0.499	0.751	0.059	1.58	2.18	-0.02
	0.500	0.250	0.059	-1.60	-0.01	2.18
	1.000	0.000	0.123	1.54	-2.22	-0.02
	0.000	0.500	0.123	-1.51	0.00	-2.23
	0.500	0.250	0.183	1.54	2.21	0.00
	0.500	0.750	0.183	-1.51	-0.01	2.24
	1.000	0.500	0.244	1.55	-2.22	-0.02
	1.000	1.000	0.244	-1.49	-0.01	-2.25
	0.500	0.750	0.308	1.60	2.17	0.01
	0.500	0.250	0.308	-1.60	-0.02	2.18
	1.000	1.000	0.361	0.13	-2.71	0.06
	1.000	0.499	0.361	-2.13	0.06	-1.58
Oxygen Ion	0.234	0.253	0.002	0.00	0.02	0.00
	0.234	0.751	0.002	0.00	0.01	0.01
	0.762	0.250	0.002	0.02	0.01	0.00
	0.763	0.750	0.002	-0.01	0.02	0.01
	0.250	0.502	0.062	-0.01	0.00	0.00
	0.752	0.500	0.062	0.00	0.01	0.01
	0.248	0.001	0.061	0.01	0.00	0.01
	0.750	0.999	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.253	0.251	0.122	0.01	0.00	-0.01
	0.747	0.750	0.122	0.01	0.00	-0.01
	0.753	0.248	0.122	-0.01	0.01	0.00
	0.251	0.001	0.183	-0.01	-0.01	0.00
	0.751	1.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.498	0.183	-0.01	-0.01	0.00
	0.247	0.252	0.244	-0.01	0.01	0.00
	0.254	0.750	0.244	0.01	0.00	-0.01
	0.747	0.248	0.245	0.01	0.00	-0.01
	0.753	0.748	0.244	-0.01	0.01	0.00
	0.249	0.501	0.305	0.00	-0.01	0.00
	0.751	0.499	0.305	0.01	0.00	0.01
	0.248	1.000	0.305	0.01	0.01	0.01
	0.750	0.998	0.305	0.00	0.00	0.00
	0.233	0.751	0.365	0.00	0.02	0.01
	0.238	0.249	0.365	0.03	0.02	-0.01
	0.761	0.747	0.365	0.01	0.01	0.01
	0.767	0.250	0.365	0.01	0.02	0.00

Table 29: The ionic positions and magnetic structure of the NpO_2 $hH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.354	0.083	0.944	0.00	0.00	0.00
	0.347	0.991	0.934	0.00	0.00	0.00
	0.662	0.009	0.433	0.00	0.00	0.00
	0.652	0.918	0.423	0.00	0.00	0.00
Actinide Ion	0.999	0.501	0.006	0.60	-2.66	0.00
	1.000	1.000	0.005	-2.29	0.39	-1.28
	0.499	0.751	0.059	1.65	2.13	0.00
	0.500	0.250	0.059	-1.63	-0.02	2.16
	0.000	0.000	0.123	1.56	-2.21	0.00
	0.000	0.500	0.123	-1.55	0.01	-2.21
	0.500	0.250	0.183	1.56	2.20	0.00
	0.500	0.750	0.183	-1.54	-0.01	2.22
	0.999	0.499	0.244	1.57	-2.20	-0.02
	1.000	1.000	0.244	-1.55	-0.03	-2.21
	0.500	0.750	0.308	1.72	2.07	0.07
	0.499	0.250	0.308	-1.64	-0.01	2.15
	0.999	1.000	0.361	1.31	-2.09	-0.15
	1.000	0.499	0.361	-2.60	-0.58	-0.04
Oxygen Ion	0.233	0.254	0.002	0.01	0.02	0.00
	0.233	0.750	0.002	0.01	0.01	0.01
	0.762	0.249	0.002	0.03	0.01	-0.01
	0.762	0.750	0.002	0.00	0.02	0.01
	0.250	0.502	0.062	0.00	0.00	0.00
	0.752	0.500	0.062	0.01	0.01	0.01
	0.248	0.001	0.061	0.01	0.00	0.00
	0.750	0.999	0.061	0.00	-0.01	0.00
	0.247	0.752	0.122	-0.01	0.01	0.00
	0.254	0.251	0.122	0.01	0.00	-0.01
	0.747	0.750	0.123	0.01	0.00	-0.01
	0.754	0.248	0.122	-0.01	0.01	0.00
	0.251	0.001	0.183	-0.01	-0.01	0.00
	0.751	1.000	0.184	0.01	0.00	0.01
	0.249	0.501	0.183	0.01	0.00	0.01
	0.749	0.498	0.183	-0.01	-0.01	0.00
	0.246	0.252	0.244	-0.01	0.01	0.00
	0.254	0.750	0.244	0.01	0.00	-0.01
	0.746	0.249	0.245	0.01	0.00	-0.01
	0.753	0.748	0.244	-0.01	0.01	0.00
	0.249	0.500	0.305	0.01	0.00	-0.01
	0.751	0.499	0.305	0.01	0.00	0.00
	0.248	1.000	0.305	0.00	0.00	0.01
	0.750	0.999	0.305	-0.01	0.00	0.00
	0.233	0.751	0.365	0.00	0.01	0.00
	0.238	0.249	0.365	0.02	0.02	-0.01
	0.761	0.747	0.365	0.00	0.01	0.00
	0.766	0.251	0.365	0.02	0.02	-0.01

Table 30: The ionic positions and magnetic structure of the NpO_2 $iH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.200	0.129	0.933	0.00	0.00	0.00
	0.143	0.060	0.919	0.00	0.00	0.00
	0.800	0.869	0.433	0.00	0.00	0.00
	0.856	0.936	0.448	0.00	0.00	0.00
Actinide Ion	0.002	0.502	0.006	0.12	-2.73	0.00
	0.001	0.000	0.006	-2.26	-0.49	-1.36
	0.500	0.751	0.059	1.73	2.06	0.03
	0.501	0.251	0.059	-1.54	-0.02	2.22
	0.999	0.000	0.123	1.56	-2.20	-0.02
	1.000	0.500	0.123	-1.59	0.06	-2.18
	0.498	0.250	0.183	1.58	2.19	0.00
	0.500	0.750	0.183	-1.50	-0.01	2.24
	0.999	0.499	0.244	1.58	-2.19	-0.03
	0.999	1.000	0.244	-1.59	0.00	-2.17
	0.500	0.749	0.308	1.76	2.03	0.07
	0.499	0.249	0.308	-1.62	-0.02	2.16
	1.000	1.000	0.361	0.41	-2.69	-0.01
	1.000	0.499	0.361	-2.23	0.04	-1.49
Oxygen Ion	0.240	0.253	0.002	0.02	0.03	0.00
	0.238	0.752	0.002	0.01	0.02	0.01
	0.769	0.251	0.002	0.03	0.02	-0.01
	0.767	0.750	0.002	0.00	0.02	0.01
	0.251	0.502	0.062	0.00	0.00	0.00
	0.753	0.501	0.062	0.01	0.01	0.01
	0.249	0.001	0.061	0.01	0.00	0.00
	0.750	0.999	0.061	0.00	0.00	0.00
	0.246	0.752	0.122	-0.01	0.01	0.00
	0.249	0.251	0.122	0.00	0.00	-0.01
	0.746	0.751	0.123	0.01	0.00	-0.01
	0.749	0.248	0.122	-0.01	0.01	0.00
	0.251	0.001	0.183	-0.01	-0.01	0.00
	0.751	0.000	0.184	0.01	0.00	0.01
	0.248	0.501	0.183	0.01	0.00	0.01
	0.748	0.497	0.183	-0.01	-0.01	0.00
	0.246	0.252	0.244	-0.01	0.01	0.00
	0.254	0.750	0.245	0.01	0.00	-0.01
	0.745	0.249	0.245	0.01	0.00	-0.01
	0.753	0.748	0.244	-0.01	0.01	0.00
	0.249	0.500	0.305	0.00	0.00	0.00
	0.751	0.499	0.305	0.01	0.00	0.00
	0.248	1.000	0.305	0.01	0.01	0.01
	0.750	0.999	0.305	0.00	0.00	0.00
	0.233	0.750	0.365	0.00	0.02	0.01
	0.238	0.249	0.365	0.03	0.02	-0.01
	0.760	0.748	0.365	0.01	0.01	0.01
	0.767	0.249	0.365	0.01	0.02	0.00

