Supplementary Information

The "Burst Effect" of Hydrogen Desorption in MgH_2 Dehydrogenation

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Table S1. Calculated data of surface formation energy of three MgH_2(110) surfaces, where E_{rel} is the energy change in the relaxation process, E_{slab} is the energy of unrelaxed slab model, E_{bulk} is the molecular conventional cell energy, A is the exposed surface area, N_{slab} is the number of atoms in the slab model, N_{bulk} is the number of protocell atoms, and σ is the surface formation energy.

Surface	E_{rel} (eV)	E_{slab} (eV)	E_{bulk} (eV)	N_{slab}	N_{bulk}	A (Å^2)	σ (eV/ Å^2)
110-1	0.687	-181.368	-23.179	60	6	38.485	0.673
110-2	1.867	-174.256	-23.179	60	6	38.485	0.796
110-3	1.897	-174.146	-23.179	60	6	38.485	0.798

Table S2. Summary of the analyzed steps and energy barrierr (E_a).

Layer	Reaction	Type	E_a (eV)
1	Process 1	Adsorption	2.52
	Process 2	Adsorption	2.53
2	Process 3 step 1	Migration	0.12
	Process 3 step 2	Migration	0.80
	Process 3 step 3	Adsorption	1.51
	Process 4 step 1	Migration	0.89
	Process 4 step 2	Migration	0.75
	Process 4 step 3	Adsorption	1.21
	Process 5 step 1	Migration	0.65
	Process 5 step 2	Adsorption	1.27
	Process 6 step 1	Migration	0.37
	Process 6 step 2	Adsorption	1.06
3	Process 7 step 1	Migration	0.42
	Process 7 step 2	Migration	0.74
	Process 7 step 3	Migration	0.83
	Process 7 step 4	Migration	0.79
	Process 7 step 5	Migration	0.46
	Process 7 step 6	Migration	0.51
	Process 7 step 7	Migration	1.23
	Process 7 step 8	Migration	0.79
	Process 8 step 1	Adsorption	1.25

Layer	Reaction	Type	E_a (eV)
	Process 8 step 2	Adsorption	1.32
	Process 8 step 3	Adsorption	1.20
	Process 8 step 4	Adsorption	1.41

Table S3. Summary of DFT calculated energies (E_e), zero-point energies (E_{ZPE}), entropic change (ΔTS), and Gibbs free energies (G) of the initial structure (IS), transition structure (TS) and final structure (FS) of the first-layer dehydrogenation process.

Process	Structure	E_e (eV)	E_{ZPE} (eV)	ΔTS (eV)	G (eV)
1	IS	-215.626	3.823	2.509	-209.294
	TS	-213.118	3.632	2.716	-206.770
	FS	-213.310	3.673	2.831	-206.806
2	IS	-206.509	3.383	2.467	-200.660
	TS	-204.009	3.227	2.657	-198.125
	FS	-204.392	3.201	2.860	-201.191

Table S4. Summary of DFT calculated energies (E_e), zero-point energies (E_{ZPE}), entropic change (ΔTS), and Gibbs free energies (G) of the initial structure (IS), transition structure (TS) and final structure (FS) of the second-layer dehydrogenation process.

Process	Structure	E_e (eV)	E_{ZPE} (eV)	ΔTS (eV)	G (eV)
3	IS	-197.570	2.926	2.497	-192.147
	TS1	-197.422	2.899	2.497	-192.026
	IM1	-198.240	2.962	2.401	-192.877
	TS2	-197.382	2.907	2.400	-192.074
	IM2	-198.258	2.992	2.405	-192.861
	TS3	-196.649	2.810	2.488	-191.351
	FS	-197.290	2.830	2.551	-191.909
4	IS	-190.476	2.528	2.280	-185.668
	TS1	-189.644	2.532	2.338	-184.774
	IM1	-190.335	2.562	2.401	-185.372
	TS2	-189.536	2.546	2.368	-184.622
	IM2	-190.805	2.598	2.342	-185.865
	TS3	-189.560	2.522	2.381	-184.658
	FS	-189.869	2.498	2.500	-184.871
5	IS	-183.051	2.201	2.242	-178.608
	TS1	-182.400	2.449	1.993	-177.959
	IM1	-183.155	2.533	1.948	-178.673
	TS2	-181.635	2.280	1.948	-177.406
	FS	-182.301	2.555	2.003	-177.744

Process	Structure	E_e (eV)	E_{ZPE} (eV)	ΔTS (eV)	G (eV)
	IS	-175.527	2.632	2.285	-170.611
6	TS1	-174.973	2.450	2.285	-170.238
	IM1	-174.995	2.450	1.580	-170.965
6	TS2	-173.937	2.466	1.568	-169.904
	FS	-174.433	2.477	1.681	-170.275

Table S5. Summary of DFT calculated energies (E_e), zero-point energies (E_{ZPE}), entropic change (ΔTS), and Gibbs free energies (G) of the initial structure (IS), transition structure (TS) and final structure (FS) of the third-layer dehydrogenation process.

Process	Structure	E_e (eV)	E_{ZPE} (eV)	ΔTS (eV)	G (eV)
7	IS	-167.699	1.529	2.042	-164.128
	TS1	-167.339	1.493	2.141	-163.705
	IM1	-167.868	1.547	2.064	-164.257
	TS2	-167.140	1.508	2.110	-163.521
	IM2	-167.539	1.534	2.110	-163.896
	TS3	-166.694	1.501	2.132	-163.061
	IM3	-167.281	1.542	2.229	-163.510
	TS4	-166.256	1.480	2.058	-162.718
	IM4	-166.698	1.495	1.832	-163.371
	TS5	-166.317	1.424	1.981	-162.912
	IM5	-166.807	1.467	2.122	-163.218
	TS6	-166.265	1.439	2.122	-162.703
	IM6	-166.855	1.288	1.993	-163.574
	TS7	-165.851	1.361	2.147	-162.343
	IM7	-166.415	1.408	1.993	-163.014
	TS8	-165.805	1.408	2.172	-162.226
	FS	-165.927	1.307	1.832	-162.788
8	IS1	-165.927	1.071	0.531	-164.324
	TS1	-164.614	1.017	0.518	-163.079

Process	Structure	E_e (eV)	E_{ZPE} (eV)	ΔTS (eV)	G (eV)
8	FS1	-165.317	1.086	0.695	-163.536
	IS2	-158.508	0.780	0.413	-157.314
	TS2	-157.111	0.710	0.411	-155.990
	FS2	-157.930	0.794	0.629	-157.137
	IS3	-151.160	0.505	0.277	-150.378
	TS3	-149.909	0.455	0.271	-149.183
	FS3	-150.623	0.565	0.526	-149.532
	IS4	-143.848	0.253	0.135	-143.460
	TS4	-142.354	0.183	0.120	-142.051
	FS4	-143.296	0.285	0.352	-142.659

Table S6. IPCOHP of the Mg-H bond in the IS of Process 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.044	-0.628
2	H28	Mg1	1.996	-0.581
3	H31	Mg1	1.870	-0.958
4	H34	Mg1	1.996	-0.581
5	H37	Mg1	2.044	-0.633
6	H43	Mg1	1.870	-0.951
7	H26	Mg2	1.926	-0.716
8	H29	Mg2	1.919	-0.795
9	H32	Mg2	1.926	-0.715
10	H35	Mg2	1.919	-0.795
11	H38	Mg2	1.926	-0.715
12	H44	Mg2	1.926	-0.716
13	H27	Mg3	1.870	-0.955
14	H30	Mg3	1.996	-0.579
15	H33	Mg3	2.044	-0.628
16	H36	Mg3	1.996	-0.579
17	H39	Mg3	1.870	-0.961
18	H45	Mg3	2.044	-0.625
19	H28	Mg4	1.936	-0.778
20	H32	Mg4	1.834	-0.772
21	H34	Mg4	1.936	-0.778

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H64	Mg4	1.936	-0.775
23	H70	Mg4	1.936	-0.780
24	H25	Mg5	1.918	-0.784
25	H29	Mg5	1.972	-0.690
26	H33	Mg5	1.918	-0.783
27	H35	Mg5	1.972	-0.694
28	H65	Mg5	1.972	-0.693
29	H71	Mg5	1.972	-0.691
30	H26	Mg6	1.834	-0.774
31	H30	Mg6	1.936	-0.779
32	H36	Mg6	1.936	-0.779
33	H66	Mg6	1.936	-0.779
34	H72	Mg6	1.936	-0.781
35	H37	Mg7	2.044	-0.625
36	H40	Mg7	1.996	-0.580
37	H43	Mg7	1.870	-0.962
38	H46	Mg7	1.996	-0.580
39	H49	Mg7	2.044	-0.630
40	H55	Mg7	1.870	-0.954
41	H38	Mg8	1.926	-0.715
42	H41	Mg8	1.919	-0.795
43	H44	Mg8	1.926	-0.716

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H47	Mg8	1.919	-0.795
45	H50	Mg8	1.926	-0.716
46	H56	Mg8	1.926	-0.714
47	H39	Mg9	1.870	-0.951
48	H42	Mg9	1.996	-0.580
49	H45	Mg9	2.044	-0.631
50	H48	Mg9	1.996	-0.580
51	H51	Mg9	1.870	-0.956
52	H57	Mg9	2.044	-0.629
53	H28	Mg10	1.936	-0.777
54	H34	Mg10	1.936	-0.778
55	H40	Mg10	1.936	-0.778
56	H44	Mg10	1.834	-0.771
57	H46	Mg10	1.936	-0.778
58	H29	Mg11	1.972	-0.694
59	H35	Mg11	1.972	-0.690
60	H37	Mg11	1.918	-0.785
61	H41	Mg11	1.972	-0.693
62	H45	Mg11	1.918	-0.784
63	H47	Mg11	1.972	-0.691
64	H30	Mg12	1.936	-0.779
65	H36	Mg12	1.936	-0.778

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H38	Mg12	1.834	-0.773
67	H42	Mg12	1.936	-0.776
68	H48	Mg12	1.936	-0.778
69	H49	Mg13	2.044	-0.631
70	H52	Mg13	1.996	-0.580
71	H55	Mg13	1.870	-0.954
72	H58	Mg13	1.996	-0.580
73	H61	Mg13	2.044	-0.626
74	H67	Mg13	1.870	-0.960
75	H50	Mg14	1.926	-0.714
76	H53	Mg14	1.919	-0.795
77	H56	Mg14	1.926	-0.717
78	H59	Mg14	1.919	-0.795
79	H62	Mg14	1.926	-0.715
80	H68	Mg14	1.926	-0.716
81	H51	Mg15	1.870	-0.953
82	H54	Mg15	1.996	-0.580
83	H57	Mg15	2.044	-0.630
84	H60	Mg15	1.996	-0.580
85	H63	Mg15	1.870	-0.954
86	H69	Mg15	2.044	-0.630
87	H40	Mg16	1.936	-0.778

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H46	Mg16	1.936	-0.778
89	H52	Mg16	1.936	-0.780
90	H56	Mg16	1.834	-0.772
91	H58	Mg16	1.936	-0.777
92	H41	Mg17	1.972	-0.691
93	H47	Mg17	1.972	-0.693
94	H49	Mg17	1.918	-0.785
95	H53	Mg17	1.972	-0.694
96	H57	Mg17	1.918	-0.786
97	H59	Mg17	1.972	-0.690
98	H42	Mg18	1.936	-0.782
99	H48	Mg18	1.936	-0.779
100	H50	Mg18	1.834	-0.774
101	H54	Mg18	1.936	-0.779
102	H60	Mg18	1.936	-0.780
103	H25	Mg19	2.044	-0.630
104	H31	Mg19	1.870	-0.954
105	H61	Mg19	2.044	-0.633
106	H64	Mg19	1.996	-0.581
107	H67	Mg19	1.870	-0.953
108	H70	Mg19	1.996	-0.581
109	H26	Mg20	1.926	-0.714

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H32	Mg20	1.926	-0.717
111	H62	Mg20	1.926	-0.715
112	H65	Mg20	1.919	-0.795
113	H68	Mg20	1.926	-0.716
114	H71	Mg20	1.919	-0.794
115	H27	Mg21	1.870	-0.958
116	H33	Mg21	2.044	-0.627
117	H63	Mg21	1.870	-0.958
118	H66	Mg21	1.996	-0.579
119	H69	Mg21	2.044	-0.625
120	H72	Mg21	1.996	-0.578
121	H52	Mg22	1.936	-0.775
122	H58	Mg22	1.936	-0.779
123	H64	Mg22	1.936	-0.780
124	H68	Mg22	1.834	-0.771
125	H70	Mg22	1.936	-0.776
126	H53	Mg23	1.972	-0.690
127	H59	Mg23	1.972	-0.694
128	H61	Mg23	1.918	-0.784
129	H65	Mg23	1.972	-0.691
130	H69	Mg23	1.918	-0.784
131	H71	Mg23	1.972	-0.693

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
132	H54	Mg24	1.936	-0.779
133	H60	Mg24	1.936	-0.778
134	H62	Mg24	1.834	-0.773
135	H66	Mg24	1.936	-0.779
136	H72	Mg24	1.936	-0.776

Table S7. IPCOHP of the Mg-H bond in the IS of Process 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.045	-0.630
2	H28	Mg1	1.997	-0.577
3	H31	Mg1	1.873	-0.951
4	H34	Mg1	1.997	-0.577
5	H37	Mg1	2.051	-0.626
6	H42	Mg1	1.870	-0.959
7	H26	Mg2	1.920	-0.719
8	H29	Mg2	1.923	-0.781
9	H32	Mg2	1.934	-0.701
10	H35	Mg2	1.923	-0.781
11	H38	Mg2	1.933	-0.733
12	H43	Mg2	1.933	-0.710
13	H27	Mg3	1.864	-0.894
14	H30	Mg3	1.988	-0.565

