QM206 - 2022
PARCIAL I

NOMBRE:

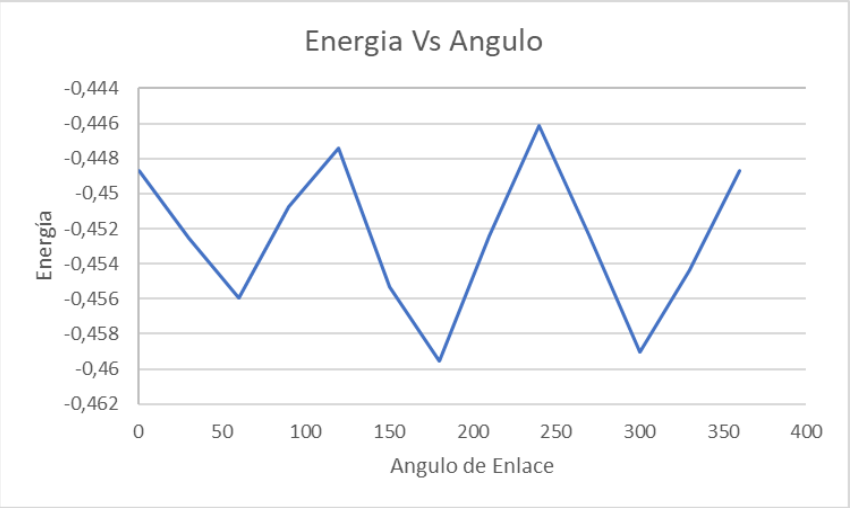
Realizar los siguientes cálculos utilizando los softwares utilizados en clases. Debe complementar sus cálculos con las imágenes correspondientes y anexar el enlace Github de los archivos generados.