Table 31: The ionic positions and magnetic structure of the NpO_2 $jH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.506	0.049	0.949	0.00	0.00	0.00
	0.506	0.949	0.949	0.00	0.00	0.00
	0.503	0.950	0.418	0.00	0.00	0.00
	0.503	0.049	0.418	0.00	0.00	0.00
Actinide Ion	0.998	0.500	0.006	0.46	-2.69	0.00
	0.999	1.000	0.005	-2.04	-0.43	-1.68
	0.498	0.750	0.059	1.67	2.11	-0.04
	0.499	0.250	0.059	-1.61	-0.01	2.17
	0.999	0.000	0.123	1.55	-2.22	-0.02
	0.999	0.500	0.123	-1.57	0.01	-2.19
	0.499	0.250	0.183	1.55	2.20	-0.01
	0.499	0.750	0.183	-1.51	0.00	2.24
	1.000	0.500	0.244	1.55	-2.21	-0.03
	1.000	0.000	0.244	-1.57	0.00	-2.19
	0.501	0.750	0.308	1.68	2.10	-0.01
	0.500	0.250	0.308	-1.61	-0.01	2.17
	0.001	0.999	0.361	0.62	-2.66	0.00
	0.000	0.500	0.361	-2.05	0.10	-1.73
Oxygen Ion	0.233	0.250	0.002	0.01	0.03	0.00
	0.233	0.750	0.001	0.01	0.02	0.01
	0.761	0.252	0.002	0.03	0.02	-0.01
	0.762	0.748	0.002	0.00	0.02	0.01
	0.250	0.502	0.061	0.00	0.00	0.00
	0.752	0.500	0.062	0.01	0.01	0.01
	0.248	0.000	0.061	0.01	0.00	0.01
	0.750	0.999	0.061	0.00	0.00	0.00
	0.246	0.752	0.122	-0.01	0.01	0.00
	0.252	0.251	0.122	0.01	0.00	-0.01
	0.746	0.750	0.123	0.01	0.00	-0.01
	0.751	0.248	0.122	-0.01	0.01	0.00
	0.251	0.002	0.183	-0.01	-0.01	0.00
	0.751	1.000	0.184	0.01	0.00	0.01
	0.249	0.500	0.183	0.01	0.00	0.01
	0.748	0.498	0.183	-0.01	-0.01	0.00
	0.247	0.252	0.245	-0.01	0.01	0.00
	0.253	0.750	0.244	0.01	0.00	-0.01
	0.746	0.249	0.245	0.01	0.00	-0.01
	0.752	0.749	0.245	-0.01	0.01	0.00
	0.250	0.502	0.305	0.00	-0.01	0.00
	0.752	0.500	0.305	0.01	0.00	0.01
	0.247	1.000	0.305	0.01	0.01	0.01
	0.750	0.999	0.306	-0.01	0.00	0.00
	0.237	0.750	0.365	-0.01	0.02	0.01
	0.238	0.250	0.365	0.03	0.02	-0.01
	0.766	0.749	0.365	0.01	0.01	0.01
	0.767	0.250	0.365	0.01	0.02	0.00

2.3 Plutonium Dioxide

2.3.1 Atomic Hydrogen

Table 32: The ionic positions and magnetic structure of the PuO_2 $aH_{(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.076	0.018	0.979	0.00	0.00	0.00
	0.924	0.982	0.385	0.00	0.00	0.00
Actinide Ion	0.517	0.743	0.001	2.10	0.24	-4.32
	0.518	0.258	0.005	1.48	-0.16	3.49
	0.999	0.999	0.061	-1.97	3.26	0.01
	0.011	0.500	0.057	-1.96	-3.25	0.07
	0.502	0.251	0.123	2.00	-0.03	-3.23
	0.502	0.748	0.121	1.95	0.01	3.26
	0.000	0.500	0.182	-2.00	3.23	0.02
	0.000	0.000	0.182	-2.01	-3.22	0.03
	0.498	0.749	0.242	2.00	-0.03	-3.23
	0.498	0.252	0.244	1.95	0.01	3.26
	0.001	0.001	0.304	-1.96	3.26	0.01
	0.989	0.500	0.307	-1.97	-3.25	0.07
	0.483	0.257	0.363	2.11	0.24	-4.32
	0.482	0.742	0.360	1.48	-0.16	3.49
Oxygen Ion	0.275	0.485	0.001	-0.01	0.02	-0.02
	0.763	0.489	0.999	-0.01	0.02	-0.01
	0.252	0.010	0.989	0.00	-0.01	0.00
	0.760	0.015	1.000	-0.01	-0.01	-0.01
	0.262	0.239	0.060	0.00	0.00	0.00
	0.758	0.253	0.063	0.00	0.00	0.00
	0.256	0.758	0.059	0.00	0.00	0.00
	0.761	0.748	0.061	0.00	0.00	0.00
	0.250	0.999	0.122	0.00	0.00	0.00
	0.752	1.000	0.121	0.00	0.00	0.00
	0.252	0.499	0.120	0.00	0.00	0.00
	0.751	0.501	0.122	0.00	0.00	0.00
	0.250	0.749	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.251	0.183	0.00	0.00	0.00
	0.249	0.499	0.243	0.00	0.00	0.00
	0.748	0.501	0.244	0.00	0.00	0.00
	0.248	0.000	0.243	0.00	0.00	0.00
	0.750	0.001	0.243	0.00	0.00	0.00
	0.239	0.252	0.304	0.00	0.00	0.00
	0.744	0.242	0.306	0.00	0.00	0.00
	0.242	0.747	0.302	0.00	0.00	0.00
	0.738	0.761	0.304	0.00	0.00	0.00
	0.240	0.985	0.365	-0.01	-0.01	-0.01
	0.748	0.990	0.376	0.00	-0.01	0.00
	0.237	0.511	0.365	-0.01	0.02	-0.01
	0.725	0.515	0.364	-0.01	0.02	-0.02