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
15	H33	Mg3	1.980	-0.503
16	H36	Mg3	1.988	-0.565
17	H44	Mg3	2.000	-0.558
18	H28	Mg4	1.936	-0.774
19	H32	Mg4	1.831	-0.766
20	H34	Mg4	1.936	-0.774
21	H62	Mg4	1.938	-0.775
22	H68	Mg4	1.938	-0.777
23	H25	Mg5	1.921	-0.791
24	H29	Mg5	1.971	-0.695
25	H33	Mg5	1.940	-0.696
26	H35	Mg5	1.971	-0.700
27	H63	Mg5	1.966	-0.707
28	H69	Mg5	1.966	-0.704
29	H26	Mg6	1.839	-0.761
30	H30	Mg6	1.939	-0.798
31	H36	Mg6	1.939	-0.797
32	H64	Mg6	1.930	-0.775
33	H70	Mg6	1.930	-0.776
34	H37	Mg7	2.049	-0.622
35	H39	Mg7	1.996	-0.574
36	H42	Mg7	1.871	-0.959

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
37	H45	Mg7	1.996	-0.574
38	H48	Mg7	2.049	-0.619
39	H53	Mg7	1.871	-0.962
40	H38	Mg8	1.930	-0.723
41	H40	Mg8	1.924	-0.784
42	H43	Mg8	1.939	-0.700
43	H46	Mg8	1.924	-0.784
44	H49	Mg8	1.930	-0.723
45	H54	Mg8	1.939	-0.701
46	H41	Mg9	1.987	-0.462
47	H44	Mg9	1.983	-0.316
48	H47	Mg9	1.987	-0.462
49	H55	Mg9	1.983	-0.320
50	H28	Mg10	1.938	-0.774
51	H34	Mg10	1.938	-0.774
52	H39	Mg10	1.936	-0.772
53	H43	Mg10	1.841	-0.775
54	H45	Mg10	1.936	-0.774
55	H29	Mg11	1.970	-0.721
56	H35	Mg11	1.970	-0.717
57	H37	Mg11	1.914	-0.801
58	H40	Mg11	1.974	-0.703

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
59	H44	Mg11	1.993	-0.666
60	H46	Mg11	1.974	-0.703
61	H30	Mg12	1.944	-0.731
62	H36	Mg12	1.944	-0.731
63	H38	Mg12	1.855	-0.710
64	H41	Mg12	1.953	-0.747
65	H47	Mg12	1.953	-0.749
66	H48	Mg13	2.051	-0.627
67	H50	Mg13	1.997	-0.577
68	H53	Mg13	1.870	-0.957
69	H56	Mg13	1.997	-0.577
70	H59	Mg13	2.045	-0.628
71	H65	Mg13	1.873	-0.955
72	H49	Mg14	1.933	-0.731
73	H51	Mg14	1.923	-0.780
74	H54	Mg14	1.933	-0.711
75	H57	Mg14	1.923	-0.781
76	H60	Mg14	1.920	-0.716
77	H66	Mg14	1.934	-0.704
78	H52	Mg15	1.988	-0.565
79	H55	Mg15	2.000	-0.555
80	H58	Mg15	1.988	-0.565

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
81	H61	Mg15	1.864	-0.898
82	H67	Mg15	1.980	-0.503
83	H39	Mg16	1.935	-0.775
84	H45	Mg16	1.935	-0.773
85	H50	Mg16	1.938	-0.776
86	H54	Mg16	1.841	-0.776
87	H56	Mg16	1.938	-0.777
88	H40	Mg17	1.973	-0.703
89	H46	Mg17	1.973	-0.704
90	H48	Mg17	1.914	-0.801
91	H51	Mg17	1.970	-0.721
92	H55	Mg17	1.993	-0.666
93	H57	Mg17	1.970	-0.716
94	H41	Mg18	1.953	-0.751
95	H47	Mg18	1.953	-0.749
96	H49	Mg18	1.855	-0.710
97	H52	Mg18	1.944	-0.729
98	H58	Mg18	1.944	-0.731
99	H25	Mg19	2.047	-0.626
100	H31	Mg19	1.872	-0.955
101	H59	Mg19	2.047	-0.626
102	H62	Mg19	1.997	-0.580

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
103	H65	Mg19	1.873	-0.953
104	H68	Mg19	1.997	-0.580
105	H26	Mg20	1.922	-0.712
106	H32	Mg20	1.928	-0.720
107	H60	Mg20	1.922	-0.713
108	H63	Mg20	1.921	-0.781
109	H66	Mg20	1.928	-0.718
110	H69	Mg20	1.921	-0.781
111	H27	Mg21	1.884	-0.969
112	H33	Mg21	2.050	-0.599
113	H61	Mg21	1.884	-0.966
114	H64	Mg21	1.991	-0.592
115	H67	Mg21	2.051	-0.598
116	H70	Mg21	1.991	-0.592
117	H50	Mg22	1.936	-0.772
118	H56	Mg22	1.936	-0.771
119	H62	Mg22	1.938	-0.776
120	H66	Mg22	1.831	-0.766
121	H68	Mg22	1.938	-0.774
122	H51	Mg23	1.971	-0.695
123	H57	Mg23	1.971	-0.700
124	H59	Mg23	1.921	-0.790

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
125	H63	Mg23	1.966	-0.705
126	H67	Mg23	1.940	-0.696
127	H69	Mg23	1.966	-0.706
128	H52	Mg24	1.939	-0.799
129	H58	Mg24	1.939	-0.798
130	H60	Mg24	1.839	-0.761
131	H64	Mg24	1.930	-0.775
132	H70	Mg24	1.930	-0.774

Table S8. IPCOHP of the Mg-H bond in the IS of Process 3 step 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.055	-0.626
2	H27	Mg1	1.996	-0.579
3	H30	Mg1	1.872	-0.960
4	H33	Mg1	1.996	-0.579
5	H36	Mg1	2.055	-0.626
6	H41	Mg1	1.872	-0.961
7	H26	Mg2	1.918	-0.730
8	H28	Mg2	1.924	-0.774
9	H31	Mg2	1.931	-0.715
10	H34	Mg2	1.924	-0.774
11	H37	Mg2	1.918	-0.730
12	H42	Mg2	1.932	-0.715
13	H29	Mg3	1.997	-0.426
14	H32	Mg3	1.995	-0.296
15	H35	Mg3	1.997	-0.426
16	H43	Mg3	1.995	-0.296
17	H27	Mg4	1.936	-0.778
18	H31	Mg4	1.831	-0.763
19	H33	Mg4	1.936	-0.775
20	H60	Mg4	1.936	-0.774
21	H66	Mg4	1.936	-0.779

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.929	-0.767
23	H28	Mg5	1.969	-0.717
24	H32	Mg5	2.032	-0.666
25	H34	Mg5	1.969	-0.712
26	H61	Mg5	1.969	-0.715
27	H67	Mg5	1.969	-0.714
28	H26	Mg6	1.849	-0.743
29	H29	Mg6	1.939	-0.765
30	H35	Mg6	1.939	-0.764
31	H62	Mg6	1.939	-0.764
32	H68	Mg6	1.939	-0.764
33	H36	Mg7	2.055	-0.627
34	H38	Mg7	1.996	-0.578
35	H41	Mg7	1.872	-0.960
36	H44	Mg7	1.996	-0.578
37	H47	Mg7	2.055	-0.623
38	H52	Mg7	1.872	-0.962
39	H37	Mg8	1.918	-0.730
40	H39	Mg8	1.924	-0.774
41	H42	Mg8	1.932	-0.714
42	H45	Mg8	1.924	-0.774
43	H48	Mg8	1.918	-0.730

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H53	Mg8	1.931	-0.715
45	H40	Mg9	1.997	-0.426
46	H43	Mg9	1.995	-0.301
47	H46	Mg9	1.997	-0.427
48	H54	Mg9	1.995	-0.297
49	H27	Mg10	1.936	-0.775
50	H33	Mg10	1.936	-0.778
51	H38	Mg10	1.936	-0.776
52	H42	Mg10	1.831	-0.762
53	H44	Mg10	1.936	-0.778
54	H28	Mg11	1.969	-0.712
55	H34	Mg11	1.969	-0.717
56	H36	Mg11	1.929	-0.767
57	H39	Mg11	1.969	-0.715
58	H43	Mg11	2.032	-0.666
59	H45	Mg11	1.969	-0.714
60	H29	Mg12	1.939	-0.764
61	H35	Mg12	1.939	-0.765
62	H37	Mg12	1.849	-0.742
63	H40	Mg12	1.939	-0.764
64	H46	Mg12	1.939	-0.765
65	H47	Mg13	2.055	-0.627

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H49	Mg13	1.996	-0.578
67	H52	Mg13	1.872	-0.960
68	H55	Mg13	1.996	-0.578
69	H58	Mg13	2.055	-0.628
70	H63	Mg13	1.872	-0.959
71	H48	Mg14	1.918	-0.730
72	H50	Mg14	1.924	-0.774
73	H53	Mg14	1.931	-0.715
74	H56	Mg14	1.924	-0.774
75	H59	Mg14	1.918	-0.730
76	H64	Mg14	1.932	-0.715
77	H51	Mg15	1.997	-0.427
78	H54	Mg15	1.995	-0.300
79	H57	Mg15	1.997	-0.426
80	H65	Mg15	1.995	-0.301
81	H38	Mg16	1.936	-0.777
82	H44	Mg16	1.936	-0.775
83	H49	Mg16	1.936	-0.777
84	H53	Mg16	1.831	-0.763
85	H55	Mg16	1.936	-0.776
86	H39	Mg17	1.969	-0.714
87	H45	Mg17	1.969	-0.715

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H47	Mg17	1.929	-0.767
89	H50	Mg17	1.969	-0.712
90	H54	Mg17	2.032	-0.666
91	H56	Mg17	1.969	-0.717
92	H40	Mg18	1.939	-0.765
93	H46	Mg18	1.939	-0.764
94	H48	Mg18	1.849	-0.743
95	H51	Mg18	1.939	-0.763
96	H57	Mg18	1.939	-0.765
97	H25	Mg19	2.055	-0.625
98	H30	Mg19	1.872	-0.962
99	H58	Mg19	2.055	-0.625
100	H60	Mg19	1.996	-0.579
101	H63	Mg19	1.872	-0.961
102	H66	Mg19	1.996	-0.579
103	H26	Mg20	1.918	-0.730
104	H31	Mg20	1.931	-0.716
105	H59	Mg20	1.918	-0.730
106	H61	Mg20	1.924	-0.774
107	H64	Mg20	1.932	-0.714
108	H67	Mg20	1.924	-0.774
109	H32	Mg21	1.995	-0.301

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H62	Mg21	1.997	-0.427
111	H65	Mg21	1.995	-0.296
112	H68	Mg21	1.997	-0.426
113	H49	Mg22	1.936	-0.777
114	H55	Mg22	1.936	-0.777
115	H60	Mg22	1.936	-0.779
116	H64	Mg22	1.831	-0.762
117	H66	Mg22	1.936	-0.774
118	H50	Mg23	1.969	-0.718
119	H56	Mg23	1.969	-0.713
120	H58	Mg23	1.929	-0.767
121	H61	Mg23	1.969	-0.714
122	H65	Mg23	2.032	-0.666
123	H67	Mg23	1.969	-0.715
124	H51	Mg24	1.939	-0.766
125	H57	Mg24	1.939	-0.763
126	H59	Mg24	1.849	-0.742
127	H62	Mg24	1.939	-0.764
128	H68	Mg24	1.939	-0.765

Table S9. IPCOHP of the Mg-H bond in the IS of Process 3 step 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.062	-0.608
2	H27	Mg1	1.995	-0.580
3	H30	Mg1	1.863	-0.981
4	H33	Mg1	2.000	-0.588
5	H36	Mg1	2.043	-0.612
6	H41	Mg1	1.872	-0.966
7	H26	Mg2	1.931	-0.769
8	H28	Mg2	1.923	-0.782
9	H31	Mg2	1.930	-0.726
10	H34	Mg2	1.927	-0.761
11	H37	Mg2	1.920	-0.729
12	H42	Mg2	1.954	-0.668
13	H29	Mg3	2.028	-0.635
14	H32	Mg3	1.859	-0.593
15	H35	Mg3	1.960	-0.554
16	H43	Mg3	1.925	-0.427
17	H27	Mg4	1.941	-0.769
18	H31	Mg4	1.839	-0.781
19	H33	Mg4	1.946	-0.778
20	H60	Mg4	1.935	-0.771
21	H66	Mg4	1.939	-0.780

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.905	-0.831
23	H28	Mg5	1.985	-0.689
24	H32	Mg5	1.953	-0.690
25	H34	Mg5	1.974	-0.694
26	H61	Mg5	1.973	-0.718
27	H67	Mg5	1.970	-0.699
28	H26	Mg6	1.917	-0.422
29	H29	Mg6	2.045	-0.511
30	H35	Mg6	2.010	-0.471
31	H62	Mg6	2.116	-0.318
32	H36	Mg7	2.039	-0.617
33	H38	Mg7	1.996	-0.576
34	H41	Mg7	1.870	-0.972
35	H44	Mg7	2.001	-0.582
36	H47	Mg7	2.059	-0.612
37	H52	Mg7	1.864	-0.975
38	H37	Mg8	1.914	-0.731
39	H39	Mg8	1.927	-0.773
40	H42	Mg8	1.936	-0.704
41	H45	Mg8	1.925	-0.751
42	H48	Mg8	1.932	-0.731
43	H53	Mg8	1.930	-0.722

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H40	Mg9	2.008	-0.487
45	H43	Mg9	1.956	-0.279
46	H46	Mg9	1.970	-0.474
47	H54	Mg9	1.950	-0.322
48	H27	Mg10	1.938	-0.766
49	H33	Mg10	1.941	-0.776
50	H38	Mg10	1.940	-0.768
51	H42	Mg10	1.834	-0.772
52	H44	Mg10	1.943	-0.773
53	H28	Mg11	1.958	-0.745
54	H34	Mg11	1.963	-0.723
55	H36	Mg11	1.895	-0.828
56	H39	Mg11	1.967	-0.720
57	H43	Mg11	2.003	-0.616
58	H45	Mg11	1.957	-0.713
59	H29	Mg12	1.960	-0.851
60	H35	Mg12	1.891	-0.825
61	H37	Mg12	1.844	-0.752
62	H40	Mg12	1.945	-0.826
63	H46	Mg12	1.952	-0.733
64	H47	Mg13	2.044	-0.626
65	H49	Mg13	1.994	-0.576

