6-31G* (10s4p1d)/[3s2p1d]

Nr	Sym	Type	Exponents	Contraction coefficients	
"s"					
1.1	Ag	1s	5484.671700	0.001831	
			825.234950	0.013950	
			188.046960	0.068445	**1s**
			52.964500	0.232714	
			16.897570	0.470193	
			5.799635	0.358521	
2.1	Ag	1s	15.539616	-0.110778	
			3.599934	-0.148026	**2s**
			1.013762	1.130767	
3.1	Ag	1s	0.270006	1.000000	**2s'**
"px", "py", "pz"					
1.2	B3u	2p	15.539616	0.070874	
			3.599934	0.339753	**2p**
			1.013762	0.727159	
2.2	B3u	2p	0.270006	1.000000	**2p'**
"d0, d2+, d2-, d1+, d1-"					
1.4	B1g	3d	0.800000	1.000000	**+polarization**

cc-pVDZ (9s4p1d)/[3s2p1d]

Nr	Sym	Type	Exponents	Contraction coefficients		
				1s	**2s**	**2s'**
1.1	Ag	1s	11720.0000	0.000710	-0.000160	0.000000
2.1	Ag		1759.0000	0.005470	-0.001263	0.000000
3.1	Ag		400.8000	0.027837	-0.006267	0.000000
			113.7000	0.104800	-0.025716	0.000000
			37.0300	0.283062	-0.070924	0.000000
			13.2700	0.448719	-0.165411	0.000000
			5.0250	0.270952	-0.116955	0.000000
			1.0130	0.015458	0.557368	0.000000
			0.3023	-0.002585	0.572759	1.000000
				2p	**2p'**	
1.2	B3u	2p	17.700000	0.043018	0.000000	
2.2	B3u		3.854000	0.228913	0.000000	
			1.046000	0.508728	0.000000	
			0.275300	0.460531	1.000000	
4.1	Ag	3d	1.185000	1.000000	**+polarization**	

LiH with a cc-pVDZ basis set

	Exponents	Contr. coefficients	
Hydrogen (4s1p)/[2s1p]			
		1s	**1s'**
1s	13.010	0.019685	0.0000
	1.9620	0.137977	0.0000
	0.4446	0.478148	0.0000
	0.1220	0.501240	1.0000
2p	0.7270	1.000000	**+polarization**

Lithium (9s4p1d)/[3s2p1d]				
		1s	**2s**	**2s'**
1s	1469.00	0.000766	-0.000120	0.0000
	220.500	0.005892	-0.000923	0.0000
	50.2600	0.029671	-0.004689	0.0000
	14.2400	0.109180	-0.017682	0.0000
	4.58100	0.282789	-0.048902	0.0000
	1.58000	0.453123	-0.096009	0.0000
	0.56400	0.274774	-0.136380	0.0000
	0.07345	0.009751	0.575102	0.0000
	0.02805	-0.003180	0.517661	1.0000
		2p	**2p'**	
2p	1.53400	0.022784	0.0000	
	0.27490	0.139107	0.0000	
	0.07362	0.500375	0.0000	
	0.02403	0.508474	1.0000	
	+polarization			
3d	0.12390	1.000000		

LiH molecular orbital coefficients

Contracted basis set: (E = –7.983642 Hartrees)

	1 1s	1 1s	1 1s	1 2pz	1 2pz	1 3d0
1σ	0.996931	-0.012108	0.004731	-0.023384	0.014673	-0.004831
	2 1s	2 1s	2 2pz			
	0.006150	0.009900	-0.001735			

	1 1s	1 1s	1 1s	1 2pz	1 2pz	1 3d0
2σ	-0.027863	0.552101	-0.175877	0.462602	-0.226484	0.056185
	2 1s	2 1s	2 2pz			
	0.670141	-0.090079	-0.013031			

Uncontracted basis set: (E = –7.985790 Hartrees)

1σ

1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s
0.00076	0.00589	0.02966	0.10904	0.28276	0.45162	0.27628	0.01058	-0.0035
1 2pz	1 2pz	1 2pz	1 2pz	1 3d0				
-0.0059	-0.0062	0.0027	-0.00067	0.00002				
2 1s	2 1s	2 1s	2 1s	2 2pz				
0.000137	0.000804	0.003692	-0.001069	-0.001469				

2σ

1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s	1 1s
-0.00008	-0.00065	-0.00321	-0.01272	-0.03248	-0.07177	-0.07380	0.26112	0.10026
1 2pz	1 2pz	1 2pz	1 2pz	1 3d0				
0.016304	0.095082	0.130581	0.034083	0.031442				
2 1s	2 1s	2 1s	2 1s	2 2pz				
0.015078	0.097154	0.303592	0.346831	-0.013078				

H_2 with a cc-pVDZ basis set

	Exponents	Contr. coefficients	
		1s	**1s'**
1s	13.010	0.019685	0.0000
	1.9620	0.137977	0.0000
	0.4446	0.478148	0.0000
	0.1220	0.501240	1.0000
2p	0.7270	1.000000	**+polarization**

Contracted basis set:

1 1s	1 1s	1 $2p_z$
0.73005	-0.24454	0.02890

2 1s	2 1s	2 $2p_z$
0.73005	-0.24454	-0.02890

Uncontracted basis set:

1 1s	1 1s	1 1s	1 1s	1 2pz
0.019390	0.132185	0.303324	0.149302	0.024021

2 1s	2 1s	2 1s	2 1s	2 2pz
0.019390	0.132185	0.303324	0.149302	-0.024021