2.3.2 Molecular Hydrogen

Table 33: The ionic positions and magnetic structure of the PuO_2 $aH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.461	0.207	0.917	0.00	0.00	0.00
	0.530	0.294	0.917	0.00	0.00	0.00
	0.539	0.793	0.448	0.00	0.00	0.00
	0.470	0.706	0.448	0.00	0.00	0.00
Actinide Ion	0.504	0.749	0.005	1.71	0.01	-3.42
	0.504	0.249	0.005	1.65	0.02	3.45
	0.002	1.000	0.058	-1.92	3.28	-0.01
	0.002	0.499	0.058	-1.92	-3.28	-0.01
	0.501	0.250	0.122	1.99	0.00	-3.24
	0.500	0.750	0.122	1.99	0.00	3.24
	0.000	0.500	0.182	-2.02	3.22	-0.01
	0.000	0.000	0.182	-2.02	-3.22	0.00
	0.499	0.750	0.242	1.99	0.00	-3.24
	0.500	0.250	0.242	1.99	0.00	3.24
	0.998	0.000	0.307	-1.92	3.28	-0.01
	0.998	0.501	0.307	-1.92	-3.28	-0.01
	0.496	0.251	0.360	1.72	0.02	-3.42
	0.496	0.751	0.360	1.65	0.03	3.45
Oxygen Ion	0.268	0.500	0.001	-0.02	0.02	0.00
	0.741	0.500	0.000	-0.02	0.02	0.00
	0.268	0.999	0.001	-0.02	-0.02	0.00
	0.741	0.999	0.001	-0.02	-0.02	0.00
	0.251	0.249	0.061	0.00	0.00	-0.01
	0.751	0.250	0.061	0.00	0.00	0.00
	0.250	0.750	0.061	0.00	0.00	0.00
	0.749	0.749	0.061	0.00	0.00	0.01
	0.251	1.000	0.121	0.00	0.00	0.00
	0.751	1.000	0.121	0.00	0.00	0.00
	0.251	0.500	0.121	0.00	0.00	0.00
	0.752	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.248	0.500	0.243	0.00	0.00	0.00
	0.749	0.500	0.243	0.00	0.00	0.00
	0.249	0.000	0.243	0.00	0.00	0.00
	0.749	0.000	0.243	0.00	0.00	0.00
	0.251	0.251	0.304	0.00	0.00	0.01
	0.750	0.250	0.304	0.00	0.00	0.00
	0.249	0.750	0.304	0.00	0.00	0.00
	0.749	0.751	0.304	0.00	0.00	-0.01
	0.259	0.001	0.364	-0.02	-0.02	0.00
	0.732	0.001	0.364	-0.02	-0.02	0.00
	0.259	0.500	0.364	-0.02	0.02	0.00
	0.732	0.500	0.363	-0.02	0.02	0.00

Table 34: The ionic positions and magnetic structure of the PuO_2 $bH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.432	0.250	0.917	0.00	0.00	0.00
	0.573	0.250	0.917	0.00	0.00	0.00
	0.568	0.750	0.448	0.00	0.00	0.00
	0.427	0.750	0.448	0.00	0.00	0.00
Actinide Ion	0.500	0.750	0.005	1.61	0.00	-3.47
	0.500	0.250	0.005	1.68	-0.01	3.44
	1.000	0.000	0.058	-1.89	3.30	0.00
	1.000	0.500	0.058	-1.89	-3.30	0.00
	0.500	0.250	0.122	1.96	0.00	-3.25
	0.499	0.750	0.122	1.96	0.00	3.25
	0.000	0.500	0.182	-1.97	3.25	0.00
	0.000	0.000	0.182	-1.97	-3.25	0.00
	0.500	0.750	0.242	1.96	0.00	-3.25
	0.501	0.250	0.242	1.96	0.00	3.25
	0.000	1.000	0.306	-1.89	3.30	0.00
	0.000	0.500	0.306	-1.89	-3.30	0.00
	0.500	0.250	0.360	1.62	0.00	-3.47
	0.500	0.750	0.360	1.68	-0.01	3.44
Oxygen Ion	0.264	0.501	0.001	-0.02	0.02	0.00
	0.737	0.500	0.001	-0.02	0.02	0.00
	0.263	1.000	0.001	-0.02	-0.02	0.00
	0.736	0.001	0.001	-0.02	-0.02	0.00
	0.252	0.250	0.061	0.00	0.00	-0.01
	0.751	0.250	0.061	0.00	0.00	0.00
	0.249	0.750	0.061	0.00	0.00	0.00
	0.747	0.750	0.061	0.00	0.00	0.01
	0.250	0.000	0.121	0.00	0.00	0.00
	0.750	1.000	0.121	0.00	0.00	0.00
	0.250	0.500	0.121	0.00	0.00	0.00
	0.750	0.501	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.250	0.499	0.243	0.00	0.00	0.00
	0.750	0.500	0.243	0.00	0.00	0.00
	0.250	0.000	0.243	0.00	0.00	0.00
	0.750	1.000	0.243	0.00	0.00	0.00
	0.253	0.250	0.304	0.00	0.00	0.01
	0.751	0.250	0.304	0.00	0.00	0.00
	0.249	0.750	0.303	0.00	0.00	0.00
	0.748	0.750	0.304	0.00	0.00	-0.01
	0.264	0.999	0.364	-0.02	-0.02	0.00
	0.737	0.000	0.364	-0.02	-0.02	0.00
	0.263	0.500	0.364	-0.02	0.02	0.00
	0.736	0.499	0.364	-0.02	0.02	0.00

Table 35: The ionic positions and magnetic structure of the PuO_2 $cH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.992	0.999	0.930	0.00	0.00	0.00
	0.996	1.000	0.906	0.00	0.00	0.00
	0.008	0.001	0.434	0.00	0.00	0.00
	0.004	0.000	0.459	0.00	0.00	0.00
Actinide Ion	0.500	0.750	0.005	1.47	0.02	-3.54
	0.500	0.251	0.005	1.46	0.02	3.54
	0.000	0.000	0.058	-1.89	3.29	0.00
	0.000	0.500	0.058	-1.89	-3.30	0.00
	0.500	0.250	0.122	1.99	0.00	-3.24
	0.500	0.750	0.122	1.99	0.00	3.24
	0.000	0.500	0.182	-2.00	3.23	-0.01
	0.000	0.000	0.182	-2.00	-3.23	-0.01
	0.500	0.750	0.242	1.99	0.00	-3.24
	0.500	0.250	0.242	1.99	0.00	3.24
	1.000	1.000	0.307	-1.89	3.29	0.00
	1.000	0.500	0.307	-1.89	-3.30	0.00
	0.500	0.250	0.360	1.48	0.02	-3.54
	0.500	0.749	0.360	1.47	0.02	3.54
Oxygen Ion	0.264	0.500	0.001	-0.02	0.02	0.00
	0.737	0.500	0.001	-0.02	0.02	0.00
	0.263	0.000	0.001	-0.02	-0.02	0.00
	0.737	0.000	0.001	-0.02	-0.02	0.00
	0.251	0.251	0.061	0.00	0.00	-0.01
	0.750	0.250	0.061	0.00	0.00	0.00
	0.251	0.750	0.061	0.00	0.00	0.00
	0.749	0.750	0.061	0.00	0.00	0.01
	0.251	0.000	0.121	0.00	0.00	0.00
	0.751	0.000	0.121	0.00	0.00	0.00
	0.251	0.500	0.121	0.00	0.00	0.00
	0.751	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.249	0.500	0.243	0.00	0.00	0.00
	0.749	0.500	0.243	0.00	0.00	0.00
	0.249	1.000	0.243	0.00	0.00	0.00
	0.749	1.000	0.243	0.00	0.00	0.00
	0.251	0.250	0.304	0.00	0.00	0.01
	0.749	0.250	0.304	0.00	0.00	0.00
	0.250	0.750	0.304	0.00	0.00	0.00
	0.749	0.749	0.304	0.00	0.00	-0.01
	0.263	1.000	0.364	-0.02	-0.02	0.00
	0.737	1.000	0.364	-0.02	-0.02	0.00
	0.263	0.500	0.364	-0.02	0.02	0.00
	0.736	0.500	0.364	-0.02	0.02	0.00