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H52	Mg13	1.871	-0.964
67	H55	Mg13	2.000	-0.586
68	H58	Mg13	2.055	-0.622
69	H63	Mg13	1.864	-0.963
70	H48	Mg14	1.938	-0.720
71	H50	Mg14	1.926	-0.783
72	H53	Mg14	1.951	-0.685
73	H56	Mg14	1.924	-0.772
74	H59	Mg14	1.922	-0.768
75	H64	Mg14	1.941	-0.706
76	H51	Mg15	2.001	-0.580
77	H54	Mg15	1.992	-0.563
78	H57	Mg15	1.980	-0.588
79	H65	Mg15	1.971	-0.523
80	H68	Mg15	1.838	-0.901
81	H38	Mg16	1.939	-0.772
82	H44	Mg16	1.942	-0.776
83	H49	Mg16	1.935	-0.769
84	H53	Mg16	1.841	-0.768
85	H55	Mg16	1.937	-0.782
86	H39	Mg17	1.972	-0.716
87	H45	Mg17	1.968	-0.693

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H47	Mg17	1.910	-0.809
89	H50	Mg17	1.967	-0.739
90	H54	Mg17	2.001	-0.645
91	H56	Mg17	1.960	-0.723
92	H40	Mg18	1.981	-0.736
93	H46	Mg18	1.960	-0.723
94	H48	Mg18	1.855	-0.727
95	H51	Mg18	1.933	-0.765
96	H57	Mg18	1.909	-0.827
97	H25	Mg19	2.044	-0.621
98	H30	Mg19	1.870	-0.963
99	H58	Mg19	2.058	-0.616
100	H60	Mg19	1.992	-0.581
101	H63	Mg19	1.865	-0.965
102	H66	Mg19	1.999	-0.588
103	H26	Mg20	1.926	-0.738
104	H31	Mg20	1.968	-0.651
105	H59	Mg20	1.933	-0.735
106	H61	Mg20	1.927	-0.750
107	H64	Mg20	1.961	-0.652
108	H67	Mg20	1.930	-0.742
109	H32	Mg21	2.201	-0.265

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H62	Mg21	2.035	-0.463
111	H65	Mg21	1.967	-0.366
112	H68	Mg21	1.902	-0.594
113	H49	Mg22	1.940	-0.764
114	H55	Mg22	1.944	-0.781
115	H60	Mg22	1.935	-0.775
116	H64	Mg22	1.840	-0.785
117	H66	Mg22	1.940	-0.785
118	H50	Mg23	1.983	-0.677
119	H56	Mg23	1.977	-0.690
120	H58	Mg23	1.915	-0.835
121	H61	Mg23	1.972	-0.700
122	H65	Mg23	1.928	-0.645
123	H67	Mg23	1.975	-0.694
124	H51	Mg24	1.986	-0.591
125	H57	Mg24	2.049	-0.556
126	H59	Mg24	1.898	-0.512
127	H62	Mg24	2.042	-0.535

Table S10. IPCOHP of the Mg-H bond in the IS of Process 3 step 3.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	1.959	-0.680
2	H27	Mg1	1.940	-0.588
3	H30	Mg1	1.959	-0.892
4	H33	Mg1	1.940	-0.591
5	H36	Mg1	1.959	-0.693
6	H41	Mg1	1.959	-0.887
7	H26	Mg2	1.959	-0.737
8	H28	Mg2	1.940	-0.739
9	H31	Mg2	1.959	-0.707
10	H34	Mg2	1.940	-0.735
11	H37	Mg2	1.959	-0.712
12	H42	Mg2	1.959	-0.710
13	H29	Mg3	1.940	-0.561
14	H32	Mg3	1.959	-0.386
15	H35	Mg3	1.940	-0.468
16	H43	Mg3	1.959	-0.391
17	H27	Mg4	1.959	-0.740
18	H31	Mg4	1.940	-0.551
19	H33	Mg4	1.959	-0.744
20	H60	Mg4	1.959	-0.743
21	H66	Mg4	1.959	-0.747

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.940	-0.727
23	H28	Mg5	1.959	-0.716
24	H32	Mg5	1.940	-0.688
25	H34	Mg5	1.959	-0.717
26	H61	Mg5	1.959	-0.745
27	H67	Mg5	1.959	-0.725
28	H26	Mg6	1.940	-0.462
29	H29	Mg6	1.959	-0.603
30	H35	Mg6	1.959	-0.519
31	H62	Mg6	1.959	-0.542
32	H36	Mg7	1.959	-0.689
33	H38	Mg7	1.940	-0.592
34	H41	Mg7	1.959	-0.887
35	H44	Mg7	1.940	-0.592
36	H47	Mg7	1.959	-0.685
37	H52	Mg7	1.959	-0.894
38	H37	Mg8	1.959	-0.716
39	H39	Mg8	1.940	-0.742
40	H42	Mg8	1.959	-0.703
41	H45	Mg8	1.940	-0.731
42	H48	Mg8	1.959	-0.734
43	H53	Mg8	1.959	-0.707

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H40	Mg9	1.940	-0.558
45	H43	Mg9	1.959	-0.620
46	H46	Mg9	1.940	-0.579
47	H54	Mg9	1.959	-0.446
48	H57	Mg9	1.722	-0.961
49	H27	Mg10	1.959	-0.737
50	H33	Mg10	1.959	-0.748
51	H38	Mg10	1.959	-0.744
52	H42	Mg10	1.940	-0.559
53	H44	Mg10	1.959	-0.747
54	H28	Mg11	1.959	-0.730
55	H34	Mg11	1.959	-0.726
56	H36	Mg11	1.940	-0.727
57	H39	Mg11	1.959	-0.746
58	H43	Mg11	1.940	-0.676
59	H45	Mg11	1.959	-0.734
60	H29	Mg12	1.959	-0.729
61	H35	Mg12	1.959	-0.773
62	H37	Mg12	1.940	-0.533
63	H40	Mg12	1.959	-0.767
64	H46	Mg12	1.959	-0.764
65	H47	Mg13	1.959	-0.680

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H49	Mg13	1.940	-0.594
67	H52	Mg13	1.959	-0.897
68	H55	Mg13	1.940	-0.595
69	H58	Mg13	1.959	-0.684
70	H63	Mg13	1.959	-0.894
71	H48	Mg14	1.959	-0.700
72	H50	Mg14	1.940	-0.731
73	H53	Mg14	1.959	-0.692
74	H56	Mg14	1.940	-0.718
75	H59	Mg14	1.959	-0.713
76	H64	Mg14	1.959	-0.700
77	H51	Mg15	1.940	-0.459
78	H54	Mg15	1.959	-0.602
79	H57	Mg15	1.994	-0.707
80	H65	Mg15	1.959	-0.531
81	H68	Mg15	1.768	-0.858
82	H38	Mg16	1.959	-0.741
83	H44	Mg16	1.959	-0.741
84	H49	Mg16	1.959	-0.744
85	H53	Mg16	1.940	-0.554
86	H55	Mg16	1.959	-0.747
87	H39	Mg17	1.959	-0.706

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H45	Mg17	1.959	-0.708
89	H47	Mg17	1.940	-0.739
90	H50	Mg17	1.959	-0.720
91	H54	Mg17	1.940	-0.707
92	H56	Mg17	1.959	-0.707
93	H40	Mg18	1.959	-0.553
94	H46	Mg18	1.959	-0.662
95	H48	Mg18	1.940	-0.478
96	H51	Mg18	1.959	-0.563
97	H25	Mg19	1.959	-0.687
98	H30	Mg19	1.959	-0.890
99	H58	Mg19	1.959	-0.688
100	H60	Mg19	1.940	-0.591
101	H63	Mg19	1.959	-0.896
102	H66	Mg19	1.940	-0.592
103	H26	Mg20	1.959	-0.697
104	H31	Mg20	1.959	-0.694
105	H59	Mg20	1.959	-0.715
106	H61	Mg20	1.940	-0.731
107	H64	Mg20	1.959	-0.702
108	H67	Mg20	1.940	-0.718
109	H32	Mg21	1.959	-0.422

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H62	Mg21	1.940	-0.522
111	H65	Mg21	1.959	-0.329
112	H68	Mg21	1.918	-0.561
113	H49	Mg22	1.959	-0.743
114	H55	Mg22	1.959	-0.745
115	H60	Mg22	1.959	-0.743
116	H64	Mg22	1.940	-0.557
117	H66	Mg22	1.959	-0.743
118	H50	Mg23	1.959	-0.712
119	H56	Mg23	1.959	-0.708
120	H58	Mg23	1.940	-0.741
121	H61	Mg23	1.959	-0.700
122	H65	Mg23	1.940	-0.716
123	H67	Mg23	1.959	-0.702
124	H51	Mg24	1.959	-0.364
125	H59	Mg24	1.940	-0.399
126	H62	Mg24	1.959	-0.369

Table S11. IPCOHP of the Mg-H bond in the IS of Process 4 step 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.068	-0.595
2	H27	Mg1	1.999	-0.587
3	H30	Mg1	1.863	-0.980
4	H33	Mg1	1.996	-0.585
5	H36	Mg1	2.039	-0.606
6	H41	Mg1	1.869	-0.976
7	H26	Mg2	1.929	-0.763
8	H28	Mg2	1.923	-0.781
9	H31	Mg2	1.944	-0.699
10	H34	Mg2	1.922	-0.737
11	H37	Mg2	1.917	-0.739
12	H42	Mg2	1.950	-0.665
13	H29	Mg3	2.033	-0.576
14	H32	Mg3	1.923	-0.428
15	H35	Mg3	1.952	-0.572
16	H43	Mg3	1.951	-0.336
17	H27	Mg4	1.945	-0.777
18	H31	Mg4	1.840	-0.783
19	H33	Mg4	1.945	-0.764
20	H59	Mg4	1.940	-0.771
21	H65	Mg4	1.938	-0.768

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.894	-0.849
23	H28	Mg5	1.975	-0.701
24	H32	Mg5	1.970	-0.629
25	H34	Mg5	1.948	-0.708
26	H60	Mg5	1.984	-0.727
27	H66	Mg5	1.972	-0.689
28	H26	Mg6	1.915	-0.460
29	H29	Mg6	2.013	-0.570
30	H35	Mg6	2.006	-0.484
31	H61	Mg6	2.134	-0.463
32	H36	Mg7	2.039	-0.608
33	H38	Mg7	1.999	-0.587
34	H41	Mg7	1.869	-0.974
35	H44	Mg7	1.996	-0.585
36	H47	Mg7	2.068	-0.594
37	H52	Mg7	1.863	-0.981
38	H37	Mg8	1.917	-0.738
39	H39	Mg8	1.923	-0.781
40	H42	Mg8	1.950	-0.666
41	H45	Mg8	1.922	-0.738
42	H48	Mg8	1.929	-0.762
43	H53	Mg8	1.944	-0.699

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H40	Mg9	2.033	-0.576
45	H43	Mg9	1.951	-0.331
46	H46	Mg9	1.952	-0.573
47	H54	Mg9	1.923	-0.427
48	H27	Mg10	1.944	-0.769
49	H33	Mg10	1.943	-0.764
50	H38	Mg10	1.944	-0.769
51	H42	Mg10	1.831	-0.764
52	H44	Mg10	1.943	-0.763
53	H28	Mg11	1.969	-0.727
54	H34	Mg11	1.964	-0.694
55	H36	Mg11	1.894	-0.810
56	H39	Mg11	1.969	-0.726
57	H43	Mg11	1.966	-0.669
58	H45	Mg11	1.964	-0.695
59	H29	Mg12	1.971	-0.835
60	H35	Mg12	1.915	-0.762
61	H37	Mg12	1.859	-0.748
62	H40	Mg12	1.971	-0.837
63	H46	Mg12	1.915	-0.761
64	H47	Mg13	2.036	-0.617
65	H49	Mg13	1.997	-0.588

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H52	Mg13	1.867	-0.971
67	H55	Mg13	1.995	-0.586
68	H57	Mg13	2.066	-0.600
69	H62	Mg13	1.861	-0.985
70	H48	Mg14	1.933	-0.731
71	H50	Mg14	1.938	-0.760
72	H53	Mg14	1.966	-0.642
73	H56	Mg14	1.931	-0.720
74	H58	Mg14	1.932	-0.757
75	H63	Mg14	1.965	-0.659
76	H51	Mg15	2.086	-0.470
77	H54	Mg15	1.979	-0.304
78	H64	Mg15	1.942	-0.393
79	H38	Mg16	1.945	-0.775
80	H44	Mg16	1.945	-0.765
81	H49	Mg16	1.940	-0.772
82	H53	Mg16	1.840	-0.783
83	H55	Mg16	1.938	-0.767
84	H39	Mg17	1.975	-0.702
85	H45	Mg17	1.948	-0.707
86	H47	Mg17	1.894	-0.849
87	H50	Mg17	1.984	-0.726

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H54	Mg17	1.970	-0.628
89	H56	Mg17	1.972	-0.689
90	H40	Mg18	2.013	-0.569
91	H46	Mg18	2.006	-0.486
92	H48	Mg18	1.915	-0.460
93	H51	Mg18	2.134	-0.467
94	H25	Mg19	2.036	-0.616
95	H30	Mg19	1.867	-0.973
96	H57	Mg19	2.066	-0.600
97	H59	Mg19	1.997	-0.588
98	H62	Mg19	1.861	-0.985
99	H65	Mg19	1.995	-0.586
100	H26	Mg20	1.933	-0.730
101	H31	Mg20	1.966	-0.642
102	H58	Mg20	1.932	-0.758
103	H60	Mg20	1.938	-0.761
104	H63	Mg20	1.965	-0.658
105	H66	Mg20	1.931	-0.721
106	H32	Mg21	1.979	-0.304
107	H61	Mg21	2.086	-0.470
108	H64	Mg21	1.942	-0.396
109	H49	Mg22	1.943	-0.776

