

Coverage-dependent adsorption, dissociation of H₂O on Al surfaces

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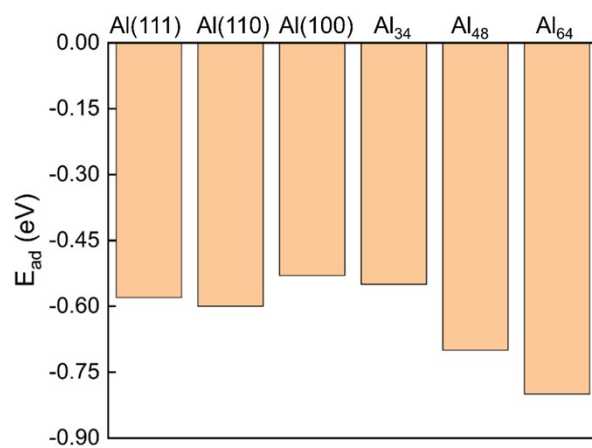


Figure S1. H₂O adsorption energy over Al surfaces and ANPs.

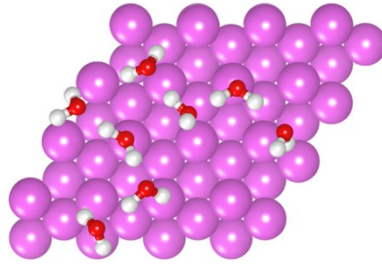


Figure S2. Adsorption configuration on eight H₂O molecules on Al(111).

Table S1. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al₃₄.

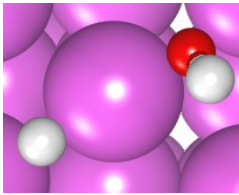
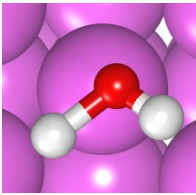
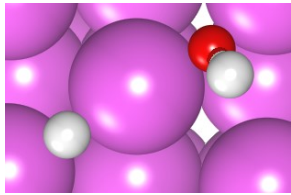
				
		IS	TS	FS
E (eV)		0.00	1.03	-0.12
Distance (Å)	H-O	0.98	0.99, 1.40	0.97
	Al-O	2.17	2.08	1.86, 2.00
	Al-H	2.68	2.46, 2.60	1.72, 1.97

Table S2. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al₄₈.

		IS	TS	FS
E (eV)		0.00	0.90	-0.43
Distance (Å)	H-O	0.98	0.98, 1.41	0.97
	Al-O	2.14	2.07	1.96
	Al-H	-	2.37	1.70, 1.95

Table S3. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al₆₄.

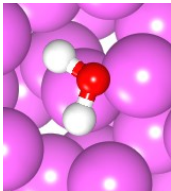
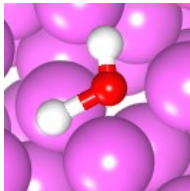
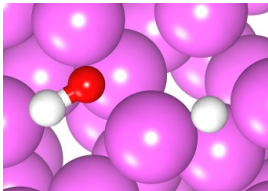
				
		IS	TS	FS
E (eV)		0.00	0.81	-0.40
Distance (Å)	H-O	0.99	0.99, 1.37	0.99
	Al-O	2.10	2.48	1.89, 1.95
	Al-H	-	-	1.71, 1.87

Table S4. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al₂O₃.

		IS	TS	FS
E (eV)		0.00	0.53	-0.44
Distance (Å)	H-O	0.99	0.98, 1.45	0.97
	Al-O	2.08	1.86	1.75
	Al-H	-	-	1.70

Table S5. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al(111).

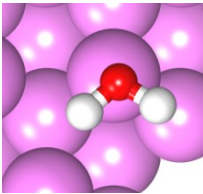
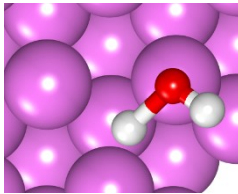
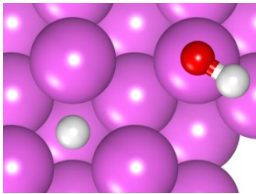
				
		IS	TS	FS
E (eV)		0.00	0.85	-1.29
Distance (Å)	H-O	0.98	0.99, 1.43	0.97
	Al-O	2.18	1.91	2.31
	Al-H	-	2.04, 2.04, 2.62	2.15

Table S6. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al(110).