Table 36: The ionic positions and magnetic structure of the PuO_2 $dH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.078	0.001	0.931	0.00	0.00	0.00
	0.072	0.001	0.907	0.00	0.00	0.00
	0.928	0.999	0.458	0.00	0.00	0.00
	0.922	0.999	0.433	0.00	0.00	0.00
Actinide Ion	0.509	0.750	0.005	1.49	0.02	-3.53
	0.510	0.250	0.005	1.46	0.02	3.54
	0.007	1.000	0.058	-1.89	3.29	-0.01
	0.008	0.500	0.058	-1.89	-3.30	-0.02
	0.503	0.250	0.122	1.99	0.00	-3.23
	0.503	0.750	0.122	1.99	0.00	3.23
	0.000	0.500	0.182	-2.00	3.23	-0.01
	0.000	0.000	0.182	-2.00	-3.23	-0.01
	0.497	0.750	0.242	1.99	0.00	-3.23
	0.497	0.250	0.242	1.99	0.00	3.23
	0.993	0.000	0.307	-1.89	3.29	-0.01
	0.992	0.500	0.307	-1.89	-3.30	-0.02
	0.491	0.250	0.360	1.49	0.02	-3.53
	0.490	0.750	0.360	1.46	0.03	3.54
Oxygen Ion	0.274	0.500	0.001	-0.02	0.02	0.00
	0.746	0.500	0.000	-0.02	0.02	0.00
	0.273	1.000	0.001	-0.02	-0.02	0.00
	0.746	0.000	0.000	-0.02	-0.02	0.00
	0.260	0.250	0.061	0.00	0.00	-0.01
	0.758	0.250	0.061	0.00	0.00	0.00
	0.259	0.750	0.061	0.00	0.00	0.00
	0.757	0.750	0.061	0.00	0.00	0.01
	0.252	0.000	0.121	0.00	0.00	0.00
	0.753	1.000	0.121	0.00	0.00	0.00
	0.252	0.500	0.121	0.00	0.00	0.00
	0.753	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.247	0.500	0.243	0.00	0.00	0.00
	0.748	0.500	0.243	0.00	0.00	0.00
	0.247	0.000	0.243	0.00	0.00	0.00
	0.748	1.000	0.243	0.00	0.00	0.00
	0.243	0.250	0.304	0.00	0.00	0.01
	0.741	0.250	0.304	0.00	0.00	0.00
	0.242	0.750	0.304	0.00	0.00	0.00
	0.740	0.750	0.304	0.00	0.00	-0.01
	0.254	1.000	0.364	-0.02	-0.02	0.00
	0.727	0.000	0.364	-0.02	-0.02	0.00
	0.254	0.500	0.364	-0.02	0.02	0.00
	0.726	0.500	0.364	-0.02	0.02	0.00

Table 37: The ionic positions and magnetic structure of the PuO_2 $eH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.241	0.998	0.926	0.00	0.00	0.00
	0.277	0.997	0.903	0.00	0.00	0.00
	0.723	0.003	0.462	0.00	0.00	0.00
	0.759	0.002	0.438	0.00	0.00	0.00
Actinide Ion	0.505	0.750	0.005	1.58	0.02	-3.49
	0.505	0.250	0.005	1.54	0.05	3.51
	0.004	1.000	0.058	-1.95	3.26	-0.01
	0.004	0.500	0.058	-1.94	-3.27	-0.01
	0.502	0.250	0.122	2.03	0.00	-3.21
	0.502	0.750	0.122	2.03	0.00	3.21
	0.000	0.500	0.182	-2.08	3.18	-0.01
	0.000	0.000	0.182	-2.07	-3.18	-0.01
	0.498	0.750	0.242	2.03	0.00	-3.21
	0.498	0.250	0.242	2.03	0.00	3.21
	0.996	0.000	0.307	-1.95	3.26	-0.01
	0.996	0.500	0.307	-1.94	-3.27	-0.01
	0.495	0.250	0.360	1.58	0.02	-3.49
	0.495	0.750	0.360	1.54	0.05	3.51
Oxygen Ion	0.270	0.500	0.001	-0.02	0.02	0.00
	0.743	0.500	0.001	-0.02	0.02	0.00
	0.268	1.000	0.001	-0.02	-0.02	0.00
	0.741	1.000	0.001	-0.02	-0.02	0.00
	0.256	0.250	0.061	0.00	0.00	-0.01
	0.754	0.250	0.061	0.00	0.00	0.00
	0.254	0.750	0.061	0.00	0.00	0.00
	0.753	0.750	0.061	0.00	0.00	0.01
	0.251	0.000	0.121	0.00	0.00	0.00
	0.752	1.000	0.121	0.00	0.00	0.00
	0.251	0.500	0.121	0.00	0.00	0.00
	0.752	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.248	0.500	0.243	0.00	0.00	0.00
	0.749	0.500	0.243	0.00	0.00	0.00
	0.248	0.000	0.243	0.00	0.00	0.00
	0.749	1.000	0.243	0.00	0.00	0.00
	0.247	0.250	0.304	0.00	0.00	0.01
	0.746	0.250	0.304	0.00	0.00	0.00
	0.246	0.750	0.304	0.00	0.00	0.00
	0.744	0.750	0.304	0.00	0.00	-0.01
	0.259	0.000	0.364	-0.02	-0.02	0.00
	0.732	0.000	0.363	-0.02	-0.02	0.00
	0.257	0.500	0.364	-0.02	0.02	0.00
	0.730	0.500	0.364	-0.02	0.02	0.00