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H55	Mg22	1.940	-0.770
111	H59	Mg22	1.943	-0.776
112	H63	Mg22	1.845	-0.809
113	H65	Mg22	1.940	-0.769
114	H50	Mg23	1.992	-0.695
115	H56	Mg23	1.961	-0.710
116	H57	Mg23	1.893	-0.897
117	H60	Mg23	1.992	-0.694
118	H64	Mg23	1.968	-0.604
119	H66	Mg23	1.961	-0.710
120	H51	Mg24	2.105	-0.433
121	H58	Mg24	1.936	-0.372
122	H61	Mg24	2.105	-0.438

Table S12. IPCOHP of the Mg-H bond in the IS of Process 4 step 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.061	-0.585
2	H27	Mg1	1.999	-0.588
3	H30	Mg1	1.860	-1.002
4	H33	Mg1	1.998	-0.583
5	H36	Mg1	2.037	-0.595
6	H41	Mg1	1.870	-0.982
7	H26	Mg2	1.920	-0.795
8	H28	Mg2	1.934	-0.758
9	H31	Mg2	1.923	-0.738
10	H34	Mg2	1.931	-0.747
11	H37	Mg2	1.916	-0.714
12	H42	Mg2	1.950	-0.669
13	H29	Mg3	1.994	-0.679
14	H32	Mg3	1.863	-0.590
15	H35	Mg3	1.970	-0.722
16	H43	Mg3	1.923	-0.529
17	H27	Mg4	1.949	-0.769
18	H31	Mg4	1.842	-0.784
19	H33	Mg4	1.949	-0.761
20	H59	Mg4	1.936	-0.775
21	H65	Mg4	1.934	-0.780

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.887	-0.868
23	H28	Mg5	1.981	-0.695
24	H32	Mg5	1.958	-0.651
25	H34	Mg5	1.982	-0.665
26	H60	Mg5	1.969	-0.714
27	H66	Mg5	1.960	-0.705
28	H26	Mg6	1.947	-0.350
29	H29	Mg6	2.095	-0.402
30	H35	Mg6	2.061	-0.417
31	H36	Mg7	2.037	-0.595
32	H38	Mg7	1.999	-0.586
33	H41	Mg7	1.871	-0.984
34	H44	Mg7	1.998	-0.585
35	H47	Mg7	2.060	-0.587
36	H52	Mg7	1.861	-0.996
37	H37	Mg8	1.914	-0.728
38	H39	Mg8	1.927	-0.767
39	H42	Mg8	1.946	-0.678
40	H45	Mg8	1.930	-0.749
41	H48	Mg8	1.925	-0.777
42	H53	Mg8	1.925	-0.734
43	H40	Mg9	2.011	-0.745

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H43	Mg9	1.909	-0.547
45	H46	Mg9	1.963	-0.676
46	H54	Mg9	1.829	-0.688
47	H27	Mg10	1.942	-0.771
48	H33	Mg10	1.942	-0.769
49	H38	Mg10	1.943	-0.766
50	H42	Mg10	1.835	-0.765
51	H44	Mg10	1.943	-0.771
52	H28	Mg11	1.960	-0.737
53	H34	Mg11	1.950	-0.736
54	H36	Mg11	1.876	-0.850
55	H39	Mg11	1.952	-0.747
56	H43	Mg11	2.019	-0.567
57	H45	Mg11	1.958	-0.736
58	H29	Mg12	1.936	-0.896
59	H35	Mg12	1.947	-0.824
60	H37	Mg12	1.836	-0.773
61	H40	Mg12	1.968	-0.869
62	H46	Mg12	1.912	-0.818
63	H47	Mg13	2.038	-0.618
64	H49	Mg13	1.996	-0.588
65	H52	Mg13	1.872	-0.957

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H55	Mg13	1.995	-0.587
67	H57	Mg13	2.061	-0.615
68	H62	Mg13	1.861	-0.981
69	H48	Mg14	1.946	-0.722
70	H50	Mg14	1.931	-0.755
71	H53	Mg14	1.977	-0.634
72	H56	Mg14	1.931	-0.740
73	H58	Mg14	1.902	-0.821
74	H63	Mg14	1.962	-0.650
75	H51	Mg15	2.095	-0.377
76	H54	Mg15	2.204	-0.222
77	H61	Mg15	1.897	-0.592
78	H64	Mg15	1.977	-0.387
79	H38	Mg16	1.948	-0.775
80	H44	Mg16	1.949	-0.763
81	H49	Mg16	1.936	-0.776
82	H53	Mg16	1.841	-0.776
83	H55	Mg16	1.934	-0.779
84	H39	Mg17	1.993	-0.677
85	H45	Mg17	1.979	-0.689
86	H47	Mg17	1.890	-0.862
87	H50	Mg17	1.966	-0.726

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H54	Mg17	1.931	-0.680
89	H56	Mg17	1.958	-0.706
90	H40	Mg18	2.116	-0.467
91	H46	Mg18	2.021	-0.476
92	H48	Mg18	1.908	-0.439
93	H51	Mg18	2.042	-0.453
94	H25	Mg19	2.039	-0.614
95	H30	Mg19	1.872	-0.962
96	H57	Mg19	2.058	-0.616
97	H59	Mg19	1.995	-0.590
98	H62	Mg19	1.860	-0.979
99	H65	Mg19	1.995	-0.588
100	H26	Mg20	1.954	-0.732
101	H31	Mg20	1.998	-0.591
102	H58	Mg20	1.928	-0.773
103	H60	Mg20	1.933	-0.741
104	H63	Mg20	1.976	-0.617
105	H66	Mg20	1.924	-0.744
106	H32	Mg21	2.081	-0.303
107	H61	Mg21	1.840	-0.704
108	H64	Mg21	1.958	-0.395
109	H49	Mg22	1.946	-0.768

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H55	Mg22	1.945	-0.771
111	H59	Mg22	1.944	-0.773
112	H63	Mg22	1.835	-0.817
113	H65	Mg22	1.943	-0.775
114	H50	Mg23	1.975	-0.700
115	H56	Mg23	1.975	-0.702
116	H57	Mg23	1.921	-0.830
117	H60	Mg23	1.984	-0.675
118	H64	Mg23	1.944	-0.652
119	H66	Mg23	1.974	-0.699
120	H51	Mg24	2.024	-0.435
121	H58	Mg24	1.964	-0.318

Table S13. IPCOHP of the Mg-H bond in the IS of Process 4 step 3.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.039	-0.579
2	H27	Mg1	2.001	-0.583
3	H30	Mg1	1.861	-1.002
4	H33	Mg1	2.001	-0.582
5	H36	Mg1	2.066	-0.569
6	H41	Mg1	1.867	-1.019
7	H26	Mg2	1.934	-0.815
8	H28	Mg2	1.929	-0.757
9	H31	Mg2	1.910	-0.765
10	H34	Mg2	1.929	-0.757
11	H37	Mg2	1.906	-0.704
12	H42	Mg2	1.957	-0.652
13	H29	Mg3	2.004	-0.714
14	H32	Mg3	1.760	-0.827
15	H35	Mg3	2.001	-0.719
16	H43	Mg3	1.961	-0.693
17	H27	Mg4	1.952	-0.765
18	H31	Mg4	1.843	-0.780
19	H33	Mg4	1.952	-0.765
20	H59	Mg4	1.932	-0.788
21	H65	Mg4	1.932	-0.788

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.857	-0.955
23	H28	Mg5	2.014	-0.628
24	H32	Mg5	1.822	-0.769
25	H34	Mg5	2.014	-0.626
26	H60	Mg5	1.981	-0.669
27	H66	Mg5	1.981	-0.672
28	H26	Mg6	1.966	-0.357
29	H29	Mg6	2.148	-0.390
30	H35	Mg6	2.153	-0.384
31	H36	Mg7	2.020	-0.614
32	H38	Mg7	2.001	-0.583
33	H41	Mg7	1.873	-0.983
34	H44	Mg7	2.001	-0.582
35	H47	Mg7	2.060	-0.581
36	H52	Mg7	1.856	-1.004
37	H37	Mg8	1.924	-0.693
38	H39	Mg8	1.946	-0.741
39	H42	Mg8	1.924	-0.738
40	H45	Mg8	1.945	-0.743
41	H48	Mg8	1.885	-0.792
42	H53	Mg8	1.916	-0.768
43	H40	Mg9	1.997	-0.687

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H43	Mg9	1.907	-0.939
45	H46	Mg9	1.993	-0.697
46	H51	Mg9	1.852	-0.912
47	H54	Mg9	1.864	-0.793
48	H27	Mg10	1.942	-0.769
49	H33	Mg10	1.942	-0.769
50	H38	Mg10	1.940	-0.771
51	H42	Mg10	1.838	-0.762
52	H44	Mg10	1.940	-0.770
53	H28	Mg11	1.934	-0.778
54	H34	Mg11	1.933	-0.781
55	H36	Mg11	1.881	-0.813
56	H39	Mg11	1.949	-0.761
57	H43	Mg11	2.190	-0.468
58	H45	Mg11	1.949	-0.758
59	H29	Mg12	1.933	-0.897
60	H35	Mg12	1.933	-0.898
61	H37	Mg12	1.813	-0.792
62	H40	Mg12	1.934	-0.813
63	H46	Mg12	1.933	-0.817
64	H47	Mg13	2.045	-0.621
65	H49	Mg13	1.995	-0.592

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H52	Mg13	1.876	-0.933
67	H55	Mg13	1.995	-0.592
68	H57	Mg13	2.052	-0.630
69	H62	Mg13	1.862	-0.983
70	H48	Mg14	1.948	-0.697
71	H50	Mg14	1.928	-0.733
72	H53	Mg14	2.007	-0.587
73	H56	Mg14	1.928	-0.734
74	H58	Mg14	1.914	-0.817
75	H63	Mg14	1.963	-0.621
76	H51	Mg15	1.872	-0.845
77	H54	Mg15	2.022	-0.517
78	H61	Mg15	1.813	-0.987
79	H64	Mg15	1.967	-0.712
80	H38	Mg16	1.950	-0.765
81	H44	Mg16	1.949	-0.759
82	H49	Mg16	1.932	-0.779
83	H53	Mg16	1.838	-0.787
84	H55	Mg16	1.932	-0.784
85	H39	Mg17	1.995	-0.676
86	H45	Mg17	1.995	-0.675
87	H47	Mg17	1.875	-0.921

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H50	Mg17	1.950	-0.707
89	H54	Mg17	1.937	-0.621
90	H56	Mg17	1.950	-0.715
91	H40	Mg18	2.024	-0.424
92	H46	Mg18	2.026	-0.427
93	H48	Mg18	1.926	-0.320
94	H25	Mg19	2.036	-0.592
95	H30	Mg19	1.878	-0.951
96	H57	Mg19	2.074	-0.607
97	H59	Mg19	1.996	-0.591
98	H62	Mg19	1.857	-1.006
99	H65	Mg19	1.996	-0.591
100	H26	Mg20	1.973	-0.737
101	H31	Mg20	2.003	-0.579
102	H58	Mg20	1.897	-0.845
103	H60	Mg20	1.928	-0.740
104	H63	Mg20	1.985	-0.593
105	H66	Mg20	1.928	-0.739
106	H61	Mg21	1.877	-0.502
107	H64	Mg21	2.054	-0.269
108	H49	Mg22	1.946	-0.773
109	H55	Mg22	1.946	-0.773

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H59	Mg22	1.949	-0.766
111	H63	Mg22	1.828	-0.829
112	H65	Mg22	1.948	-0.767
113	H50	Mg23	1.983	-0.679
114	H56	Mg23	1.983	-0.677
115	H57	Mg23	1.962	-0.732
116	H60	Mg23	1.964	-0.724
117	H64	Mg23	1.985	-0.680
118	H66	Mg23	1.964	-0.725
119	H58	Mg24	1.986	-0.231

Table S14. IPCOHP of the Mg-H bond in the IS of Process 5 step 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.053	-0.581
2	H27	Mg1	1.999	-0.583
3	H30	Mg1	1.860	-0.997
4	H33	Mg1	1.999	-0.583
5	H36	Mg1	2.041	-0.587
6	H41	Mg1	1.868	-0.988
7	H26	Mg2	1.918	-0.793
8	H28	Mg2	1.931	-0.749
9	H31	Mg2	1.921	-0.746
10	H34	Mg2	1.931	-0.749
11	H37	Mg2	1.929	-0.697
12	H42	Mg2	1.946	-0.676
13	H29	Mg3	1.979	-0.771
14	H32	Mg3	1.817	-0.692
15	H35	Mg3	1.979	-0.771
16	H43	Mg3	1.909	-0.614
17	H27	Mg4	1.952	-0.757
18	H31	Mg4	1.840	-0.778
19	H33	Mg4	1.952	-0.759
20	H58	Mg4	1.935	-0.774
21	H63	Mg4	1.935	-0.775

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.874	-0.907
23	H28	Mg5	1.993	-0.667
24	H32	Mg5	1.907	-0.665
25	H34	Mg5	1.993	-0.669
26	H59	Mg5	1.965	-0.704
27	H64	Mg5	1.965	-0.702
28	H26	Mg6	1.965	-0.346
29	H29	Mg6	2.128	-0.412
30	H35	Mg6	2.127	-0.411
31	H36	Mg7	2.041	-0.595
32	H38	Mg7	1.999	-0.582
33	H41	Mg7	1.868	-0.982
34	H44	Mg7	1.999	-0.583
35	H47	Mg7	2.053	-0.583
36	H51	Mg7	1.860	-0.996
37	H37	Mg8	1.929	-0.701
38	H39	Mg8	1.931	-0.749
39	H42	Mg8	1.946	-0.675
40	H45	Mg8	1.931	-0.749
41	H48	Mg8	1.918	-0.794
42	H52	Mg8	1.921	-0.746
43	H40	Mg9	1.979	-0.770