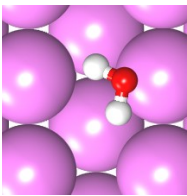
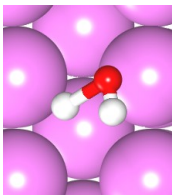
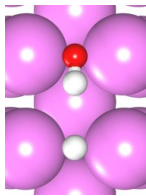
				
		IS	TS	FS
E (eV)		0.00	0.58	-0.75
Distance (Å)	H-O	0.98	0.98, 1.57	0.98
	Al-O	2.44	2.25	1.96
	Al-H	-	1.98, 2.69, 2.81	1.87

Table S7. Energetics and structures of IS, TS and FS during the H₂O dissociation on Al(100).

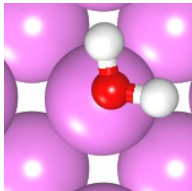
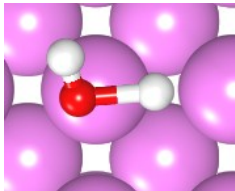
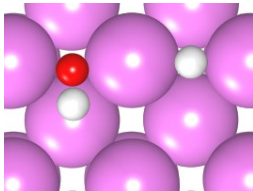
				
		IS	TS	FS
E (eV)		0.00	0.67	-0.81
	H-O	0.98	0.98, 1.53	0.98
Distance (Å)	Al-O	2.18	2.06	1.91, 1.93
	Al-H	-	2.32, 2.61, 2.66	1.75, 1.82

Table S8. Energetics and structures of IS, TS and FS during the (H₂O)₂ dissociation on Al(110).

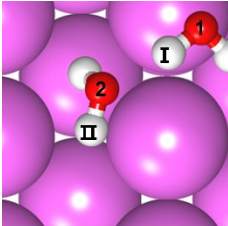
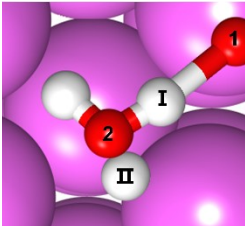
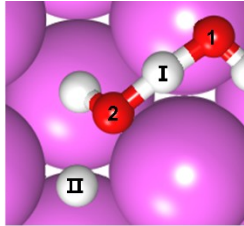
				
		IS	TS	FS
E (eV)		0.00	0.36	-0.52
Distance (Å)	H _I -O ₁	1.00	1.63	1.20
	H _I -O ₂	1.75	1.00	1.21
	H _{II} -O ₂	0.97	1.59	-
	Al-O ₁	2.40	1.80	2.26
	Al-O ₂	-	-	-
	Al-H _{II}	-	1.81, 2.40, 2.70	2.08, 2.09

Table S9. Energetics and structures of IS, TS and FS during the (H₂O)₃ dissociation on Al(111).

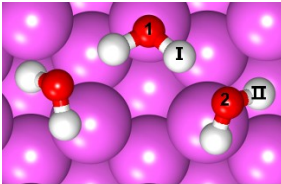
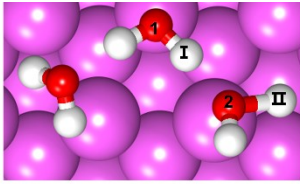
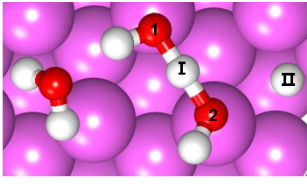
				
		IS	TS	FS
E (eV)		0.00	0.64	-0.23
Distance (Å)	H _I -O ₁	1.01	1.02	1.18
	H _I -O ₂	1.67	1.63	1.23
	H _{II} -O ₂	0.98	1.34	-
	Al-O ₁	1.97	2.00	1.88
	Al-O ₂	-	2.06	1.91
	Al-H _{II}	2.99	2.18, 2.62	1.85, 2.08

Table S10. Energetics and structures of IS, TS and FS during the (H₂O)₃ dissociation on Al(110).