Table 38: The ionic positions and magnetic structure of the PuO_2 $fH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.226	0.151	0.939	0.00	0.00	0.00
	0.256	0.234	0.926	0.00	0.00	0.00
	0.744	0.766	0.438	0.00	0.00	0.00
	0.774	0.849	0.425	0.00	0.00	0.00
Actinide Ion	0.503	0.748	0.005	1.69	0.00	-3.43
	0.503	0.249	0.005	1.82	-0.02	3.36
	0.002	0.999	0.058	-1.91	3.28	-0.01
	0.002	0.498	0.058	-1.92	-3.28	0.00
	0.502	0.249	0.122	1.99	0.00	-3.24
	0.500	0.749	0.122	1.98	0.00	3.24
	0.000	0.500	0.182	-2.01	3.22	-0.01
	0.000	0.000	0.182	-2.01	-3.22	0.01
	0.498	0.751	0.242	1.99	0.00	-3.24
	0.500	0.251	0.242	1.98	0.00	3.24
	0.998	0.001	0.307	-1.91	3.28	-0.01
	0.998	0.502	0.307	-1.92	-3.28	0.00
	0.497	0.252	0.360	1.69	0.00	-3.43
	0.497	0.751	0.360	1.82	-0.02	3.36
Oxygen Ion	0.267	0.500	0.001	-0.02	0.02	0.00
	0.740	0.497	0.001	-0.02	0.02	0.00
	0.265	0.996	0.001	-0.02	-0.02	0.00
	0.739	1.000	0.001	-0.02	-0.02	0.00
	0.255	0.248	0.061	0.00	0.00	-0.01
	0.754	0.248	0.061	0.00	0.00	0.00
	0.251	0.748	0.061	0.00	0.00	0.00
	0.750	0.748	0.061	0.00	0.00	0.01
	0.251	1.000	0.121	0.00	0.00	0.00
	0.751	0.999	0.121	0.00	0.00	0.00
	0.251	0.499	0.121	0.00	0.00	0.00
	0.751	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.249	0.500	0.243	0.00	0.00	0.00
	0.749	0.501	0.243	0.00	0.00	0.00
	0.249	0.001	0.243	0.00	0.00	0.00
	0.749	0.000	0.243	0.00	0.00	0.00
	0.250	0.252	0.304	0.00	0.00	0.01
	0.749	0.252	0.303	0.00	0.00	0.00
	0.246	0.752	0.303	0.00	0.00	0.00
	0.745	0.752	0.304	0.00	0.00	-0.01
	0.261	0.000	0.364	-0.02	-0.02	0.00
	0.735	0.004	0.364	-0.02	-0.02	0.01
	0.260	0.503	0.364	-0.02	0.02	0.00
	0.733	0.500	0.363	-0.02	0.02	0.00

Table 39: The ionic positions and magnetic structure of the PuO_2 $gH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.296	0.126	0.934	0.00	0.00	0.00
	0.350	0.196	0.919	0.00	0.00	0.00
	0.704	0.874	0.431	0.00	0.00	0.00
	0.650	0.804	0.445	0.00	0.00	0.00
Actinide Ion	0.504	0.748	0.005	1.80	0.00	-3.37
	0.505	0.249	0.005	1.93	-0.04	3.29
	0.003	0.999	0.058	-2.02	3.22	-0.02
	0.004	0.498	0.058	-2.02	-3.22	0.00
	0.502	0.249	0.122	2.09	0.00	-3.17
	0.502	0.749	0.122	2.08	0.00	3.18
	0.000	0.500	0.182	-2.17	3.12	-0.01
	0.000	0.000	0.182	-2.17	-3.12	0.00
	0.498	0.751	0.242	2.09	0.00	-3.17
	0.498	0.251	0.242	2.08	0.00	3.18
	0.997	0.001	0.307	-2.02	3.22	-0.02
	0.996	0.502	0.307	-2.02	-3.22	0.00
	0.496	0.252	0.360	1.80	0.01	-3.37
	0.495	0.751	0.360	1.93	-0.04	3.29
Oxygen Ion	0.269	0.499	0.001	-0.02	0.02	0.00
	0.742	0.498	0.001	-0.02	0.02	0.00
	0.266	0.997	0.001	-0.02	-0.02	0.00
	0.740	0.998	0.001	-0.02	-0.02	0.00
	0.255	0.248	0.061	0.00	0.00	-0.01
	0.754	0.248	0.061	0.00	0.00	0.00
	0.254	0.749	0.061	0.00	0.00	0.00
	0.753	0.748	0.061	0.00	0.00	0.01
	0.251	1.000	0.121	0.00	0.00	0.00
	0.752	0.999	0.121	0.00	0.00	0.00
	0.251	0.499	0.121	0.00	0.00	0.00
	0.752	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.248	0.500	0.243	0.00	0.00	0.00
	0.749	0.501	0.243	0.00	0.00	0.00
	0.248	0.001	0.243	0.00	0.00	0.00
	0.749	0.000	0.243	0.00	0.00	0.00
	0.247	0.252	0.304	0.00	0.00	0.01
	0.746	0.251	0.304	0.00	0.00	0.00
	0.246	0.752	0.304	0.00	0.00	0.00
	0.745	0.752	0.304	0.00	0.00	-0.01
	0.260	0.002	0.364	-0.03	-0.02	0.00
	0.734	0.003	0.364	-0.02	-0.02	0.01
	0.258	0.502	0.364	-0.02	0.02	0.00
	0.731	0.501	0.364	-0.02	0.02	0.00

Table 40: The ionic positions and magnetic structure of the PuO_2 $hH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.178	0.297	0.940	0.00	0.00	0.00
	0.175	0.196	0.941	0.00	0.00	0.00
	0.822	0.703	0.424	0.00	0.00	0.00
	0.825	0.804	0.423	0.00	0.00	0.00
Actinide Ion	0.508	0.750	0.005	1.81	0.00	-3.37
	0.506	0.250	0.004	1.92	-0.01	3.30
	0.005	0.000	0.058	-1.97	3.25	-0.02
	0.005	0.500	0.058	-1.97	-3.25	-0.02
	0.503	0.250	0.122	2.06	0.00	-3.19
	0.502	0.750	0.122	2.04	0.00	3.21
	0.000	0.500	0.182	-2.10	3.16	-0.01
	0.000	0.000	0.182	-2.10	-3.16	-0.01
	0.497	0.750	0.242	2.06	0.00	-3.19
	0.498	0.250	0.242	2.04	0.00	3.21
	0.995	1.000	0.307	-1.97	3.25	-0.02
	0.995	0.500	0.307	-1.97	-3.25	-0.02
	0.492	0.250	0.360	1.82	0.01	-3.37
	0.494	0.750	0.360	1.93	0.00	3.30
Oxygen Ion	0.272	0.503	0.001	-0.02	0.02	0.00
	0.745	0.498	0.000	-0.02	0.02	0.00
	0.271	0.997	0.001	-0.02	-0.02	0.00
	0.745	0.002	0.000	-0.02	-0.02	0.00
	0.259	0.250	0.060	0.00	0.00	-0.01
	0.758	0.250	0.061	0.00	0.00	0.00
	0.255	0.750	0.061	0.00	0.00	0.00
	0.754	0.750	0.061	0.00	0.00	0.01
	0.252	0.000	0.121	0.00	0.00	0.00
	0.752	1.000	0.121	0.00	0.00	0.00
	0.252	0.500	0.121	0.00	0.00	0.00
	0.752	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.248	0.500	0.243	0.00	0.00	0.00
	0.748	0.500	0.243	0.00	0.00	0.00
	0.248	0.000	0.243	0.00	0.00	0.00
	0.748	1.000	0.243	0.00	0.00	0.00
	0.246	0.250	0.304	0.00	0.00	0.01
	0.745	0.250	0.304	0.00	0.00	0.00
	0.242	0.750	0.304	0.00	0.00	0.00
	0.741	0.750	0.304	0.00	0.00	-0.01
	0.255	0.998	0.364	-0.03	-0.02	0.00
	0.729	0.003	0.364	-0.02	-0.02	0.01
	0.255	0.502	0.364	-0.02	0.02	0.00
	0.728	0.497	0.364	-0.02	0.02	0.01

