HyperChem – cząsteczka H_2

Metoda obliczeniowa: Ab initio – Medium (6-31G*), MP2

Długość wiązania H – H, A	Energia z MP2, kcal/mol	MP2, kcal/mol
0.1	1620.100170	-5.404141
0.2	48.9910057	-6.360758
0.3	-404.840648	-7.395402
0.4	-585.469167	-8.338947
0.5	-663.920796	-9.178993
0.6	-696.555011	-9.934714
0.7	-706.653032	-10.634219
0.8	-705.140992	-11.317057
0.9	-697.593822	-12.026894
1	-687.002449	-12.804157
1.1	-675.003031	-13.682178
1.2	-662.499036	-14.686717
1.3	-649.9990797	-15.837394
1.4	-637.754106	-17.149273
1.5	-625.939112	-18.634229
Geometry optymalization	Single point energy	MP2 correlation energy
0.72995	-707.09522	-10.8385