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H43	Mg9	1.909	-0.614
45	H46	Mg9	1.979	-0.770
46	H53	Mg9	1.817	-0.689
47	H27	Mg10	1.943	-0.768
48	H33	Mg10	1.943	-0.770
49	H38	Mg10	1.943	-0.769
50	H42	Mg10	1.838	-0.755
51	H44	Mg10	1.943	-0.768
52	H28	Mg11	1.948	-0.747
53	H34	Mg11	1.948	-0.747
54	H36	Mg11	1.878	-0.829
55	H39	Mg11	1.948	-0.747
56	H43	Mg11	2.076	-0.532
57	H45	Mg11	1.948	-0.748
58	H29	Mg12	1.953	-0.858
59	H35	Mg12	1.953	-0.856
60	H37	Mg12	1.832	-0.809
61	H40	Mg12	1.952	-0.857
62	H46	Mg12	1.952	-0.857
63	H47	Mg13	2.043	-0.592
64	H49	Mg13	1.995	-0.589
65	H51	Mg13	1.871	-0.966

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H54	Mg13	1.995	-0.589
67	H56	Mg13	2.064	-0.610
68	H60	Mg13	1.859	-0.994
69	H48	Mg14	1.959	-0.736
70	H50	Mg14	1.930	-0.731
71	H52	Mg14	2.016	-0.548
72	H55	Mg14	1.930	-0.731
73	H57	Mg14	1.919	-0.837
74	H61	Mg14	1.985	-0.589
75	H53	Mg15	2.133	-0.099
76	H62	Mg15	1.981	-0.247
77	H38	Mg16	1.952	-0.755
78	H44	Mg16	1.952	-0.761
79	H49	Mg16	1.935	-0.777
80	H52	Mg16	1.840	-0.778
81	H54	Mg16	1.935	-0.773
82	H39	Mg17	1.993	-0.669
83	H45	Mg17	1.993	-0.670
84	H47	Mg17	1.874	-0.905
85	H50	Mg17	1.965	-0.703
86	H53	Mg17	1.906	-0.666
87	H55	Mg17	1.965	-0.701

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H40	Mg18	2.127	-0.412
89	H46	Mg18	2.127	-0.412
90	H48	Mg18	1.965	-0.347
91	H25	Mg19	2.043	-0.594
92	H30	Mg19	1.871	-0.964
93	H56	Mg19	2.064	-0.598
94	H58	Mg19	1.995	-0.589
95	H60	Mg19	1.859	-1.005
96	H63	Mg19	1.995	-0.589
97	H26	Mg20	1.959	-0.736
98	H31	Mg20	2.017	-0.549
99	H57	Mg20	1.919	-0.836
100	H59	Mg20	1.930	-0.731
101	H61	Mg20	1.985	-0.592
102	H64	Mg20	1.930	-0.731
103	H32	Mg21	2.131	-0.099
104	H62	Mg21	1.981	-0.243
105	H49	Mg22	1.948	-0.766
106	H54	Mg22	1.948	-0.763
107	H58	Mg22	1.948	-0.763
108	H61	Mg22	1.837	-0.834
109	H63	Mg22	1.948	-0.765

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H50	Mg23	1.983	-0.688
111	H55	Mg23	1.983	-0.688
112	H56	Mg23	1.923	-0.824
113	H59	Mg23	1.983	-0.688
114	H62	Mg23	1.939	-0.695
115	H64	Mg23	1.983	-0.687
116	H57	Mg24	2.003	-0.231

Table S15. IPCOHP of the Mg-H bond in the IS of Process 5 step 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.053	-0.585
2	H27	Mg1	1.999	-0.585
3	H30	Mg1	1.860	-1.003
4	H33	Mg1	1.999	-0.584
5	H36	Mg1	2.041	-0.593
6	H41	Mg1	1.869	-0.992
7	H26	Mg2	1.918	-0.790
8	H28	Mg2	1.931	-0.752
9	H31	Mg2	1.921	-0.754
10	H34	Mg2	1.931	-0.749
11	H37	Mg2	1.929	-0.721
12	H42	Mg2	1.946	-0.687
13	H29	Mg3	1.979	-0.813
14	H32	Mg3	1.817	-0.768
15	H35	Mg3	1.979	-0.801
16	H43	Mg3	1.909	-0.727
17	H27	Mg4	1.952	-0.758
18	H31	Mg4	1.840	-0.778
19	H33	Mg4	1.952	-0.763
20	H58	Mg4	1.935	-0.781
21	H63	Mg4	1.935	-0.777

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.874	-0.905
23	H28	Mg5	1.994	-0.681
24	H32	Mg5	1.907	-0.658
25	H34	Mg5	1.994	-0.680
26	H59	Mg5	1.965	-0.712
27	H64	Mg5	1.965	-0.709
28	H26	Mg6	1.965	-0.336
29	H29	Mg6	2.128	-0.411
30	H35	Mg6	2.128	-0.426
31	H36	Mg7	2.041	-0.598
32	H38	Mg7	1.999	-0.591
33	H41	Mg7	1.868	-0.982
34	H44	Mg7	1.999	-0.588
35	H47	Mg7	2.053	-0.586
36	H51	Mg7	1.860	-1.001
37	H37	Mg8	1.929	-0.665
38	H39	Mg8	1.931	-0.729
39	H42	Mg8	1.946	-0.685
40	H45	Mg8	1.931	-0.741
41	H48	Mg8	1.918	-0.764
42	H52	Mg8	1.921	-0.755
43	H40	Mg9	1.979	-0.588

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H43	Mg9	1.909	-0.590
45	H46	Mg9	2.160	-0.672
46	H53	Mg9	1.817	-0.661
47	H27	Mg10	1.943	-0.770
48	H33	Mg10	1.943	-0.766
49	H38	Mg10	1.943	-0.770
50	H42	Mg10	1.838	-0.754
51	H44	Mg10	1.943	-0.771
52	H28	Mg11	1.948	-0.743
53	H34	Mg11	1.948	-0.746
54	H36	Mg11	1.878	-0.839
55	H39	Mg11	1.948	-0.755
56	H43	Mg11	2.076	-0.536
57	H45	Mg11	1.948	-0.744
58	H29	Mg12	1.953	-0.659
59	H35	Mg12	1.953	-0.715
60	H37	Mg12	1.832	-0.635
61	H40	Mg12	1.952	-0.677
62	H47	Mg13	2.043	-0.601
63	H49	Mg13	1.995	-0.592
64	H51	Mg13	1.871	-0.962
65	H54	Mg13	1.995	-0.589

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H56	Mg13	2.064	-0.603
67	H60	Mg13	1.859	-0.999
68	H48	Mg14	1.959	-0.774
69	H50	Mg14	1.930	-0.738
70	H52	Mg14	2.016	-0.559
71	H55	Mg14	1.930	-0.734
72	H57	Mg14	1.919	-0.821
73	H61	Mg14	1.985	-0.604
74	H46	Mg15	2.092	-0.849
75	H53	Mg15	2.133	-0.410
76	H62	Mg15	1.981	-0.448
77	H38	Mg16	1.952	-0.763
78	H44	Mg16	1.952	-0.758
79	H49	Mg16	1.935	-0.780
80	H52	Mg16	1.840	-0.790
81	H54	Mg16	1.935	-0.776
82	H39	Mg17	1.993	-0.671
83	H45	Mg17	1.993	-0.665
84	H47	Mg17	1.874	-0.918
85	H50	Mg17	1.965	-0.702
86	H53	Mg17	1.906	-0.640
87	H55	Mg17	1.965	-0.705

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H40	Mg18	2.127	-0.311
89	H48	Mg18	1.965	-0.292
90	H25	Mg19	2.043	-0.600
91	H30	Mg19	1.871	-0.969
92	H56	Mg19	2.064	-0.604
93	H58	Mg19	1.995	-0.591
94	H60	Mg19	1.859	-0.998
95	H63	Mg19	1.995	-0.589
96	H26	Mg20	1.959	-0.730
97	H31	Mg20	2.016	-0.558
98	H57	Mg20	1.919	-0.847
99	H59	Mg20	1.930	-0.725
100	H61	Mg20	1.985	-0.594
101	H64	Mg20	1.930	-0.727
102	H32	Mg21	2.131	-0.145
103	H62	Mg21	1.980	-0.178
104	H49	Mg22	1.948	-0.774
105	H54	Mg22	1.948	-0.767
106	H58	Mg22	1.948	-0.767
107	H61	Mg22	1.837	-0.833
108	H63	Mg22	1.948	-0.768
109	H50	Mg23	1.983	-0.697

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H55	Mg23	1.983	-0.705
111	H56	Mg23	1.923	-0.821
112	H59	Mg23	1.983	-0.682
113	H62	Mg23	1.940	-0.696
114	H64	Mg23	1.983	-0.683
115	H57	Mg24	2.003	-0.208

Table S16. IPCOHP of the Mg-H bond in the IS of Process 6 step 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.036	-0.582
2	H27	Mg1	2.002	-0.578
3	H30	Mg1	1.861	-1.016
4	H33	Mg1	2.000	-0.579
5	H36	Mg1	2.036	-0.582
6	H40	Mg1	1.862	-1.011
7	H26	Mg2	1.909	-0.772
8	H28	Mg2	1.957	-0.735
9	H31	Mg2	1.935	-0.723
10	H34	Mg2	1.965	-0.725
11	H37	Mg2	1.909	-0.771
12	H41	Mg2	1.933	-0.725
13	H29	Mg3	1.984	-0.878
14	H32	Mg3	1.824	-0.930
15	H35	Mg3	2.009	-0.806
16	H42	Mg3	1.826	-0.928
17	H27	Mg4	1.947	-0.762
18	H31	Mg4	1.845	-0.791
19	H33	Mg4	1.948	-0.759
20	H56	Mg4	1.942	-0.778
21	H61	Mg4	1.941	-0.777

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.865	-0.922
23	H28	Mg5	1.985	-0.696
24	H32	Mg5	1.991	-0.549
25	H34	Mg5	1.993	-0.688
26	H57	Mg5	1.942	-0.737
27	H62	Mg5	1.942	-0.720
28	H26	Mg6	1.910	-0.354
29	H29	Mg6	2.103	-0.443
30	H35	Mg6	2.070	-0.471
31	H36	Mg7	2.061	-0.568
32	H38	Mg7	1.998	-0.590
33	H40	Mg7	1.866	-1.002
34	H43	Mg7	1.999	-0.591
35	H45	Mg7	2.042	-0.593
36	H49	Mg7	1.861	-1.006
37	H37	Mg8	1.938	-0.710
38	H39	Mg8	1.933	-0.708
39	H41	Mg8	2.000	-0.582
40	H44	Mg8	1.932	-0.714
41	H46	Mg8	1.906	-0.843
42	H50	Mg8	1.962	-0.624
43	H42	Mg9	2.012	-0.248

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H51	Mg9	1.955	-0.199
45	H27	Mg10	1.947	-0.763
46	H33	Mg10	1.948	-0.759
47	H38	Mg10	1.942	-0.778
48	H41	Mg10	1.845	-0.792
49	H43	Mg10	1.941	-0.776
50	H28	Mg11	1.982	-0.698
51	H34	Mg11	1.994	-0.684
52	H36	Mg11	1.866	-0.924
53	H39	Mg11	1.941	-0.737
54	H42	Mg11	1.992	-0.546
55	H44	Mg11	1.942	-0.724
56	H29	Mg12	2.092	-0.448
57	H35	Mg12	2.082	-0.468
58	H37	Mg12	1.911	-0.352
59	H45	Mg13	2.047	-0.578
60	H47	Mg13	1.997	-0.588
61	H49	Mg13	1.868	-1.004
62	H52	Mg13	1.998	-0.589
63	H54	Mg13	2.050	-0.581
64	H58	Mg13	1.866	-0.998
65	H46	Mg14	1.920	-0.816

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H48	Mg14	1.937	-0.724
67	H50	Mg14	1.996	-0.579
68	H53	Mg14	1.937	-0.729
69	H55	Mg14	1.920	-0.814
70	H59	Mg14	1.995	-0.583
71	H51	Mg15	1.939	-0.315
72	H60	Mg15	1.937	-0.313
73	H38	Mg16	1.953	-0.763
74	H43	Mg16	1.954	-0.758
75	H47	Mg16	1.945	-0.767
76	H50	Mg16	1.833	-0.813
77	H52	Mg16	1.945	-0.772
78	H39	Mg17	1.987	-0.668
79	H44	Mg17	1.988	-0.672
80	H45	Mg17	1.886	-0.875
81	H48	Mg17	1.965	-0.706
82	H51	Mg17	1.906	-0.671
83	H53	Mg17	1.967	-0.711
84	H46	Mg18	2.008	-0.222
85	H25	Mg19	2.062	-0.567
86	H30	Mg19	1.866	-0.995
87	H54	Mg19	2.040	-0.589

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H56	Mg19	1.998	-0.590
89	H58	Mg19	1.862	-1.013
90	H61	Mg19	1.998	-0.591
91	H26	Mg20	1.939	-0.708
92	H31	Mg20	1.998	-0.586
93	H55	Mg20	1.906	-0.844
94	H57	Mg20	1.932	-0.709
95	H59	Mg20	1.961	-0.624
96	H62	Mg20	1.932	-0.713
97	H32	Mg21	2.014	-0.249
98	H60	Mg21	1.957	-0.195
99	H47	Mg22	1.945	-0.764
100	H52	Mg22	1.944	-0.775
101	H56	Mg22	1.953	-0.765
102	H59	Mg22	1.833	-0.811
103	H61	Mg22	1.954	-0.755
104	H48	Mg23	1.967	-0.704
105	H53	Mg23	1.966	-0.708
106	H54	Mg23	1.885	-0.873
107	H57	Mg23	1.985	-0.673
108	H60	Mg23	1.906	-0.674
109	H62	Mg23	1.988	-0.672