Table 41: The ionic positions and magnetic structure of the PuO_2 $iH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.501	0.000	0.923	0.00	0.00	0.00
	0.500	1.000	0.899	0.00	0.00	0.00
	0.500	0.000	0.466	0.00	0.00	0.00
	0.499	1.000	0.441	0.00	0.00	0.00
Actinide Ion	0.500	0.750	0.005	1.53	0.02	-3.51
	0.500	0.250	0.005	1.53	0.02	3.51
	1.000	1.000	0.058	-1.94	3.27	0.00
	1.000	0.500	0.058	-1.93	-3.27	0.00
	0.500	0.250	0.122	2.02	0.00	-3.21
	0.500	0.750	0.122	2.02	0.00	3.21
	0.000	0.500	0.182	-2.06	3.19	0.00
	0.000	0.000	0.182	-2.06	-3.19	0.00
	0.500	0.750	0.242	2.02	0.00	-3.21
	0.500	0.250	0.242	2.02	0.00	3.21
	0.000	0.000	0.307	-1.94	3.27	0.00
	0.000	0.500	0.307	-1.93	-3.27	0.00
	0.500	0.250	0.360	1.53	0.02	-3.51
	0.500	0.750	0.360	1.53	0.03	3.51
Oxygen Ion	0.263	0.500	0.001	-0.02	0.02	0.00
	0.737	0.500	0.001	-0.02	0.02	0.00
	0.263	0.000	0.001	-0.02	-0.02	0.00
	0.736	0.000	0.001	-0.02	-0.02	0.00
	0.251	0.250	0.061	0.00	0.00	-0.01
	0.749	0.250	0.061	0.00	0.00	0.00
	0.250	0.750	0.061	0.00	0.00	0.00
	0.749	0.750	0.061	0.00	0.00	0.01
	0.249	0.000	0.121	0.00	0.00	0.00
	0.750	1.000	0.121	0.00	0.00	0.00
	0.250	0.500	0.121	0.00	0.00	0.00
	0.750	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.250	0.500	0.243	0.00	0.00	0.00
	0.750	0.500	0.243	0.00	0.00	0.00
	0.250	0.000	0.243	0.00	0.00	0.00
	0.751	1.000	0.243	0.00	0.00	0.00
	0.251	0.250	0.304	0.00	0.00	0.01
	0.750	0.250	0.304	0.00	0.00	0.00
	0.251	0.750	0.304	0.00	0.00	0.00
	0.749	0.750	0.304	0.00	0.00	-0.01
	0.264	1.000	0.364	-0.02	-0.02	0.00
	0.737	1.000	0.364	-0.02	-0.02	0.00
	0.263	0.500	0.364	-0.02	0.02	0.00
	0.737	0.500	0.364	-0.02	0.02	0.00

Table 42: The ionic positions and magnetic structure of the PuO_2 $jH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.571	0.000	0.914	0.00	0.00	0.00
	0.430	0.000	0.914	0.00	0.00	0.00
	0.429	1.000	0.451	0.00	0.00	0.00
	0.570	1.000	0.451	0.00	0.00	0.00
Actinide Ion	0.500	0.750	0.005	1.49	0.00	-3.53
	0.500	0.250	0.005	1.50	0.00	3.52
	0.000	0.000	0.058	-1.91	3.28	0.00
	0.000	0.500	0.058	-1.90	-3.29	0.00
	0.500	0.250	0.122	2.00	0.00	-3.23
	0.500	0.750	0.122	2.00	0.00	3.23
	0.000	0.500	0.182	-2.02	3.21	0.00
	0.000	0.000	0.182	-2.02	-3.22	0.00
	0.500	0.750	0.242	2.00	0.00	-3.23
	0.500	0.250	0.242	2.00	0.00	3.23
	1.000	1.000	0.307	-1.91	3.28	0.00
	1.000	0.500	0.307	-1.90	-3.29	0.00
	0.500	0.250	0.360	1.50	0.00	-3.53
	0.500	0.750	0.360	1.50	0.00	3.52
Oxygen Ion	0.263	0.500	0.001	-0.02	0.02	0.00
	0.737	0.500	0.001	-0.02	0.02	0.00
	0.263	0.000	0.001	-0.02	-0.02	0.00
	0.737	0.000	0.001	-0.02	-0.02	0.00
	0.251	0.251	0.061	0.00	0.00	-0.01
	0.750	0.250	0.061	0.00	0.00	0.00
	0.250	0.750	0.061	0.00	0.00	0.00
	0.749	0.750	0.061	0.00	0.00	0.01
	0.250	0.000	0.121	0.00	0.00	0.00
	0.750	0.000	0.121	0.00	0.00	0.00
	0.250	0.500	0.121	0.00	0.00	0.00
	0.750	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.250	0.500	0.243	0.00	0.00	0.00
	0.750	0.500	0.243	0.00	0.00	0.00
	0.250	1.000	0.243	0.00	0.00	0.00
	0.750	1.000	0.243	0.00	0.00	0.00
	0.251	0.250	0.304	0.00	0.00	0.01
	0.750	0.250	0.304	0.00	0.00	0.00
	0.250	0.750	0.304	0.00	0.00	0.00
	0.749	0.749	0.304	0.00	0.00	-0.01
	0.263	1.000	0.364	-0.02	-0.02	0.00
	0.737	1.000	0.364	-0.02	-0.02	0.00
	0.263	0.500	0.364	-0.02	0.02	0.00
	0.737	0.500	0.364	-0.02	0.02	0.00

Table 43: The ionic positions and magnetic structure of the PuO_2 $kH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.009	0.251	0.941	0.00	0.00	0.00
	0.019	0.250	0.916	0.00	0.00	0.00
	0.981	0.750	0.448	0.00	0.00	0.00
	0.991	0.749	0.424	0.00	0.00	0.00
Actinide Ion	0.500	0.750	0.005	1.63	0.00	-3.46
	0.499	0.250	0.005	1.71	0.00	3.43
	0.999	1.000	0.058	-1.97	3.25	0.00
	0.999	0.500	0.058	-1.97	-3.25	0.00
	0.500	0.250	0.122	2.05	0.00	-3.20
	0.499	0.750	0.122	2.05	0.00	3.20
	0.000	0.500	0.182	-2.11	3.16	0.00
	0.000	0.000	0.182	-2.11	-3.16	0.00
	0.500	0.750	0.242	2.05	0.00	-3.20
	0.501	0.250	0.242	2.05	0.00	3.20
	0.001	0.000	0.307	-1.97	3.25	0.00
	0.001	0.500	0.306	-1.97	-3.25	0.00
	0.500	0.250	0.360	1.64	0.00	-3.46
	0.501	0.750	0.360	1.71	0.00	3.43
Oxygen Ion	0.263	0.501	0.001	-0.02	0.02	0.00
	0.736	0.499	0.001	-0.02	0.02	0.00
	0.263	0.999	0.001	-0.02	-0.02	0.00
	0.736	0.001	0.001	-0.02	-0.02	0.00
	0.252	0.250	0.061	0.00	0.00	-0.01
	0.750	0.250	0.061	0.00	0.00	0.00
	0.248	0.750	0.061	0.00	0.00	0.00
	0.747	0.750	0.061	0.00	0.00	0.01
	0.249	0.000	0.121	0.00	0.00	0.00
	0.749	1.000	0.121	0.00	0.00	0.00
	0.249	0.500	0.121	0.00	0.00	0.00
	0.750	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.250	0.500	0.243	0.00	0.00	0.00
	0.751	0.500	0.243	0.00	0.00	0.00
	0.251	0.000	0.243	0.00	0.00	0.00
	0.751	1.000	0.243	0.00	0.00	0.00
	0.253	0.250	0.304	0.00	0.00	0.01
	0.752	0.250	0.303	0.00	0.00	0.00
	0.250	0.750	0.304	0.00	0.00	0.00
	0.748	0.750	0.304	0.00	0.00	-0.01
	0.264	0.999	0.364	-0.02	-0.02	0.00
	0.737	0.001	0.364	-0.02	-0.02	0.00
	0.264	0.501	0.364	-0.02	0.02	0.00
	0.737	0.499	0.364	-0.02	0.02	0.00