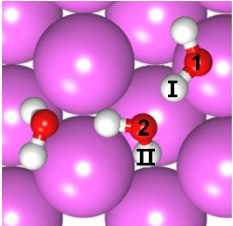
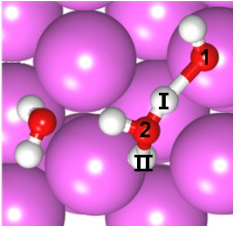
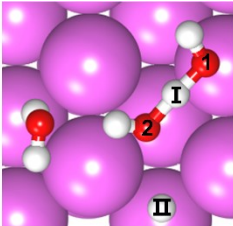
				
		IS	TS	FS
E (eV)		0.00	0.26	-0.38
Distance (Å)	H _I -O ₁	1.05	1.68	1.20
	H _I -O ₂	1.51	1.01	1.27
	H _{II} -O ₂	0.98	1.62	-
	Al-O ₁	2.94	1.85	2.19
	Al-O ₂	-	-	2.89
	Al-H _{II}	2.91	1.81, 2.45	1.66, 2.27, 2.27

Table S11. Energetics and structures of IS, TS and FS during the (H₂O)₂ dissociation on Al₃₄.

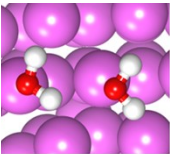
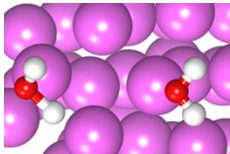
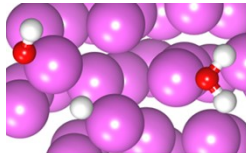
			
	IS	TS	FS
E (eV)	0.00	0.84	-0.86

Table S12. Energetics and structures of IS, TS and FS during the $(\text{H}_2\text{O})_2$ dissociation on Al_{48} .

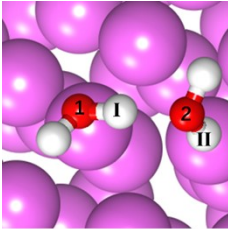
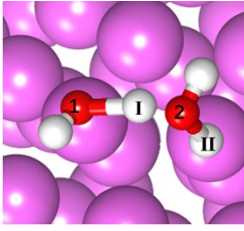
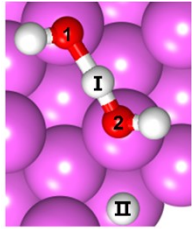
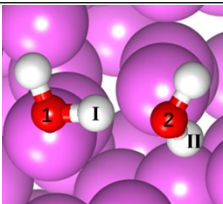
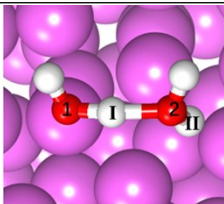
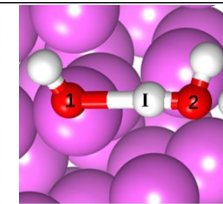
				
		IS	TS	FS
E (eV)		0.00	0.74	-0.50
Distance (Å)	H _I -O ₁	1.03	1.51	1.67
	H _I -O ₂	1.58	1.08	1.02
	H _{II} -O ₂	0.99	1.54	-
	Al-O ₁	2.01	1.79	1.79
	Al-O ₂	-	-	-
	Al-H _{II}	-	1.79	1.71, 1.84

Table S13. Energetics and structures of IS, TS and FS during the (H₂O)₂ dissociation on Al₆₄.

