Supplementary Information

Incorporating Magnesium and Calcium Cations in Porous Organic Frameworks for High-Capacity Hydrogen Storage

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Table S1. The total and increment hydrogen binding energies (in kJ/mol) of $C_6H_4O_2Mg$ and $C_6H_4O_2Ca$ with hydrogen molecules calculated at the RIMP2/def2-TZVPP level of theory with BSSE corrections.

n (H_2)	$C_6H_4O_2Mg$			$C_6H_4O_2Ca$		
	Total	Ave	Incr.	Total	Ave	Incr.
1	22.74	22.74	-	13.33	13.33	-
2	41.82	20.91	19.09	31.15	15.57	17.82
3	54.93	18.31	13.11	44.12	14.71	12.97
4	64.71	16.18	9.77	52.74	13.18	8.62
5	70.49	14.10	5.78	57.92	11.58	5.18
6	75.91	12.65	5.42	72.25	12.04	14.33
7	80.32	11.47	4.41	77.15	11.02	4.91
8	84.04	10.51	3.72	82.51	10.31	5.36
9				88.73	9.86	6.22
10				95.05	9.51	6.32

Figure S1. RI-MP2/def2-TZVPP optimized structures of H_2 molecules bound to $C_6H_4O_2Mg$. The distances are labeled in Å

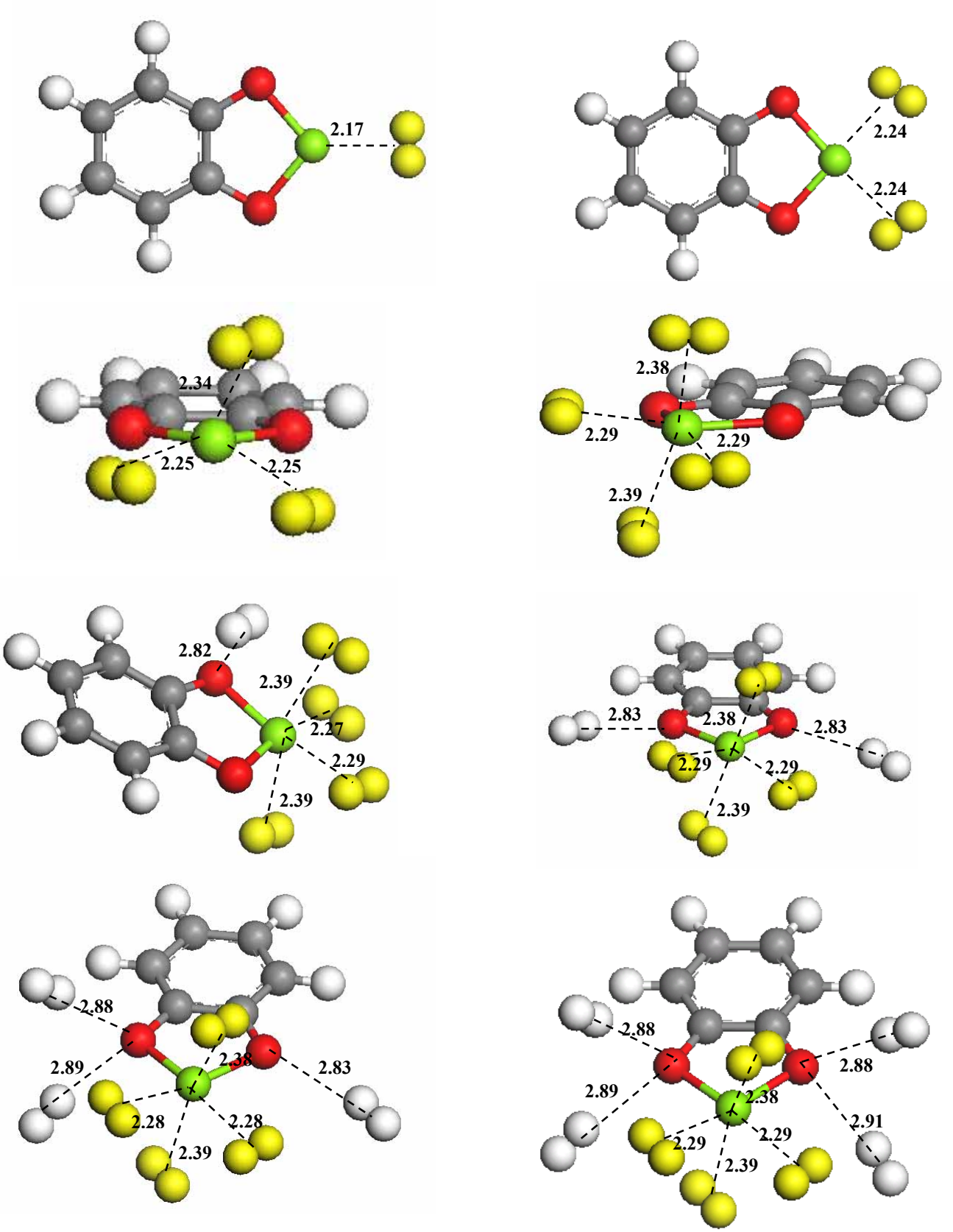

Figure S2. RI-MP2/def2-TZVPP optimized structures of H_2 molecules bound to $C_6H_4O_2Ca$. The distances are labeled in Å