Table 44: The ionic positions and magnetic structure of the PuO_2 $lH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.017	0.300	0.948	0.00	0.00	0.00
	0.017	0.200	0.948	0.00	0.00	0.00
	0.983	0.700	0.417	0.00	0.00	0.00
	0.983	0.800	0.417	0.00	0.00	0.00
Actinide Ion	0.501	0.750	0.005	1.56	0.00	-3.50
	0.500	0.250	0.005	1.63	-0.01	3.46
	0.000	1.000	0.058	-1.93	3.27	-0.01
	0.000	0.500	0.058	-1.93	-3.27	-0.01
	0.501	0.250	0.122	2.02	0.00	-3.22
	0.500	0.750	0.122	2.01	0.00	3.22
	0.000	0.500	0.182	-2.05	3.20	0.00
	0.000	0.000	0.182	-2.05	-3.20	0.00
	0.499	0.750	0.242	2.02	0.00	-3.22
	0.500	0.250	0.242	2.01	0.00	3.22
	1.000	0.000	0.307	-1.93	3.27	-0.01
	1.000	0.500	0.307	-1.93	-3.27	-0.01
	0.499	0.250	0.360	1.57	0.00	-3.50
	0.500	0.750	0.360	1.63	0.00	3.46
Oxygen Ion	0.265	0.502	0.001	-0.02	0.02	0.00
	0.737	0.499	0.001	-0.02	0.02	0.00
	0.264	0.998	0.001	-0.02	-0.02	0.00
	0.737	0.000	0.001	-0.02	-0.02	0.00
	0.253	0.250	0.061	0.00	0.00	-0.01
	0.751	0.250	0.061	0.00	0.00	0.00
	0.249	0.750	0.061	0.00	0.00	0.00
	0.748	0.750	0.061	0.00	0.00	0.01
	0.250	0.001	0.121	0.00	0.00	0.00
	0.750	1.000	0.121	0.00	0.00	0.00
	0.250	0.499	0.121	0.00	0.00	0.00
	0.750	0.500	0.121	0.00	0.00	0.00
	0.250	0.750	0.182	0.00	0.00	0.00
	0.750	0.750	0.182	0.00	0.00	0.00
	0.250	0.250	0.182	0.00	0.00	0.00
	0.750	0.250	0.182	0.00	0.00	0.00
	0.250	0.500	0.243	0.00	0.00	0.00
	0.750	0.501	0.243	0.00	0.00	0.00
	0.250	0.000	0.243	0.00	0.00	0.00
	0.750	0.999	0.243	0.00	0.00	0.00
	0.252	0.250	0.304	0.00	0.00	0.01
	0.751	0.250	0.303	0.00	0.00	0.00
	0.249	0.750	0.304	0.00	0.00	0.00
	0.747	0.750	0.304	0.00	0.00	-0.01
	0.263	1.000	0.364	-0.02	-0.02	0.00
	0.736	0.002	0.364	-0.02	-0.02	0.00
	0.263	0.501	0.364	-0.02	0.02	0.00
	0.735	0.498	0.363	-0.02	0.02	0.00

Table 45: The ionic positions and magnetic structure of the PuO_2 $mH_{2(011)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.018	1.000	0.980	0.00	0.00	0.00
	0.722	0.000	0.938	0.00	0.00	0.00
	0.982	0.000	0.385	0.00	0.00	0.00
	0.278	1.000	0.426	0.00	0.00	0.00
Actinide Ion	0.481	0.739	0.001	1.53	-0.01	-4.56
	0.482	0.262	0.001	1.84	0.40	4.41
	0.004	0.000	0.065	-1.89	3.28	0.25
	0.990	0.500	0.056	-2.02	-3.20	0.07
	0.499	0.254	0.121	1.90	-0.05	-3.29
	0.499	0.746	0.121	1.96	-0.08	3.25
	0.000	0.500	0.182	-2.02	3.22	-0.01
	0.000	0.000	0.182	-2.01	-3.22	-0.01
	0.501	0.746	0.243	1.90	-0.05	-3.29
	0.501	0.254	0.243	1.96	-0.08	3.25
	0.996	1.000	0.300	-1.89	3.29	0.25
	0.010	0.500	0.309	-2.02	-3.21	0.07
	0.519	0.261	0.364	1.53	0.00	-4.56
	0.518	0.738	0.364	1.84	0.40	4.41
Oxygen Ion	0.233	0.500	0.998	0.00	0.01	0.00
	0.731	0.500	0.001	0.00	0.01	0.00
	0.182	1.000	0.995	0.00	-0.01	0.00
	0.709	0.000	0.969	-0.01	0.00	0.00
	0.243	0.247	0.062	0.00	-0.01	0.00
	0.745	0.232	0.059	0.01	-0.01	0.00
	0.243	0.753	0.062	0.00	0.00	0.00
	0.744	0.769	0.058	0.00	-0.01	0.00
	0.251	0.000	0.122	0.00	0.00	0.00
	0.749	1.000	0.123	0.00	0.00	0.00
	0.251	0.500	0.121	0.00	0.00	0.00
	0.750	0.500	0.119	0.00	0.00	0.00
	0.250	0.748	0.182	0.00	0.00	0.00
	0.750	0.747	0.182	0.00	0.00	0.00
	0.250	0.253	0.182	0.00	0.00	0.00
	0.750	0.252	0.182	0.00	0.00	0.00
	0.250	0.500	0.245	0.00	0.00	0.00
	0.749	0.500	0.243	0.00	0.00	0.00
	0.251	0.000	0.242	0.00	0.00	0.00
	0.749	1.000	0.242	0.00	0.00	0.00
	0.256	0.231	0.306	0.00	-0.01	0.00
	0.757	0.247	0.303	0.00	0.00	0.00
	0.255	0.768	0.306	0.01	-0.01	0.00
	0.757	0.753	0.303	0.00	-0.01	0.00
	0.291	1.000	0.396	-0.01	0.00	0.00
	0.818	0.000	0.370	0.00	-0.01	0.00
	0.269	0.500	0.364	0.00	0.01	0.00
	0.767	0.500	0.366	0.00	0.01	0.00

2.4 Bader Charge Distribution

A Bader charge analysis with the Henkleman *et al*[2-4] code has been completed.[5] The inequivalent actinide (An(a)-An(d)) and oxygen (O(e)-O(l)) ions for the (011) surface are labelled (**Figure 3**). Note: as an inherent issue common to DFT-based methods, the Bader charges of the ions are often underestimated.[6]

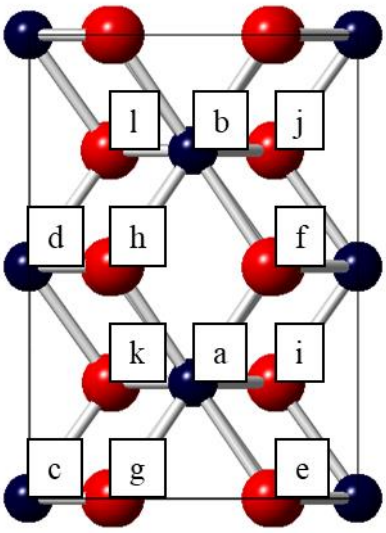

Figure 3: The inequivalent actinide (An_a-An_d) and oxygen (O_e-O_l) ions for the low-index AnO_2 (011) surface are indicated (initial 3 monolayers).

