APPENDIX
D

MOLECULAR INTEGRALS FOR H_2 AS A FUNCTION OF BOND LENGTH

All quantities are in atomic units. The integrals are for a minimal basis STO-3G calculation with Slater exponent $\zeta = 1.24$, as described in the text (Subsection 3.5.2).

R	ε_1	ε_2	J_{11}	J_{12}	J_{22}	K_{12}
0.6	−0.7927	1.3327	0.7496	0.7392	0.7817	0.1614
0.8	−0.7321	1.1233	0.7330	0.7212	0.7607	0.1655
1.0	−0.6758	0.9418	0.7144	0.7019	0.7388	0.1702
1.2	−0.6245	0.7919	0.6947	0.6824	0.7176	0.1755
1.4	−0.5782	0.6703	0.6746	0.6636	0.6975	0.1813
1.6	−0.5368	0.5715	0.6545	0.6457	0.6786	0.1874
1.8	−0.4998	0.4898	0.6349	0.6289	0.6608	0.1938
2.0	−0.4665	0.4209	0.6162	0.6131	0.6439	0.2005
2.5	−0.3954	0.2889	0.5751	0.5789	0.6057	0.2179
3.0	−0.3377	0.1981	0.5432	0.5512	0.5734	0.2351
4.0	−0.2542	0.0916	0.5026	0.5121	0.5259	0.2651
5.0	−0.2028	0.0387	0.4808	0.4873	0.4947	0.2877
7.5	−0.1478	−0.0114	0.4533	0.4540	0.4547	0.3206
10.0	−0.1293	−0.0292	0.4373	0.4373	0.4373	0.3373
20.0	−0.1043	−0.0543	0.4123	0.4123	0.4123	0.3623
100.0	−0.0843	−0.0743	0.3923	0.3923	0.3923	0.3823
∞	−0.0793	−0.0793	0.3873	0.3873	0.3873	0.3873