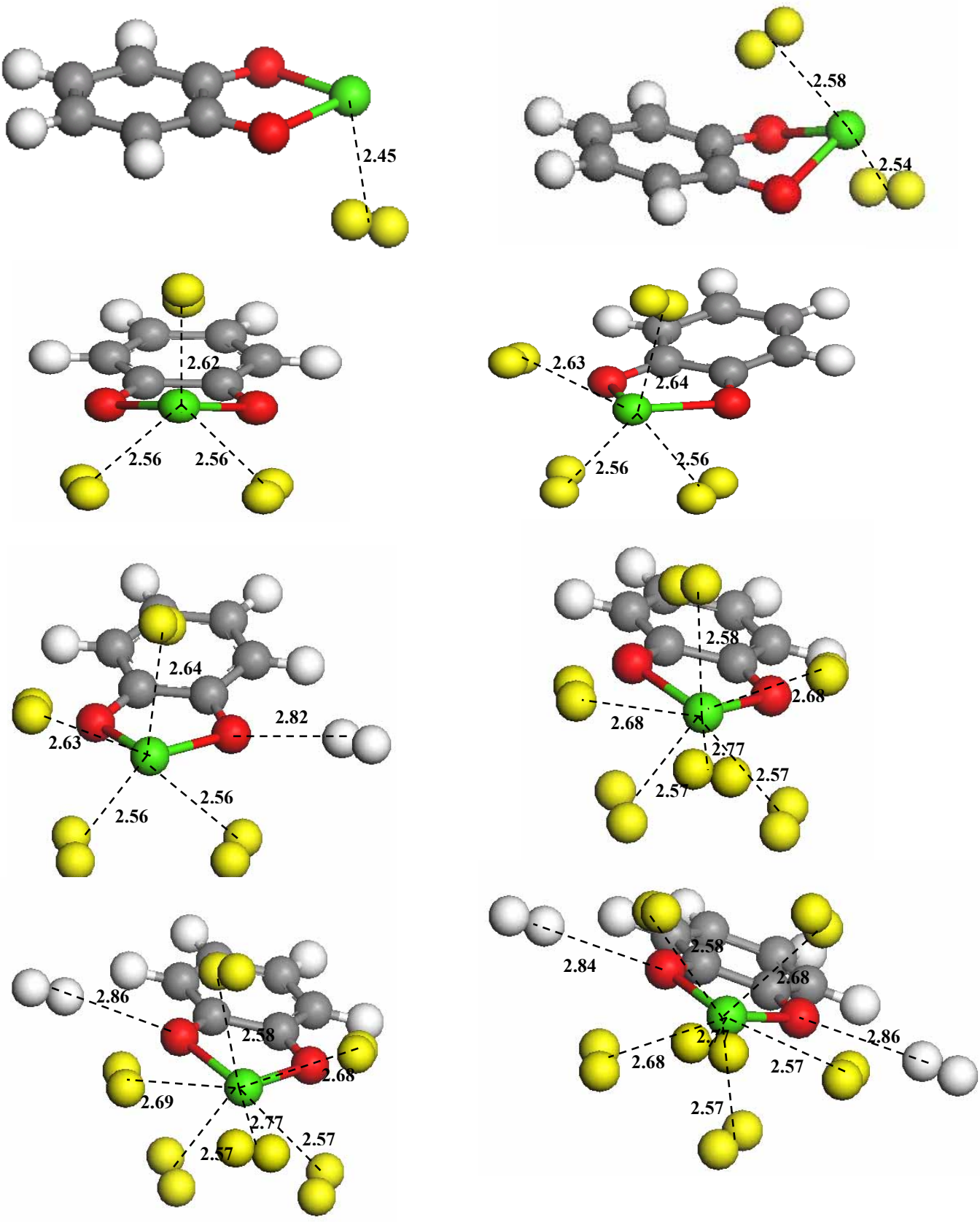

Table S2. Chemical potential (K) of hydrogen calculated at different temperatures and pressures

Pressure(MPa)	temperature		
	77K	233K	298K
0.00001	-1345.174	-4179.166	-5528.168
0.00005	-1221.172	-3803.914	-5048.297
0.0001	-1167.897	-3642.367	-4841.795
0.0005	-1043.95	-3267.241	-4362.284
0.001	-990.615	-3105.713	-4155.558
0.005	-866.661	-2730.885	-3676.03
0.01	-813.268	-2569.35	-3469.56
0.05	-689.435	-2193.404	-2989.217
0.1	-636.206	-2031.229	-2781.616
0.5	-513.24	-1868.533	-2573.716
1	-460.988	-1772.798	-2450.931
2	-409.694	-1704.161	-2363.936
3	-380.807	-1651.067	-2295.484
4	-360.582	-1607.052	-2239.541
5	-345.522	-1569.937	-2192.061
6	-333.587	-1537.342	-2150.32
7	-323.417	-1508.735	-2113.925
8	-315.325	-1482.496	-2080.929
9	-307.109	-1380.936	-1951.585
10	-301.909	-1305.855	-1857.724
15	-277.82	-1245.957	-1782.512
20	-251.917	-1195.885	-1719.47
25	-232.13	-2193.404	-3469.56
30	-213.979	-2031.229	-2989.217