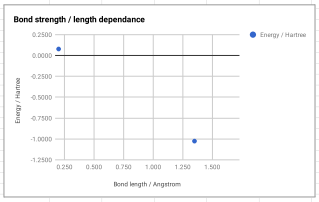
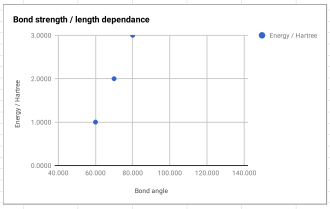
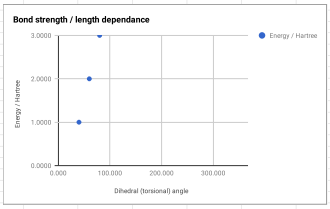
user	Bond length / Angstrom	Energy / Hartree	Energy / kJ/mol
	0.200	0.0781	204.97
	0.300		
	0.350		
	0.400		
	0.450		
	0.500		
	0.550		
	0.600		
	0.650		
	0.700		
	0.715		
	0.730		
	0.740		
	0.750		
	0.800		
	0.850		
	0.900		
	0.950		
	1.000		
	1.050		
	1.100		
	1.150		
	1.200		
	1.250		
	1.300		
Jon	1.350	-1.0260	-2,693.68
	1.400		
	1.450		
	1.500		
	1.550		
	1.600		
	1.650		
	1.700		



user	Bond length / Angstrom	Energy / Hartree
	40.000	
	50.000	
	60.000	1.0000
	70.000	2.0000
	80.000	3.0000
	90.000	
	95.000	
	98.000	
	100.000	
	102.000	
	104.000	
	106.000	
	108.000	
	110.000	
	112.000	
	115.000	
	120.000	
	130.000	
	140.000	



user	Torsional angle / degrees	Energy / Hartree
	0.000	
	20.000	
	40.000	1.0000
	60.000	2.0000
	80.000	3.0000
	100.000	
	120.000	
	140.000	
	160.000	
	180.000	
	200.000	
	220.000	
	240.000	
	260.000	
	280.000	
	300.000	
	320.000	
	340.000	
	360.000	



Name	Independent variable (what to dial up/down)	Dependent variable (what to observe)	RQ	Hypothesis	Comment
Jon	Bond length of H-H	Total energy of molecule	How does the H-H bond enthalpy varies with bond length, as calculated at the RHF / 6-311 level of theory?	The shorter the bond length, the higher the bond enthalpy --- if the atoms are closer then they will form stronger bonds	Too narrow a scope for an actual IA, but can be a suitable base to build on.
Aiste	Bond length of C=O bonds in diff molecules	C=O bond stretching frequency (from SDBS)	How does the empirical C=O stretch freq. (from IR) varies with bond length?	The shorter the bond, the higher the frequency (linear, proportional). This is what Hooke's law predicts.	