				
		IS	TS	FS
E (eV)		0.00	0.71	-0.41
Distance (Å)	H _I -O ₁	1.03	1.51	1.88
	H _I -O ₂	1.59	1.01	1.98
	H _{II} -O ₂	0.99	1.37	-
	Al-O ₁	2.00	1.83	1.77
	Al-O ₂	-	-	-
	Al-H _{II}	-	-	1.77, 1.79

Coordinates of ANPs

Al₃₄

-3.818	-0.022	1.654
1.926	-1.447	4.079
2.061	0.965	-4.139
-1.984	-2.123	1.185
-0.609	1.337	-4.270
3.026	-0.379	0.045
0.176	-1.771	-3.506
1.488	4.316	0.462
2.625	-1.127	-2.509
-3.909	-1.405	-0.700
2.755	0.553	2.539
0.302	-0.602	1.881
-4.124	1.032	-1.761
-0.196	-2.972	3.225
0.250	0.716	4.317
0.442	0.553	-2.023
2.393	-2.426	1.650
-1.935	-0.825	3.555
0.790	3.301	-1.989
-1.723	2.362	-1.951
0.809	2.830	2.673
-2.072	-0.485	-2.795
-1.643	0.249	-0.164
0.451	-4.078	-2.046
-1.074	3.575	0.567
2.966	1.694	-1.682
3.440	2.483	0.864
-1.532	1.520	2.266
0.466	-1.622	-0.624
2.730	-3.255	-0.839
-3.437	2.388	0.428
-1.880	-2.969	-1.381
-0.015	-3.916	0.663
0.856	1.550	0.327
	Al ₄₈	
-4.601	0.053	-0.461
-1.029	1.799	3.926
1.602	1.929	3.064
-0.056	-2.694	3.461
-0.449	-3.104	-4.254
-1.923	-4.512	0.026
1.709	1.456	0.229
-2.848	4.081	2.434
3.141	-1.233	3.689

-0.145	4.205	3.327
-1.262	-0.237	1.664
1.641	3.989	1.274
0.687	-0.554	-4.559
2.553	-3.714	-0.527
1.407	-0.674	1.789
-3.667	1.980	-2.388
-2.187	-0.790	4.198
1.389	2.123	-4.314
-3.525	-1.009	-2.693
1.783	-1.036	-0.821
2.201	-3.407	2.251
4.404	0.520	-0.754
-0.809	2.483	1.203
-2.081	3.839	-0.943
-0.643	-1.457	-2.084
0.202	-4.153	-1.786
0.612	-0.251	4.391
-3.352	1.373	2.791
4.248	-2.044	-1.795
0.648	3.715	-1.240
-1.068	2.874	-3.208
-1.788	0.777	-0.786
-2.371	-3.140	2.280
-0.060	-2.559	0.561
0.649	-5.188	0.736
1.972	-2.611	-3.127
4.040	-1.751	0.987
3.940	2.930	0.363
3.092	0.037	-3.287
3.005	2.515	-2.117
-3.822	2.435	0.399
-2.474	-3.468	-2.432
0.556	0.946	-2.113
-2.689	-1.855	-0.182
-1.739	0.397	-4.016
-0.753	5.247	0.834
-4.048	-1.057	2.028
3.904	0.794	1.982
	Al ₆₄	
0.337	-0.395	4.370
1.362	-4.027	-3.058
-0.301	-2.598	-4.759
-3.662	-3.188	-1.554

-0.463	5.057	-2.368
3.571	0.140	4.158
-1.394	-4.016	-2.694
-5.190	0.635	0.759
-3.346	-3.353	1.671
-1.645	0.066	2.363
3.557	-2.738	-2.264
-5.318	-2.040	0.326
1.714	2.039	3.930
2.912	-4.912	-0.647
3.692	2.475	-2.467
0.005	2.202	1.699
2.533	4.009	2.155
4.294	3.732	0.043
-2.373	1.784	0.372
4.182	1.948	2.240
-2.545	-1.569	-3.572
-1.064	1.989	4.362
0.102	-1.552	-2.230
1.491	-2.669	-0.127
0.145	-1.950	2.097
1.761	-4.447	2.069
-0.257	2.742	-1.037
0.494	4.953	0.667
-1.721	0.616	-2.005
0.188	4.303	3.504
-3.457	1.088	-3.984
-2.864	3.547	-2.233
5.416	-1.452	-0.809
-1.153	-2.774	-0.123
-2.050	-2.375	3.873
-0.197	0.107	-4.588
4.734	-0.647	1.789
-2.276	3.847	2.552
-0.121	-0.141	0.077
2.119	-1.508	-4.196
-2.067	4.830	0.006
-2.879	-0.833	0.025
2.176	4.558	-1.440
-4.280	-1.034	2.772
-4.718	-0.765	-2.113
0.256	-5.147	-0.724
-2.819	0.055	4.840
-4.457	3.446	0.709