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
110	H55	Mg24	2.008	-0.221

Table S17. IPCOHP of the Mg-H bond in the IS of Process 6 step 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.052	-0.593
2	H27	Mg1	1.999	-0.585
3	H30	Mg1	1.867	-0.980
4	H33	Mg1	1.998	-0.578
5	H36	Mg1	2.049	-0.605
6	H40	Mg1	1.867	-0.984
7	H26	Mg2	1.923	-0.760
8	H28	Mg2	1.943	-0.758
9	H31	Mg2	1.946	-0.688
10	H34	Mg2	1.932	-0.718
11	H37	Mg2	1.903	-0.766
12	H41	Mg2	1.949	-0.679
13	H29	Mg3	2.058	-0.486
14	H32	Mg3	1.941	-0.552
15	H35	Mg3	1.981	-0.717
16	H42	Mg3	1.974	-0.498
17	H27	Mg4	1.945	-0.770
18	H31	Mg4	1.841	-0.778
19	H33	Mg4	1.942	-0.765
20	H56	Mg4	1.943	-0.769
21	H61	Mg4	1.941	-0.768

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H25	Mg5	1.886	-0.862
23	H28	Mg5	1.966	-0.742
24	H32	Mg5	1.984	-0.607
25	H34	Mg5	1.953	-0.708
26	H57	Mg5	1.979	-0.709
27	H62	Mg5	1.965	-0.690
28	H26	Mg6	1.926	-0.312
29	H29	Mg6	1.952	-0.452
30	H36	Mg7	2.060	-0.587
31	H38	Mg7	1.999	-0.586
32	H40	Mg7	1.864	-0.993
33	H43	Mg7	1.998	-0.585
34	H45	Mg7	2.044	-0.588
35	H49	Mg7	1.867	-0.985
36	H37	Mg8	1.938	-0.730
37	H39	Mg8	1.933	-0.735
38	H41	Mg8	1.976	-0.613
39	H44	Mg8	1.928	-0.728
40	H46	Mg8	1.932	-0.805
41	H50	Mg8	1.959	-0.632
42	H35	Mg9	1.937	-0.793
43	H42	Mg9	2.122	-0.334

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H51	Mg9	1.913	-0.461
45	H27	Mg10	1.948	-0.762
46	H33	Mg10	1.944	-0.761
47	H38	Mg10	1.944	-0.769
48	H41	Mg10	1.833	-0.779
49	H43	Mg10	1.942	-0.768
50	H28	Mg11	1.991	-0.692
51	H34	Mg11	1.968	-0.679
52	H36	Mg11	1.894	-0.862
53	H39	Mg11	1.974	-0.688
54	H42	Mg11	1.915	-0.713
55	H44	Mg11	1.969	-0.681
56	H29	Mg12	1.974	-0.496
57	H37	Mg12	1.931	-0.337
58	H45	Mg13	2.041	-0.593
59	H47	Mg13	1.998	-0.586
60	H49	Mg13	1.864	-0.992
61	H52	Mg13	1.997	-0.586
62	H54	Mg13	2.056	-0.581
63	H58	Mg13	1.862	-0.994
64	H46	Mg14	1.921	-0.810
65	H48	Mg14	1.935	-0.709

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H50	Mg14	1.983	-0.603
67	H53	Mg14	1.936	-0.729
68	H55	Mg14	1.937	-0.785
69	H59	Mg14	1.982	-0.612
70	H51	Mg15	1.968	-0.192
71	H60	Mg15	1.926	-0.339
72	H38	Mg16	1.946	-0.768
73	H43	Mg16	1.945	-0.766
74	H47	Mg16	1.947	-0.767
75	H50	Mg16	1.839	-0.797
76	H52	Mg16	1.945	-0.765
77	H39	Mg17	1.973	-0.709
78	H44	Mg17	1.963	-0.707
79	H45	Mg17	1.878	-0.887
80	H48	Mg17	1.977	-0.692
81	H51	Mg17	1.931	-0.619
82	H53	Mg17	1.975	-0.694
83	H46	Mg18	1.991	-0.237
84	H25	Mg19	2.052	-0.587
85	H30	Mg19	1.863	-0.993
86	H54	Mg19	2.042	-0.594
87	H56	Mg19	1.999	-0.585

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H58	Mg19	1.864	-0.992
89	H61	Mg19	1.998	-0.581
90	H26	Mg20	1.931	-0.737
91	H31	Mg20	1.972	-0.636
92	H55	Mg20	1.923	-0.800
93	H57	Mg20	1.946	-0.724
94	H59	Mg20	1.957	-0.660
95	H62	Mg20	1.927	-0.725
96	H32	Mg21	1.996	-0.276
97	H60	Mg21	1.928	-0.352
98	H47	Mg22	1.946	-0.769
99	H52	Mg22	1.944	-0.774
100	H56	Mg22	1.948	-0.765
101	H59	Mg22	1.844	-0.803
102	H61	Mg22	1.945	-0.769
103	H48	Mg23	1.953	-0.723
104	H53	Mg23	1.966	-0.722
105	H54	Mg23	1.879	-0.885
106	H57	Mg23	1.985	-0.700
107	H60	Mg23	1.983	-0.580
108	H62	Mg23	1.959	-0.720
109	H55	Mg24	1.987	-0.232

Table S18. IPCOHP of Mg-H bond in tHe IS of Process 8 step 1.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.035	-0.516
2	H27	Mg1	2.011	-0.573
3	H29	Mg1	1.865	-1.028
4	H32	Mg1	2.008	-0.567
5	H34	Mg1	2.033	-0.521
6	H38	Mg1	1.866	-1.025
7	H28	Mg2	1.948	-0.368
8	H30	Mg2	1.964	-0.363
9	H33	Mg2	2.029	-0.428
10	H39	Mg2	1.961	-0.359
11	H26	Mg3	2.084	-0.410
12	H31	Mg3	2.234	-0.313
13	H27	Mg4	1.953	-0.767
14	H30	Mg4	1.884	-0.811
15	H32	Mg4	1.950	-0.779
16	H54	Mg4	1.949	-0.769
17	H59	Mg4	1.952	-0.777
18	H25	Mg5	1.864	-0.703
19	H28	Mg5	1.941	-0.580
20	H33	Mg5	1.978	-0.667
21	H55	Mg5	1.991	-0.676

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H60	Mg5	1.945	-0.585
23	H26	Mg6	2.036	-0.584
24	H31	Mg6	2.018	-0.623
25	H53	Mg6	2.008	-0.636
26	H58	Mg6	2.041	-0.578
27	H34	Mg7	2.026	-0.515
28	H36	Mg7	2.004	-0.566
29	H38	Mg7	1.867	-1.030
30	H41	Mg7	2.012	-0.571
31	H43	Mg7	2.035	-0.518
32	H47	Mg7	1.865	-1.028
33	H37	Mg8	2.042	-0.429
34	H39	Mg8	1.960	-0.367
35	H42	Mg8	1.948	-0.376
36	H48	Mg8	1.963	-0.364
37	H40	Mg9	2.022	-0.448
38	H27	Mg10	1.954	-0.767
39	H32	Mg10	1.949	-0.777
40	H36	Mg10	1.948	-0.773
41	H39	Mg10	1.882	-0.809
42	H41	Mg10	1.954	-0.772
43	H28	Mg11	1.945	-0.577

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H33	Mg11	1.977	-0.668
45	H34	Mg11	1.863	-0.706
46	H37	Mg11	1.986	-0.664
47	H42	Mg11	1.945	-0.587
48	H26	Mg12	2.021	-0.600
49	H31	Mg12	2.039	-0.595
50	H35	Mg12	2.004	-0.642
51	H40	Mg12	2.043	-0.556
52	H43	Mg13	2.031	-0.517
53	H45	Mg13	2.009	-0.566
54	H47	Mg13	1.865	-1.030
55	H50	Mg13	2.007	-0.572
56	H52	Mg13	2.033	-0.514
57	H56	Mg13	1.865	-1.036
58	H46	Mg14	1.945	-0.371
59	H48	Mg14	1.961	-0.365
60	H51	Mg14	2.043	-0.435
61	H57	Mg14	1.964	-0.367
62	H44	Mg15	2.012	-0.451
63	H36	Mg16	1.949	-0.773
64	H41	Mg16	1.952	-0.775
65	H45	Mg16	1.950	-0.770

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H48	Mg16	1.884	-0.813
67	H50	Mg16	1.951	-0.775
68	H37	Mg17	1.982	-0.668
69	H42	Mg17	1.944	-0.584
70	H43	Mg17	1.865	-0.711
71	H46	Mg17	1.943	-0.581
72	H51	Mg17	1.986	-0.675
73	H35	Mg18	2.022	-0.629
74	H40	Mg18	2.023	-0.585
75	H44	Mg18	2.020	-0.576
76	H49	Mg18	2.023	-0.627
77	H25	Mg19	2.028	-0.517
78	H29	Mg19	1.867	-1.028
79	H52	Mg19	2.034	-0.521
80	H54	Mg19	2.004	-0.568
81	H56	Mg19	1.864	-1.027
82	H59	Mg19	2.013	-0.567
83	H30	Mg20	1.960	-0.368
84	H55	Mg20	2.053	-0.436
85	H57	Mg20	1.963	-0.364
86	H60	Mg20	1.949	-0.370
87	H53	Mg21	2.269	-0.301

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H58	Mg21	2.062	-0.434
89	H45	Mg22	1.948	-0.771
90	H50	Mg22	1.952	-0.775
91	H54	Mg22	1.950	-0.772
92	H57	Mg22	1.884	-0.812
93	H59	Mg22	1.950	-0.776
94	H46	Mg23	1.939	-0.587
95	H51	Mg23	1.988	-0.668
96	H52	Mg23	1.864	-0.711
97	H55	Mg23	1.987	-0.683
98	H60	Mg23	1.944	-0.583
99	H44	Mg24	2.038	-0.552
100	H49	Mg24	2.003	-0.654
101	H53	Mg24	2.027	-0.621
102	H58	Mg24	2.025	-0.602

Table S19. IPCOHP of the Mg-H bond in the IS of Process 8 step 2.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.035	-0.527
2	H26	Mg1	2.011	-0.571
3	H28	Mg1	1.865	-1.020
4	H30	Mg1	2.008	-0.570
5	H32	Mg1	2.033	-0.521
6	H36	Mg1	1.866	-1.027
7	H27	Mg2	1.948	-0.464
8	H29	Mg2	1.964	-0.385
9	H31	Mg2	2.029	-0.447
10	H37	Mg2	1.961	-0.380
11	H26	Mg4	1.953	-0.771
12	H29	Mg4	1.884	-0.794
13	H30	Mg4	1.950	-0.787
14	H52	Mg4	1.949	-0.774
15	H57	Mg4	1.952	-0.776
16	H25	Mg5	1.864	-0.679
17	H27	Mg5	1.941	-0.628
18	H31	Mg5	1.978	-0.685
19	H53	Mg5	1.991	-0.671
20	H58	Mg5	1.945	-0.577
21	H51	Mg6	2.001	-0.502

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H56	Mg6	2.029	-0.466
23	H32	Mg7	2.026	-0.516
24	H34	Mg7	2.004	-0.571
25	H36	Mg7	1.867	-1.028
26	H39	Mg7	2.012	-0.574
27	H41	Mg7	2.035	-0.520
28	H45	Mg7	1.865	-1.033
29	H35	Mg8	2.042	-0.389
30	H37	Mg8	1.960	-0.345
31	H40	Mg8	1.948	-0.341
32	H46	Mg8	1.963	-0.331
33	H38	Mg9	2.046	-0.403
34	H26	Mg10	1.954	-0.772
35	H30	Mg10	1.949	-0.783
36	H34	Mg10	1.948	-0.777
37	H37	Mg10	1.882	-0.793
38	H39	Mg10	1.954	-0.772
39	H27	Mg11	1.945	-0.624
40	H31	Mg11	1.977	-0.685
41	H32	Mg11	1.863	-0.679
42	H35	Mg11	1.986	-0.657
43	H40	Mg11	1.945	-0.577

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H33	Mg12	1.993	-0.506
45	H38	Mg12	2.027	-0.457
46	H41	Mg13	2.031	-0.516
47	H43	Mg13	2.009	-0.562
48	H45	Mg13	1.865	-1.022
49	H48	Mg13	2.007	-0.569
50	H50	Mg13	2.033	-0.520
51	H54	Mg13	1.865	-1.022
52	H44	Mg14	1.945	-0.386
53	H46	Mg14	1.961	-0.370
54	H49	Mg14	2.043	-0.450
55	H55	Mg14	1.964	-0.373
56	H42	Mg15	2.011	-0.434
57	H34	Mg16	1.949	-0.773
58	H39	Mg16	1.952	-0.772
59	H43	Mg16	1.950	-0.768
60	H46	Mg16	1.884	-0.806
61	H48	Mg16	1.951	-0.776
62	H35	Mg17	1.982	-0.655
63	H40	Mg17	1.944	-0.573
64	H41	Mg17	1.865	-0.710
65	H44	Mg17	1.943	-0.580

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H49	Mg17	1.986	-0.666
67	H33	Mg18	2.030	-0.640
68	H38	Mg18	2.051	-0.570
69	H42	Mg18	2.022	-0.566
70	H47	Mg18	2.014	-0.634
71	H25	Mg19	2.028	-0.511
72	H28	Mg19	1.867	-1.039
73	H50	Mg19	2.034	-0.516
74	H52	Mg19	2.004	-0.572
75	H54	Mg19	1.864	-1.041
76	H57	Mg19	2.013	-0.570
77	H29	Mg20	1.960	-0.343
78	H53	Mg20	2.053	-0.399
79	H55	Mg20	1.963	-0.329
80	H58	Mg20	1.949	-0.337
81	H51	Mg21	2.264	-0.289
82	H56	Mg21	2.082	-0.389
83	H43	Mg22	1.948	-0.772
84	H48	Mg22	1.952	-0.776
85	H52	Mg22	1.950	-0.767
86	H55	Mg22	1.884	-0.805
87	H57	Mg22	1.950	-0.775