Table 46: The Bader charge distribution (e) of the UO_2 (011) surface for each configuration.

Configuration	H		U				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.48	2.48	2.57	2.56	-1.25	-1.24	-1.25	-1.25	-1.27	-1.27	-1.27	-1.27
Atomic Interaction														
a	-0.44	-	2.57	2.57	2.51	2.66	-1.26	-1.27	-1.26	-1.27	-1.21	-1.20	-1.21	-1.20
b	-0.47	-	2.71	2.58	2.51	2.51	-1.25	-1.26	-1.25	-1.26	-1.20	-1.20	-1.23	-1.22
c	-0.40	-	2.56	2.72	2.47	2.48	-1.24	-1.25	-1.24	-1.26	-1.24	-1.24	-1.21	-1.19
d	0.63	-	2.54	2.55	2.46	2.13	-1.29	-1.27	-1.30	-1.28	-1.29	-1.36	-1.26	-1.26
Molecular Interaction														
a	0.01	0.00	2.57	2.57	2.47	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.24	-1.25
b	0.03	-0.02	2.57	2.57	2.47	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.25
c	0.03	-0.02	2.57	2.57	2.47	2.49	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.25
d	-0.01	0.00	2.56	2.56	2.48	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.24	-1.25	-1.24
e	-0.03	0.03	2.57	2.57	2.48	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.25
f	-0.06	0.06	2.57	2.56	2.48	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.24
g	-0.01	0.00	2.57	2.57	2.48	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.24	-1.25	-1.24
h	-0.04	0.04	2.57	2.57	2.47	2.48	-1.28	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.25
i	-0.04	0.04	2.57	2.57	2.47	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.24
j	-0.03	0.03	2.57	2.57	2.47	2.48	-1.27	-1.27	-1.27	-1.27	-1.25	-1.25	-1.25	-1.25

Table 47: The Bader charge distribution (e) of the NpO_2 (011) surface for each configuration.

Configuration	H		Np				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.51	2.51	2.42	2.42	-1.25	-1.24	-1.24	-1.24	-1.22	-1.22	-1.22	-1.22
Atomic Interaction														
a	-0.22	-	2.51	2.51	2.46	2.44	-1.24	-1.24	-1.23	-1.23	-1.19	-1.19	-1.19	-1.19
b	0.64	-	2.50	2.50	2.42	2.06	-1.26	-1.26	-1.24	-1.25	-1.27	-1.24	-1.36	-1.23
Molecular Interaction														
a	-0.04	0.06	2.51	2.51	2.42	2.42	-1.24	-1.24	-1.25	-1.25	-1.22	-1.22	-1.22	-1.22
b	0.02	-0.01	2.51	2.51	2.42	2.42	-1.24	-1.24	-1.25	-1.25	-1.22	-1.22	-1.22	-1.22
c	-0.01	0.00	2.51	2.51	2.42	2.43	-1.24	-1.24	-1.24	-1.24	-1.22	-1.22	-1.23	-1.22
d	-0.04	0.03	2.51	2.51	2.42	2.43	-1.24	-1.24	-1.24	-1.24	-1.22	-1.22	-1.22	-1.22
e	-0.06	0.05	2.51	2.51	2.42	2.43	-1.24	-1.24	-1.24	-1.24	-1.22	-1.22	-1.22	-1.22
f	-0.03	0.04	2.52	2.51	2.42	2.42	-1.24	-1.24	-1.24	-1.25	-1.23	-1.22	-1.22	-1.22
g	-0.03	0.03	2.51	2.51	2.42	2.42	-1.24	-1.24	-1.25	-1.25	-1.23	-1.22	-1.22	-1.22
h	-0.05	-0.04	2.51	2.51	2.43	2.42	-1.24	-1.24	-1.25	-1.24	-1.23	-1.22	-1.22	-1.22
i	0.04	-0.04	2.51	2.51	2.42	2.42	-1.24	-1.24	-1.25	-1.25	-1.22	-1.22	-1.22	-1.22
j	0.04	-0.05	2.51	2.51	2.43	2.43	-1.24	-1.24	-1.25	-1.24	-1.22	-1.22	-1.22	-1.22

Table 48: The Bader charge distribution (e) of the PuO_2 (011) surface for each configuration.

Configuration	H		Pu				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.38	2.38	2.48	2.48	-1.20	-1.20	-1.20	-1.20	-1.22	-1.23	-1.23	-1.22
Atomic Interaction														
a	0.64	-	2.47	2.48	2.03	2.40	-1.25	-1.24	-1.22	-1.24	-1.26	-1.36	-1.22	-1.22
Molecular Interaction														
a	0.03	-0.02	2.48	2.48	2.39	2.39	-1.23	-1.22	-1.22	-1.23	-1.20	-1.21	-1.20	-1.21
b	-0.02	0.04	2.47	2.47	2.38	2.38	-1.23	-1.22	-1.22	-1.23	-1.20	-1.20	-1.20	-1.20
c	0.00	-0.01	2.47	2.47	2.39	2.39	-1.23	-1.22	-1.22	-1.23	-1.20	-1.20	-1.19	-1.20
d	-0.06	0.06	2.48	2.48	2.39	2.40	-1.23	-1.22	-1.22	-1.23	-1.20	-1.20	-1.20	-1.20
e	-0.06	0.05	2.48	2.48	2.40	2.39	-1.23	-1.22	-1.22	-1.23	-1.20	-1.21	-1.20	-1.20
f	-0.03	0.04	2.48	2.48	2.39	2.39	-1.23	-1.21	-1.22	-1.23	-1.20	-1.21	-1.21	-1.20
g	0.02	-0.02	2.48	2.48	2.39	2.39	-1.23	-1.22	-1.22	-1.23	-1.20	-1.20	-1.21	-1.20
h	-0.02	0.02	2.48	2.48	2.39	2.39	-1.23	-1.22	-1.22	-1.24	-1.21	-1.20	-1.21	-1.20
i	-0.01	0.01	2.47	2.47	2.38	2.38	-1.23	-1.22	-1.21	-1.23	-1.20	-1.19	-1.19	-1.20
J	0.05	-0.05	2.47	2.47	2.38	2.38	-1.23	-1.22	-1.22	-1.23	-1.20	-1.20	-1.20	-1.20
k	0.01	-0.01	2.47	2.48	2.39	2.39	-1.23	-1.22	-1.22	-1.23	-1.20	-1.19	-1.20	-1.19
l	-0.06	0.05	2.48	2.48	2.39	2.40	-1.20	-1.22	-1.22	-1.23	-1.20	-1.21	-1.20	-1.21
m	0.64	0.56	2.44	2.47	2.01	2.01	-1.26	-1.23	-1.25	-1.24	-1.30	-1.36	-1.25	-1.24

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