-4.701	1.836	-1.580
5.072	1.159	-0.362
-2.330	-5.207	-0.138
-1.098	2.561	-3.982
0.444	-3.226	4.452
4.285	-0.143	-2.988
2.494	1.162	-4.711
2.797	-0.490	-0.639
2.740	-2.250	3.357
2.136	2.044	0.023
-0.971	-4.535	2.280
1.233	0.943	-2.329
1.432	3.392	-3.753
-3.886	1.752	2.972
4.008	-3.116	1.057
1.923	0.084	1.905
	Al ₉₂	
-0.284	-0.033	0.006
0.532	1.633	2.119
2.258	-0.638	2.111
2.074	1.561	-0.072
-3.683	-6.191	-5.941
-0.152	-6.210	-5.795
-5.631	-4.125	-6.198
-3.367	-4.188	-7.931
-3.916	-1.950	-6.211
-1.944	-4.055	-5.690
-1.951	-1.761	-8.177
-0.480	-4.234	-7.912
0.038	-1.986	-6.244
1.770	-4.197	-6.179
-5.852	0.080	-6.179
-3.666	0.384	-7.886
-3.967	2.183	-5.847
-2.031	0.146	-5.760
-0.334	0.428	-7.828
-0.088	2.205	-5.739
1.900	0.110	-6.185
-5.977	-6.016	-4.077
-4.137	-7.969	-3.900
-4.218	-5.957	-1.950
-2.456	-8.188	-1.800
-1.993	-6.161	-3.786
0.018	-8.048	-3.248

0.071	-5.783	-1.881
1.963	-6.138	-3.881
-7.747	-4.054	-4.460
-8.124	-2.106	-2.622
-6.076	-3.967	-2.172
-5.890	-2.032	-4.340
-3.972	-4.043	-3.971
-4.014	-2.004	-2.214
-2.046	-4.046	-1.984
-1.999	-1.977	-4.056
0.064	-4.004	-3.973
-0.055	-2.036	-2.184
2.098	-3.994	-2.073
1.980	-2.055	-4.364
3.782	-4.156	-4.288
4.152	-2.073	-2.579
-7.857	-0.064	-4.347
-6.158	-0.093	-2.113
-6.112	1.963	-3.938
-4.083	-0.009	-4.026
-4.199	1.802	-1.934
-2.095	-0.032	-2.059
-2.088	2.129	-3.847
0.061	-0.124	-4.110
0.032	1.610	-2.037
2.099	-0.175	-2.207
2.055	1.943	-3.936
3.883	-0.036	-4.350
-4.251	3.919	-3.702
-2.344	3.999	-1.782
0.078	3.882	-3.441
-6.215	-5.602	0.077
-4.439	-7.784	0.086
-4.253	-5.860	2.012
-2.159	-6.126	0.063
-0.045	-7.948	-0.301
0.049	-6.104	1.876
2.098	-5.685	0.123
-7.778	-3.299	-0.090
-6.015	-3.384	2.081
-5.513	-1.748	-0.088
-3.984	-3.960	-0.055
-3.653	-1.915	1.914
-2.050	-4.209	1.990