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H44	Mg23	1.939	-0.584
89	H49	Mg23	1.988	-0.663
90	H50	Mg23	1.864	-0.710
91	H53	Mg23	1.987	-0.671
92	H58	Mg23	1.944	-0.573
93	H42	Mg24	2.035	-0.553
94	H47	Mg24	2.005	-0.656
95	H51	Mg24	2.030	-0.635

Table S20. IPCOHP of the Mg-H bond in the IS of Process 8 step 3.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.035	-0.523
2	H26	Mg1	2.011	-0.566
3	H28	Mg1	1.865	-1.015
4	H30	Mg1	2.008	-0.564
5	H32	Mg1	2.033	-0.522
6	H36	Mg1	1.866	-1.016
7	H27	Mg2	1.948	-0.476
8	H29	Mg2	1.964	-0.389
9	H31	Mg2	2.029	-0.454
10	H37	Mg2	1.961	-0.385
11	H26	Mg4	1.953	-0.773
12	H29	Mg4	1.884	-0.785
13	H30	Mg4	1.950	-0.785
14	H50	Mg4	1.949	-0.771
15	H55	Mg4	1.952	-0.776
16	H25	Mg5	1.864	-0.678
17	H27	Mg5	1.941	-0.629
18	H31	Mg5	1.978	-0.688
19	H51	Mg5	1.991	-0.655
20	H56	Mg5	1.945	-0.568
21	H49	Mg6	2.005	-0.484

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H54	Mg6	2.057	-0.458
23	H32	Mg7	2.026	-0.518
24	H34	Mg7	2.004	-0.572
25	H36	Mg7	1.867	-1.029
26	H39	Mg7	2.012	-0.573
27	H41	Mg7	2.035	-0.517
28	H44	Mg7	1.865	-1.026
29	H35	Mg8	2.042	-0.331
30	H37	Mg8	1.960	-0.293
31	H40	Mg8	1.948	-0.297
32	H45	Mg8	1.963	-0.284
33	H33	Mg9	2.278	-0.249
34	H38	Mg9	2.067	-0.355
35	H26	Mg10	1.954	-0.771
36	H30	Mg10	1.949	-0.786
37	H34	Mg10	1.948	-0.775
38	H37	Mg10	1.882	-0.784
39	H39	Mg10	1.954	-0.770
40	H27	Mg11	1.945	-0.627
41	H31	Mg11	1.977	-0.687
42	H32	Mg11	1.863	-0.677
43	H35	Mg11	1.986	-0.642

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H40	Mg11	1.945	-0.568
45	H33	Mg12	1.998	-0.495
46	H38	Mg12	2.052	-0.443
47	H41	Mg13	2.031	-0.522
48	H42	Mg13	2.009	-0.559
49	H44	Mg13	1.865	-1.020
50	H46	Mg13	2.007	-0.570
51	H48	Mg13	2.033	-0.526
52	H52	Mg13	1.865	-1.016
53	H43	Mg14	1.945	-0.478
54	H45	Mg14	1.961	-0.395
55	H47	Mg14	2.043	-0.459
56	H53	Mg14	1.964	-0.395
57	H34	Mg16	1.949	-0.775
58	H39	Mg16	1.952	-0.774
59	H42	Mg16	1.950	-0.773
60	H45	Mg16	1.884	-0.786
61	H46	Mg16	1.951	-0.784
62	H35	Mg17	1.982	-0.647
63	H40	Mg17	1.944	-0.566
64	H41	Mg17	1.865	-0.683
65	H43	Mg17	1.943	-0.626

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H47	Mg17	1.986	-0.692
67	H33	Mg18	2.020	-0.482
68	H38	Mg18	2.027	-0.470
69	H25	Mg19	2.028	-0.517
70	H28	Mg19	1.867	-1.031
71	H48	Mg19	2.034	-0.514
72	H50	Mg19	2.004	-0.575
73	H52	Mg19	1.864	-1.035
74	H55	Mg19	2.013	-0.570
75	H29	Mg20	1.960	-0.290
76	H51	Mg20	2.053	-0.343
77	H53	Mg20	1.963	-0.288
78	H56	Mg20	1.949	-0.293
79	H49	Mg21	2.213	-0.281
80	H54	Mg21	2.114	-0.337
81	H42	Mg22	1.948	-0.776
82	H46	Mg22	1.952	-0.783
83	H50	Mg22	1.950	-0.773
84	H53	Mg22	1.884	-0.787
85	H55	Mg22	1.950	-0.774
86	H43	Mg23	1.939	-0.633
87	H47	Mg23	1.988	-0.692

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
88	H48	Mg23	1.864	-0.685
89	H51	Mg23	1.987	-0.663
90	H56	Mg23	1.944	-0.564
91	H49	Mg24	2.021	-0.470
92	H54	Mg24	2.020	-0.482

Table S21. IPCOHP of the Mg-H bond in the IS of Process 8 step 4.

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
1	H25	Mg1	2.035	-0.527
2	H26	Mg1	2.011	-0.572
3	H28	Mg1	1.865	-1.017
4	H30	Mg1	2.008	-0.569
5	H32	Mg1	2.033	-0.528
6	H36	Mg1	1.866	-1.016
7	H27	Mg2	1.948	-0.426
8	H29	Mg2	1.964	-0.358
9	H31	Mg2	2.029	-0.417
10	H37	Mg2	1.961	-0.355
11	H26	Mg4	1.953	-0.777
12	H29	Mg4	1.884	-0.782
13	H30	Mg4	1.950	-0.787
14	H49	Mg4	1.949	-0.776
15	H53	Mg4	1.952	-0.783
16	H25	Mg5	1.864	-0.653
17	H27	Mg5	1.941	-0.609
18	H31	Mg5	1.978	-0.676
19	H50	Mg5	1.991	-0.693
20	H54	Mg5	1.945	-0.601
21	H32	Mg7	2.026	-0.521

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
22	H34	Mg7	2.004	-0.572
23	H36	Mg7	1.867	-1.026
24	H39	Mg7	2.012	-0.575
25	H41	Mg7	2.035	-0.518
26	H44	Mg7	1.865	-1.025
27	H35	Mg8	2.042	-0.356
28	H37	Mg8	1.960	-0.303
29	H40	Mg8	1.948	-0.321
30	H45	Mg8	1.963	-0.294
31	H33	Mg9	2.258	-0.253
32	H38	Mg9	2.066	-0.343
33	H26	Mg10	1.954	-0.772
34	H30	Mg10	1.949	-0.784
35	H34	Mg10	1.948	-0.778
36	H37	Mg10	1.882	-0.786
37	H39	Mg10	1.954	-0.772
38	H27	Mg11	1.945	-0.616
39	H31	Mg11	1.977	-0.685
40	H32	Mg11	1.863	-0.680
41	H35	Mg11	1.986	-0.634
42	H40	Mg11	1.945	-0.562
43	H33	Mg12	1.996	-0.473

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
44	H38	Mg12	2.041	-0.424
45	H41	Mg13	2.031	-0.527
46	H42	Mg13	2.009	-0.565
47	H44	Mg13	1.865	-1.024
48	H46	Mg13	2.007	-0.575
49	H48	Mg13	2.033	-0.527
50	H51	Mg13	1.865	-1.025
51	H43	Mg14	1.945	-0.427
52	H45	Mg14	1.961	-0.366
53	H47	Mg14	2.043	-0.421
54	H52	Mg14	1.964	-0.365
55	H34	Mg16	1.949	-0.777
56	H39	Mg16	1.952	-0.775
57	H42	Mg16	1.950	-0.772
58	H45	Mg16	1.884	-0.790
59	H46	Mg16	1.951	-0.785
60	H35	Mg17	1.982	-0.636
61	H40	Mg17	1.944	-0.559
62	H41	Mg17	1.865	-0.689
63	H43	Mg17	1.943	-0.617
64	H47	Mg17	1.986	-0.691
65	H33	Mg18	2.015	-0.464

No.	Atom H	Atom Mg	Distance (Å)	IPCOHP (arb. units)
66	H38	Mg18	2.025	-0.443
67	H25	Mg19	2.028	-0.533
68	H28	Mg19	1.867	-1.027
69	H48	Mg19	2.034	-0.532
70	H49	Mg19	2.004	-0.578
71	H51	Mg19	1.864	-1.025
72	H53	Mg19	2.013	-0.575
73	H29	Mg20	1.960	-0.304
74	H50	Mg20	2.053	-0.348
75	H52	Mg20	1.963	-0.302
76	H54	Mg20	1.949	-0.330
77	H42	Mg22	1.948	-0.780
78	H46	Mg22	1.952	-0.783
79	H49	Mg22	1.950	-0.778
80	H52	Mg22	1.884	-0.783
81	H53	Mg22	1.950	-0.785
82	H43	Mg23	1.939	-0.611
83	H47	Mg23	1.988	-0.681
84	H48	Mg23	1.864	-0.659
85	H50	Mg23	1.987	-0.703
86	H54	Mg23	1.944	-0.597

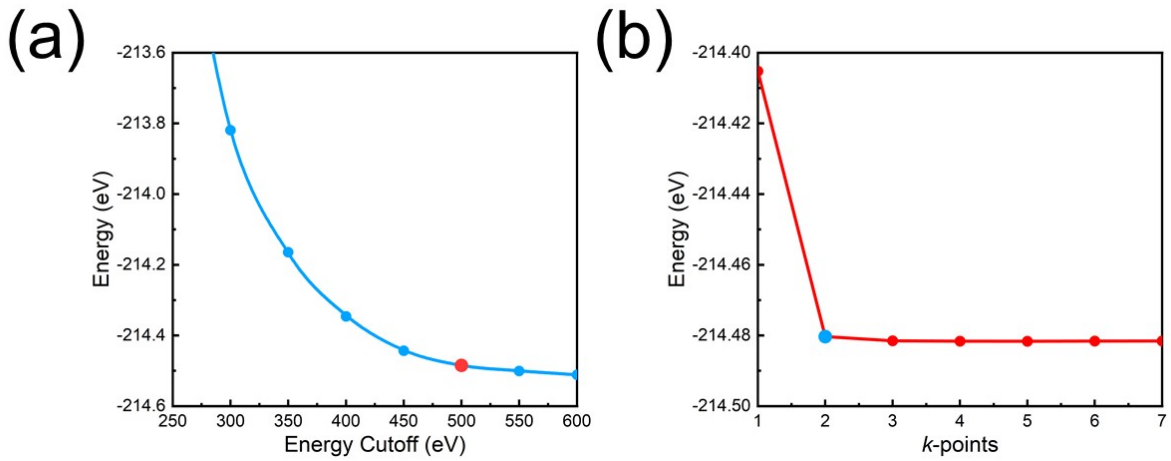

Figure S1. Convergence tests of the calculation settings of (a) energy cutoff and (b) *k*-points. The points with the color different from others are the *k*-points and energy cutoff selected for this study.

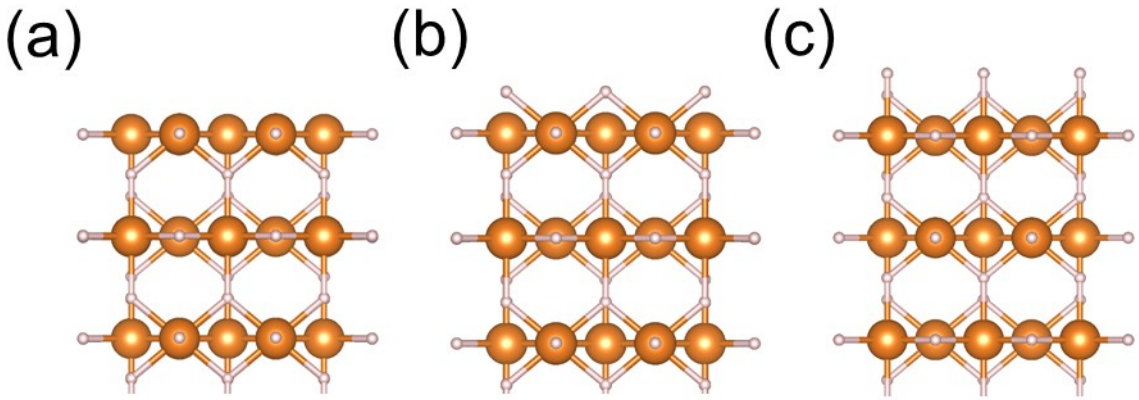

Figure S2. The three MgH_2(110) surfaces considered for surface energy calculations. (a) MgH_2(110-1). (b) MgH_2(110-2). (c) MgH_2(110-3).

