

Table S1: Observed and Calculated Frequencies (cm^{-1}) for Li_2H_2 (${}^1\text{A}_g$ in D_{2h} symmetry).

		${}^7\text{Li}_2\text{H}_2$	${}^6\text{Li}_2\text{H}_2$	${}^7\text{Li}_2\text{D}_2$	${}^6\text{Li}_2\text{D}_2$
mode	obsd ^a	calcd ^b	obsd	calcd	obsd
(a_g)	1180.7(0)		1182.5(0)		844.4(0)
(b_{2u})	986.2	1076.6(972)	994.2	1087.8(992)	748.6
(b_{1u})	905.0	982.9(1009)	913.2	993.1(1030)	691.2
(b_{3g})		896.6(0)	908.9(0)		684.9(0)
(b_{3u})		603.8(764)	610.1(780)		453.1(430)
(a_g)		521.0(0)	561.8(0)		515.3(0)

^aObserved frequencies from solid H_2 . ^bCalculated at the MP2/6-311++G(3df,3pd) level of theory; intensities (km/mol).

Table S2: Calculated and Observed Frequencies (cm^{-1}) for Cyclic Li_3H (${}^1\text{A}_1$ in C_{2v} symmetry).

	${}^7\text{Li}_3\text{H}$			${}^6\text{Li}_3\text{H}$			${}^7\text{Li}_2\text{D}_2$			${}^6\text{Li}_2\text{D}_2$	
mode	calcd ^a	obsd ^b	calcd	obsd	calcd	obsd	calcd	obsd	calcd	obsd	obsd
b_2	1068.5(35)		1079.1		799.8					814.0	
a_1	1061.8(893)	981.4	1071.0	991.0	791.3	743	805.4	756			
a_1	401.8(137)		432.5		393.7				422.2		
b_1	373.7(37)		378.3		283.3				299.1		
a_1	280.5(4)		302.5		277.8				289.4		
b_2	192.2(47)		207.4		191.6				206.8		

^aCalculated at the B3LYP/6-311++G(3df,3pd) level of theory; intensities (km/mol). ^bObserved frequencies from solid H_2 .

Figure S1. Structures of Li_4H_4 isomers calculated at the B3LYP/6-311++G(3df,3pd) level of theory.