-2.024	-2.048	-0.199
-0.132	-3.992	0.053
-0.201	-1.947	1.884
2.051	-3.566	2.052
1.638	-1.989	-0.181
3.931	-3.453	-0.034
-7.935	-0.563	0.043
-5.997	-0.488	2.309
-6.003	1.453	0.283
-3.542	0.219	0.185
-4.032	1.926	2.317
-1.804	0.333	2.388
-1.710	2.338	0.456
3.940	-0.606	-0.141
-4.206	3.533	0.179
0.326	3.875	-0.674
-3.971	-3.837	3.892
-1.854	-2.063	4.185
-0.007	-4.036	3.772
-3.920	-0.227	4.089
0.307	-0.319	4.051
	Al ₂₂₅	
-9.867	-1.957	0.001
-9.866	0.000	-1.957
-9.863	1.957	-0.000
-9.863	0.001	1.957
-5.948	-5.946	-0.009
-5.997	-2.066	-4.034
-5.997	-4.034	-2.066
-7.918	-2.055	-2.054
-7.926	-3.964	-0.007
-5.935	-2.009	-0.008
-5.997	-4.036	2.051
-7.915	-2.056	2.048
-5.989	-2.066	4.020
-5.947	-0.009	-5.946
-7.926	-0.008	-3.964
-5.997	2.050	-4.037
-5.936	-0.008	-2.009
-7.916	2.048	-2.058
-7.795	-0.001	-0.002
-5.930	1.997	-0.007
-5.930	-0.006	1.996
-7.914	2.054	2.052

-7.916	-0.005	3.955
-5.987	2.052	4.022
-5.939	-0.008	5.934
-5.989	4.020	-2.069
-7.917	3.956	-0.008
-5.942	5.935	-0.011
-5.987	4.024	2.051
-1.960	-9.865	-0.000
-2.068	-5.997	-4.035
-2.057	-7.918	-2.056
-4.036	-5.997	-2.067
-3.966	-7.924	-0.008
-2.010	-5.935	-0.008
-2.058	-7.915	2.048
-4.037	-5.997	2.051
-2.067	-5.990	4.020
-2.057	-2.057	-7.920
-2.068	-4.035	-5.997
-4.035	-2.067	-5.996
-4.126	-4.125	-4.126
-2.041	-2.041	-4.005
-2.041	-4.006	-2.041
-4.005	-2.041	-2.040
-3.974	-3.975	-0.010
-1.997	-1.999	-0.012
-2.041	-4.006	2.020
-4.004	-2.041	2.020
-4.130	-4.130	4.111
-2.043	-2.044	3.982
-2.069	-4.033	5.981
-4.032	-2.069	5.981
-2.058	-2.059	7.903
-1.960	-0.002	-9.870
-3.966	-0.009	-7.926
-2.059	2.046	-7.919
-2.010	-0.009	-5.937
-4.037	2.050	-5.998
-3.975	-0.010	-3.975
-2.041	2.019	-4.007
-1.998	-0.013	-1.999
-4.005	2.020	-2.042
-3.966	-0.011	-0.011
-1.997	1.977	-0.013
-1.996	-0.012	1.976

-4.002	2.023	2.021
-3.969	-0.010	3.958
-2.037	2.022	3.982
-2.007	-0.008	5.916
-4.031	2.053	5.978
-3.961	-0.006	7.912
-2.059	2.047	7.899
-1.962	-0.005	9.854
-2.068	4.019	-5.992
-4.130	4.110	-4.133
-2.070	5.980	-4.036
-2.043	3.983	-2.045
-4.033	5.981	-2.072
-3.969	3.959	-0.012
-2.008	5.917	-0.011
-2.038	3.985	2.019
-4.032	5.980	2.049
-4.125	4.111	4.109
-2.066	5.975	4.013
-2.065	4.017	5.972
-2.059	7.903	-2.063
-3.962	7.913	-0.010
-1.963	9.855	-0.010
-2.060	7.901	2.043
-0.002	-9.866	-1.959
1.955	-9.863	-0.002
-0.002	-9.863	1.956
-0.011	-5.947	-5.948
-0.010	-7.926	-3.966
2.049	-5.998	-4.038
2.046	-7.916	-2.059
-0.008	-5.936	-2.010
-0.002	-7.796	-0.002
1.996	-5.932	-0.008
2.053	-7.915	2.052
-0.006	-5.931	1.996
-0.007	-7.917	3.955
2.053	-5.989	4.022
-0.008	-5.941	5.934
-0.003	-1.959	-9.871
-0.010	-3.965	-7.927
2.045	-2.059	-7.920
2.049	-4.038	-5.999
-0.009	-2.010	-5.938