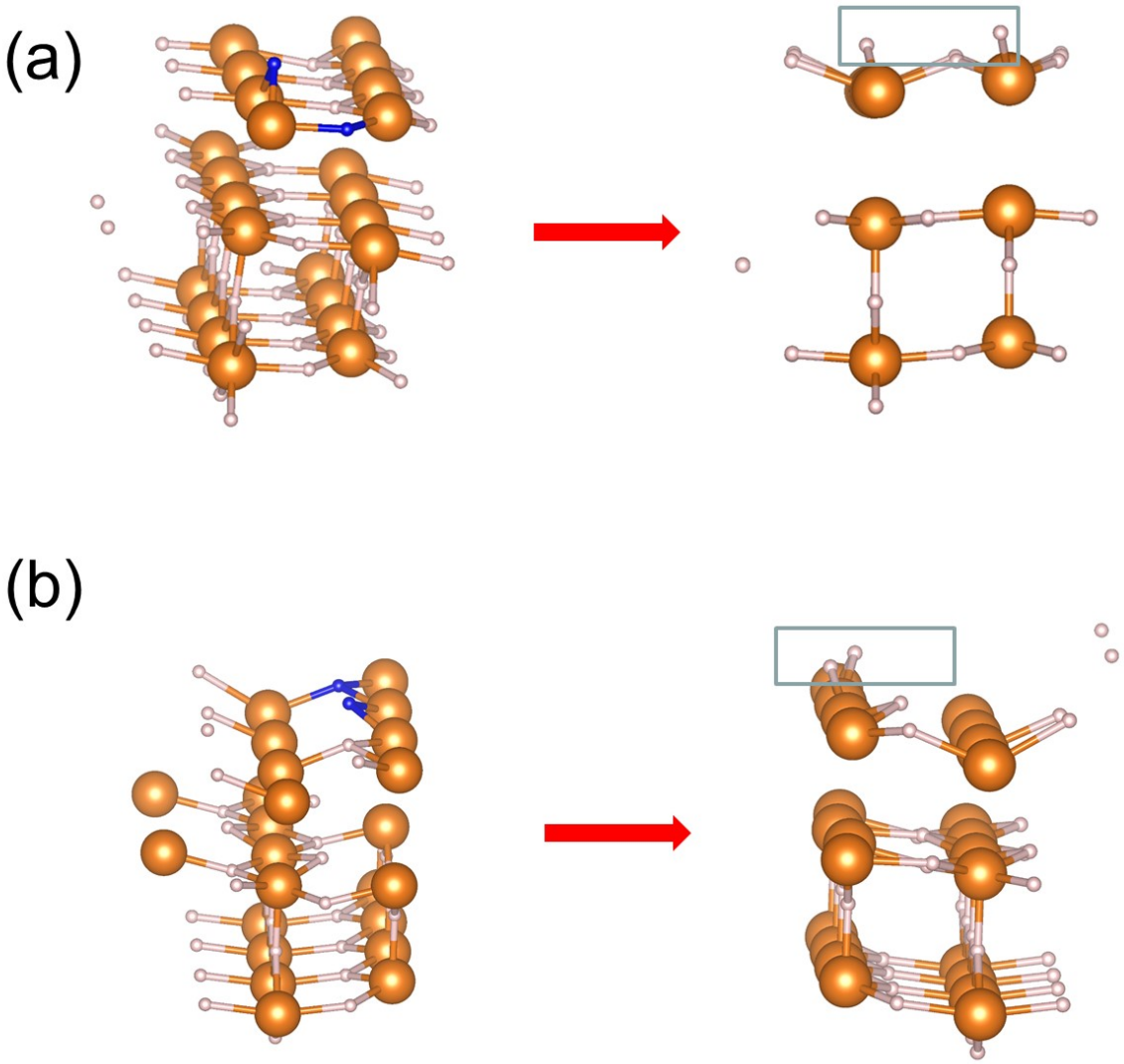

Figure S3. (a) On the left is the ideal structure for SBH migration to FBH, and on the right is the structure after relaxation. (b) The blue sphere on the left is H before H_2 formation, and the relaxation structure after H_2 formation is on the right.

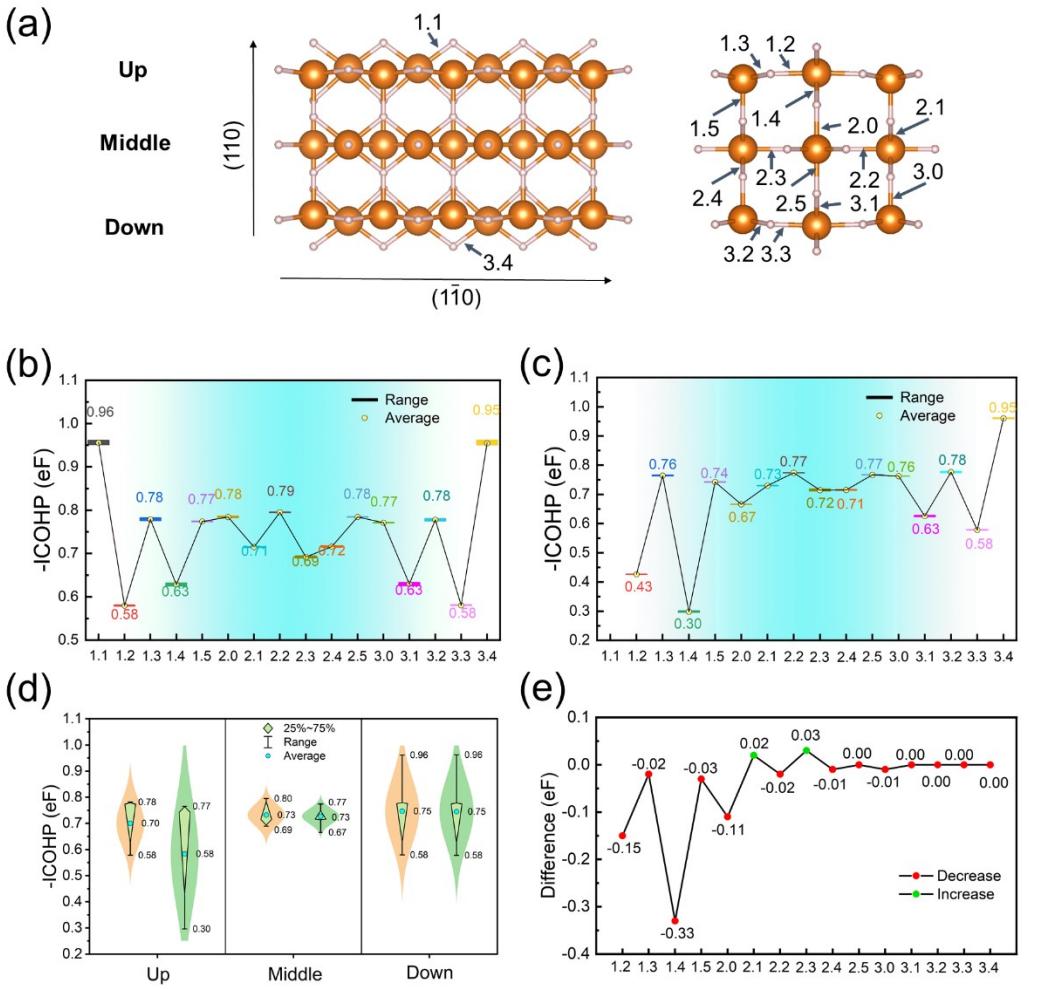

Figure S4. (a) Numbering of Mg-H bonds according to the position and number of layers. (b, c) Mg-H bonding strength before and after dehydrogenation of FBHs. (d) Comparative violin plot of the bond strength of the three Mg-H layers. The orange and green points represent the bond strength distribution before and after the dehydrogenation of FBHs, respectively. (e) The difference in Mg-H bond strength before and after the dehydrogenation of FBHs.

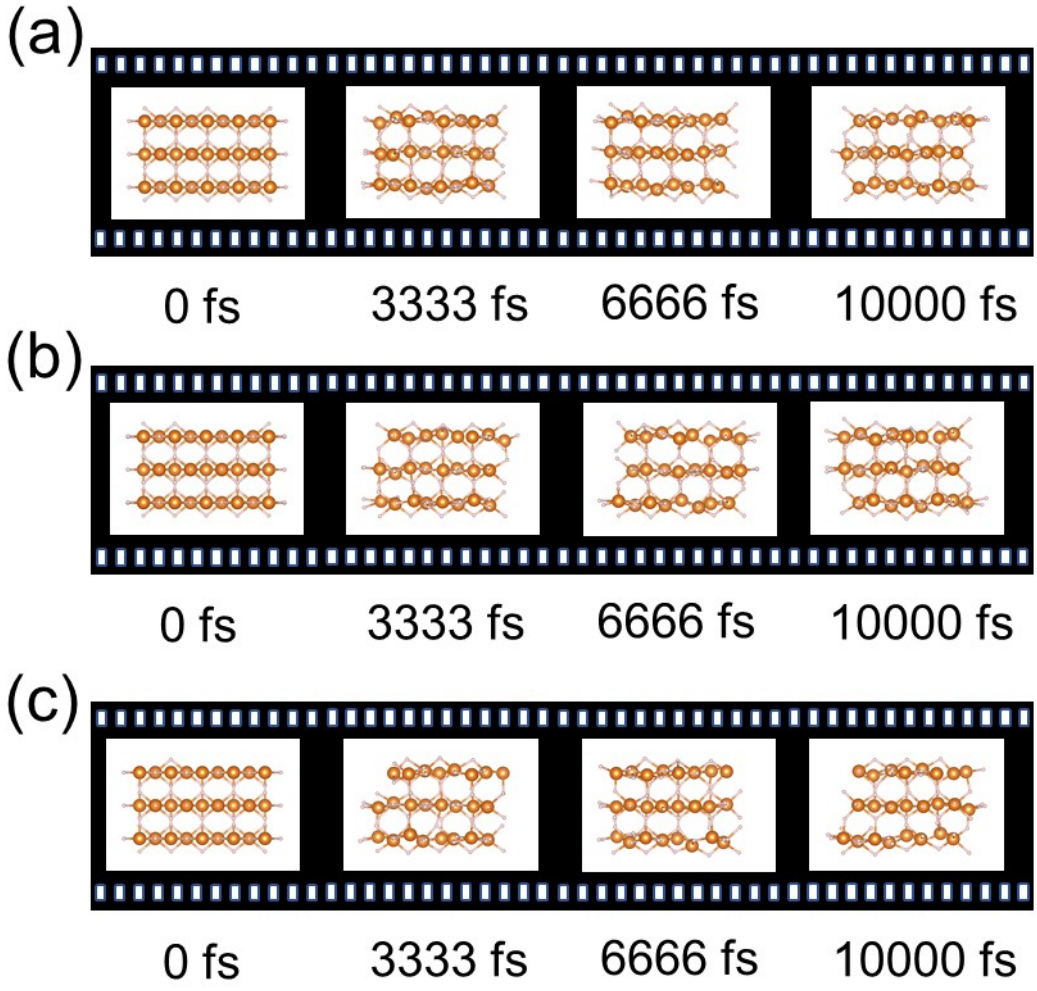

Figure S5. (a) Structural changes of MgH_2 at 500 K with 25% surface H defect within 10ps. (b) Structural changes of MgH_2 at 500 K with 50% surface H defect within 10ps. (c) Structural changes of MgH_2 at 500 K with 75% surface H defect within 10ps. White and orange spheres represent H and Mg, respectively.

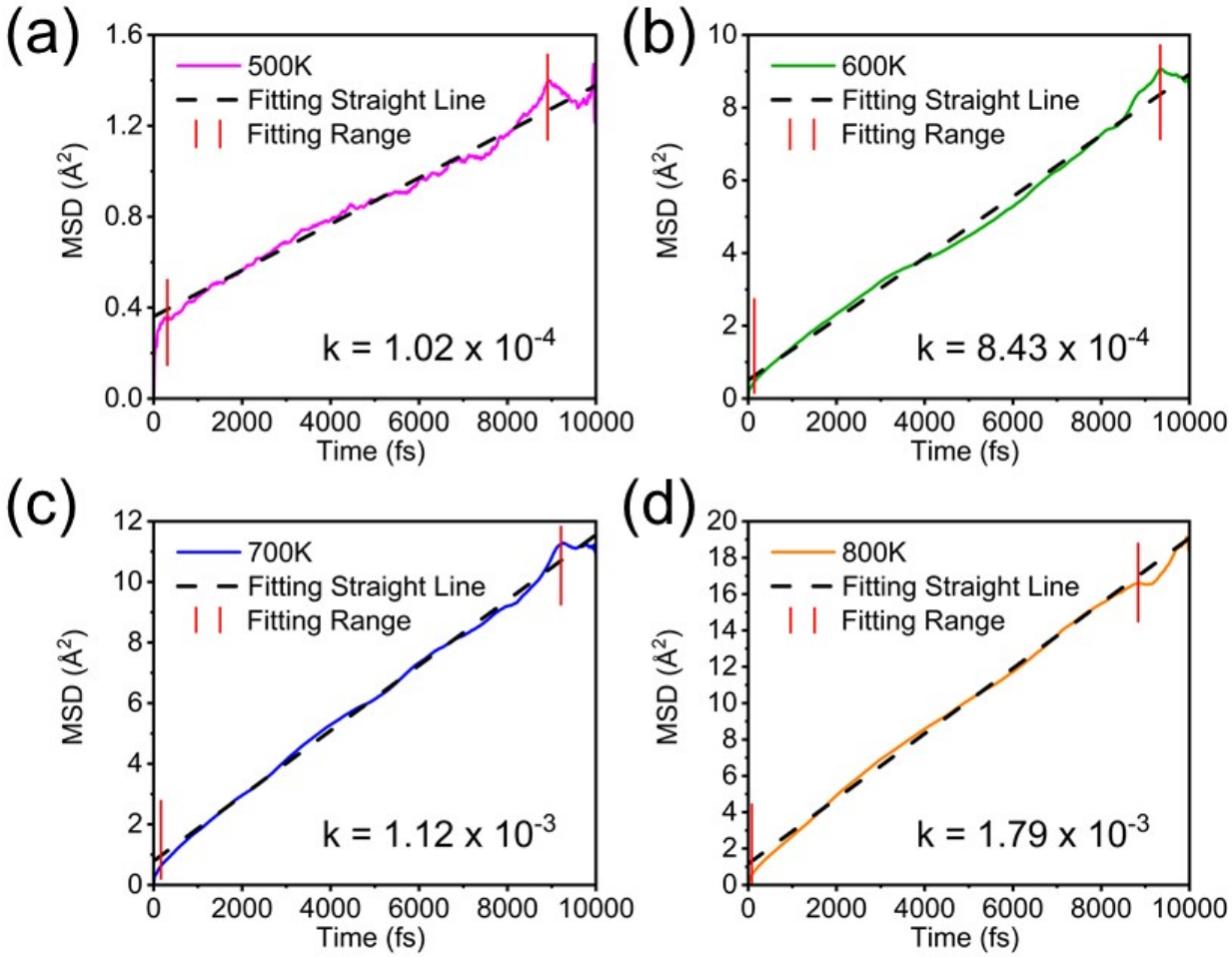

Figure S6. Linear fitting of H diffusion curves at 500K(a), 600K(b), 700K(c), and 800K(d).