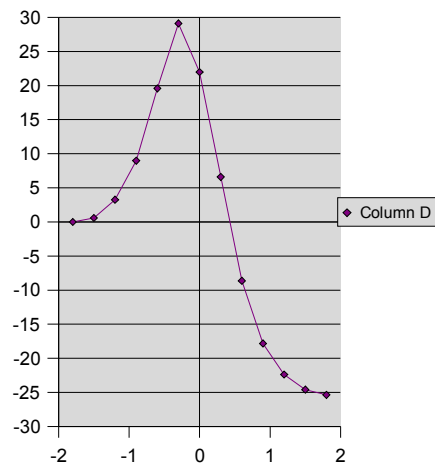This is an example spreadsheet for the practical. It is **not** a good example of a spreadsheet as it does not have any labels for the graphs, units, axis labels etc
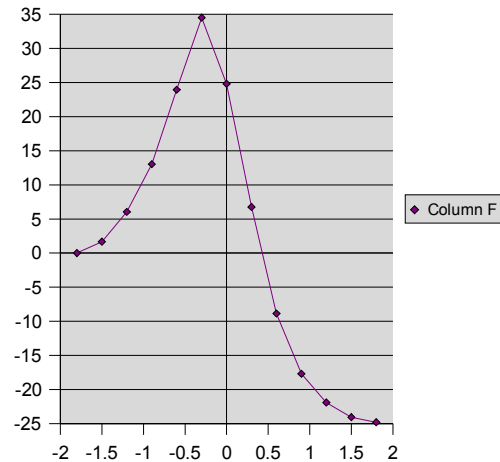Please ensure that your spreadsheet does have labels, units and a clear layout.
Please ensure that you clearly record on your spreadsheet your **starting structure**

RC	Nsteps	QM/MM	Relative QM/MM	QM	Relative QM	Stabilisation	Arg90 QM/MM	Relative QM/MM	QM	Relative QM	Stabilisation
-1.8	52	-3267.76	0	-188.39	0	0	-2912.08	0	-162.57	0	0
-1.5	62	-3267.16	0.59	-186.71	1.68	1.09					
-1.2	48	-3264.49	3.27	-182.35	6.04	2.77					
-0.9	42	-3258.77	8.98	-175.34	13.04	4.06					
-0.6	33	-3248.17	19.59	-164.44	23.95	4.36					
-0.3	24	-3238.64	29.11	-153.86	34.53	5.42	-2882.07	30.01	-131.22	31.35	1.34
0	38	-3245.78	21.98	-163.56	24.83	2.85					
0.3	37	-3261.15	6.61	-181.63	6.76	0.15					
0.6	34	-3276.39	-8.63	-197.25	-8.87	-0.23					
0.9	34	-3285.57	-17.82	-206.09	-17.7	0.12					
1.2	37	-3290.12	-22.36	-210.3	-21.91	0.45					
1.5	34	-3292.34	-24.58	-212.45	-24.06	0.52					
1.8	43	-3293.1	-25.34	-213.19	-24.81	0.54	-2936.52	-24.44	-188.1	-25.53	-1.08

Main Title — Column D

Main Title — Column F

Main Title — Column G