-0.010	-3.976	-3.975
2.019	-2.043	-4.007
2.020	-4.007	-2.043
-0.012	-2.000	-1.999
-0.010	-3.968	-0.011
1.978	-1.999	-0.014
2.023	-4.005	2.021
-0.010	-1.999	1.976
-0.009	-3.971	3.958
2.023	-2.040	3.982
2.053	-4.033	5.977
-0.007	-2.009	5.916
-0.006	-3.962	7.911
2.048	-2.060	7.899
-0.004	-1.963	9.854
1.952	-0.003	-9.870
-0.004	1.953	-9.869
-0.004	-0.003	-7.799
2.050	2.050	-7.919
1.995	-0.008	-5.935
-0.008	1.995	-5.934
-0.011	-0.012	-3.968
2.021	2.020	-4.006
1.977	-0.013	-2.000
-0.011	1.976	-1.999
-0.011	-0.013	-0.013
1.978	1.976	-0.014
1.978	-0.012	1.973
-0.009	1.977	1.974
-0.009	-0.011	3.950
2.023	2.021	3.981
1.995	-0.008	5.913
-0.006	1.993	5.913
-0.005	-0.007	7.782
2.049	2.047	7.894
1.958	-0.005	9.848
-0.003	1.956	9.848
-0.009	3.953	-7.923
2.050	4.020	-5.992
-0.010	5.932	-5.945
-0.011	3.958	-3.973
2.051	5.977	-4.038
2.021	3.983	-2.042
-0.008	5.917	-2.012

-0.009	3.952	-0.013
1.994	5.915	-0.012
2.023	3.984	2.018
-0.007	5.916	1.990
-0.007	3.957	3.953
2.055	5.975	4.014
2.055	4.019	5.970
-0.006	5.927	5.922
-0.005	3.952	7.904
-0.007	7.911	-3.966
2.047	7.900	-2.066
-0.006	9.854	-1.969
-0.006	7.783	-0.011
1.956	9.851	-0.010
2.048	7.898	2.042
-0.004	9.851	1.951
-0.006	7.907	3.947
4.019	-5.991	-2.070
3.955	-7.919	-0.009
5.935	-5.944	-0.012
4.024	-5.990	2.050
4.018	-2.069	-5.993
4.109	-4.132	-4.134
5.979	-2.072	-4.037
5.980	-4.035	-2.073
3.983	-2.045	-2.046
3.959	-3.971	-0.013
5.918	-2.010	-0.012
5.980	-4.035	2.048
3.986	-2.041	2.018
4.112	-4.127	4.108
5.976	-2.068	4.012
4.018	-2.067	5.971
3.952	-0.009	-7.923
5.932	-0.011	-5.946
4.021	2.050	-5.993
3.958	-0.012	-3.974
5.978	2.049	-4.038
5.917	-0.010	-2.013
3.984	2.020	-2.042
3.953	-0.012	-0.014
5.916	1.992	-0.013
5.917	-0.009	1.989
3.986	2.021	2.018

3.958	-0.009	3.953
5.976	2.052	4.014
5.928	-0.008	5.922
4.021	2.053	5.970
3.953	-0.007	7.903
4.109	4.107	-4.131
5.975	4.014	-2.072
4.016	5.973	-2.072
3.958	3.956	-0.013
5.927	5.926	-0.014
5.976	4.019	2.048
4.021	5.974	2.048
4.112	4.109	4.105
3.952	7.906	-0.013
7.904	-2.061	-2.064
7.913	-3.964	-0.012
9.856	-1.966	-0.011
7.902	-2.063	2.041
7.912	-0.009	-3.968
9.855	-0.008	-1.970
7.901	2.044	-2.066
7.785	-0.009	-0.012
9.852	1.953	-0.011
9.852	-0.007	1.949
7.899	2.046	2.041
7.908	-0.008	3.946
7.907	3.949	-0.014