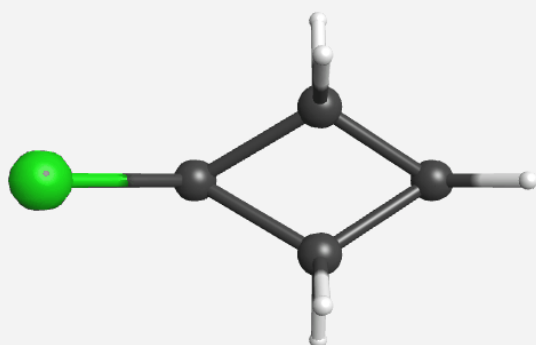











b) Encontrar las energías de los diferentes modos de vibración

Step	Energy (au)			
0	-608.008383032			
1	-608.122185075			
2	-608.229776756			
3	-608.271400555			
4	-608.278459588			
5	-608.278843010			
6	-608.279122881			
7	-608.279268264			
8	-608.279283950			
9	-608.279286233			
10	-608.279286291			
Animation speed		<input type="text" value="5"/>		
Loop		<input type="button" value="Loop"/>		



Show all						
Mode	Symmetry	Frequency (cm <sup>-1</sup> )	IR Intensity	Raman Intensity	Actions	
1	A"	-2157.19 (-2399.5415)	17.7372	13.4873		
2	A"	-677.76 (-753.9091)	370.0056	13.7055		
3	A'	-341.86 (-380.2642)	344.3117	7.6294		
4	A'	131.77 (146.5750)	15.6957	2.9139		
5	A"	349.98 (389.3025)	0.0319	2.7570		
6	A'	377.09 (419.4497)	48.7904	5.1652		
7	A'	558.96 (621.7610)	151.3800	5.7862		
8	A'	640.07 (711.9830)	40.5274	16.0138		
9	A'	778.50 (865.9670)	113.9000	17.6410		
10	A"	791.59 (880.5270)	14.8647	4.8686		
11	A"	922.21 (1025.8205)	10.7142	11.1998		
12	A'	953.03 (1060.1017)	2.5569	35.9865		
13	A'	976.94 (1086.6944)	30.1691	5.9565		
14	A"	1038.35 (1155.0032)	0.6806	8.3354		
15	A'	1079.06 (1200.2910)	1.5411	2.0956		

16	A''	1183.83 (1316.8295)	0.2345	0.3461		
17	A'	1214.71 (1351.1838)	10.3124	14.9524		
18	A''	1297.19 (1442.9267)	2.7623	3.1934		
19	A'	1335.35 (1485.3780)	56.1056	5.9279		
20	A''	1338.26 (1488.6078)	23.4985	6.3123		
21	A'	1374.34 (1528.7448)	17.8736	8.5644		
22	A''	1482.11 (1648.6209)	3.9885	7.0990		
23	A'	1501.06 (1669.6995)	9.6937	21.9949		
24	A''	2582.09 (2872.1776)	101.1600	72.3121		
25	A'	2586.09 (2876.6350)	93.3957	182.5737		
26	A'	2641.84 (2938.6443)	51.3642	236.0558		
27	A''	2671.45 (2971.5750)	32.8909	131.6977		
28	A'	2675.91 (2976.5450)	1.1068	69.0995		
29	A'	2683.39 (2984.8656)	45.8732	101.6607		
30	A''	2699.99 (3003.3309)	13.9565	100.4284		
Frequency Scale Factor					<input type="text" value="0.899"/>	
Normal Mode Amplitude					<input type="text" value="1.0"/>	
Animation Speed					<input type="text" value="50"/>	
IR Spectrum						
Raman Spectrum						
Peak Width (cm <sup>-1</sup> )					<input type="text" value="40"/>	