PROBLEMA 1: DIAGRAMA DE ENERGÍA

Construya un diagrama de energía vs ángulo de enlace para el 2,3-diclorobutano

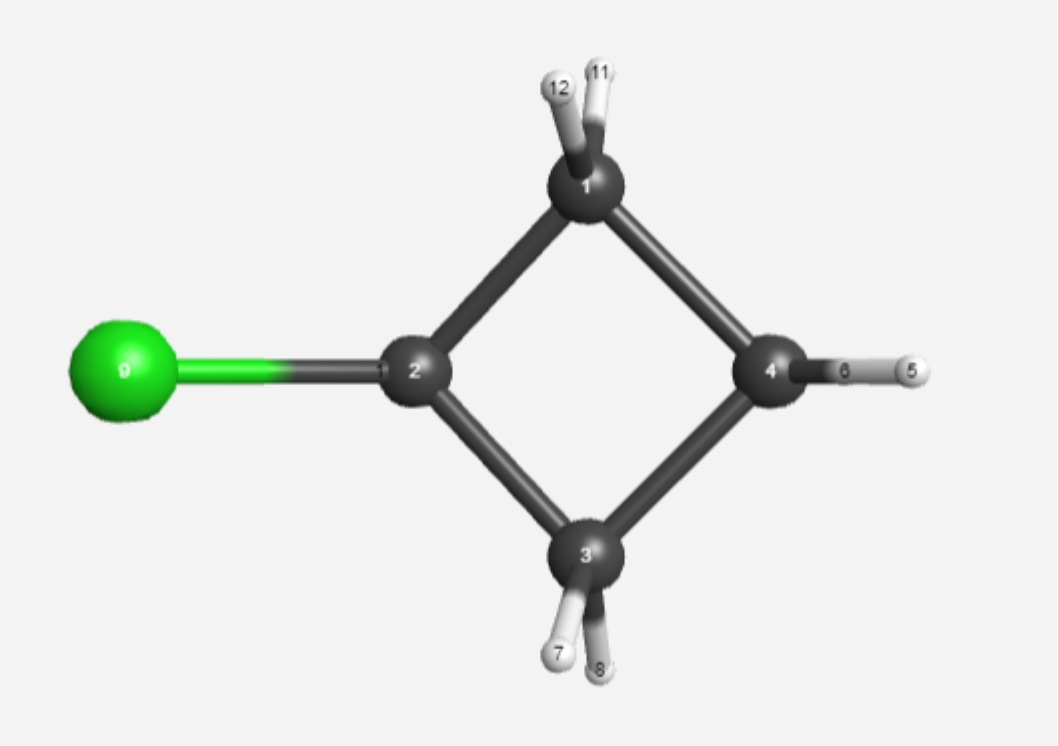
Coordinate Scan

Coordinate	Energy (au)
0.0000	-0.44866
30.0000	-0.45254
60.0000	-0.45592
90.0000	-0.45074
120.0000	-0.44739
150.0000	-0.45530
180.0000	-0.45953
210.0000	-0.45241
240.0000	-0.44615
270.0000	-0.45233
300.0000	-0.45904
330.0000	-0.45434
360.0000	-0.44866
Animation speed	5
Loop	None



PROBLEMA 2: OPTIMIZACIÓN DE LA GEOMETRÍA

a) Optimizar la geometría de la molécula de 1-clorociclobutano



Geometry Sequence Energies

Step	Energy (au)
0	-608.008071102
1	-608.121933559
2	-608.229637548
3	-608.271370538
4	-608.278459234
5	-608.278842557
6	-608.279122288
7	-608.279268196
8	-608.279283947
9	-608.279286234
10	-608.279286291
Animation speed	5
Loop	None

b) Encontrar las energías de los diferentes modos de vibración

Vibrational Modes

Show all

Mode	Symmetry	Frequency (cm^{-1})	IR Intensity	Raman Intensity	Actions
1	A'	95.79 (117.2508)	1.0483	0.2436	
2	A"	266.77 (326.5245)	3.2872	1.9047	
3	A'	323.87 (396.4117)	3.2959	2.8874	
4	A'	549.58 (672.6752)	5.6564	7.8453	
5	A'	712.08 (871.5799)	7.3258	3.6257	
6	A"	751.50 (919.8276)	0.2139	0.3271	
7	A'	820.95 (1004.8408)	18.7560	7.1956	
8	A'	928.64 (1136.6511)	9.2848	5.6033	
9	A"	931.90 (1140.6411)	0.2556	0.5356	
10	A"	951.02 (1164.0379)	0.0541	15.8326	
11	A'	1010.56 (1236.9187)	9.1000	11.6399	
12	A"	1042.28 (1275.7369)	0.7810	4.2080	
13	A'	1070.49 (1310.2717)	1.8116	3.6193	
14	A'	1181.67 (1446.3492)	3.0784	10.7544	
15	A"	1184.12 (1449.3539)	0.0052	9.6984	

16	A"	1223.10 (1497.0657)	0.2214	4.4679		
17	A'	1239.55 (1517.1968)	38.8729	9.2284		
18	A"	1243.10 (1521.5472)	0.0181	0.3087		
19	A"	1294.26 (1584.1603)	1.1228	2.3906		
20	A'	1322.40 (1618.6018)	10.3787	4.2446		
21	A"	1460.47 (1787.5965)	0.1680	3.5089		
22	A'	1463.24 (1790.9969)	0.2330	20.3427		
23	A'	1486.37 (1819.2963)	0.0729	15.7621		
24	A'	2959.25 (3622.0956)	0.1661	23.8940		
25	A"	2962.95 (3626.6276)	0.0347	0.9415		
26	A'	2967.88 (3632.6609)	0.3754	85.1714		
27	A'	2996.52 (3667.7152)	0.0255	42.1254		
28	A'	3065.46 (3752.0880)	0.4817	27.9609		
29	A"	3068.64 (3755.9859)	0.4985	52.1627		
30	A'	3071.06 (3758.9428)	0.0769	14.5515		

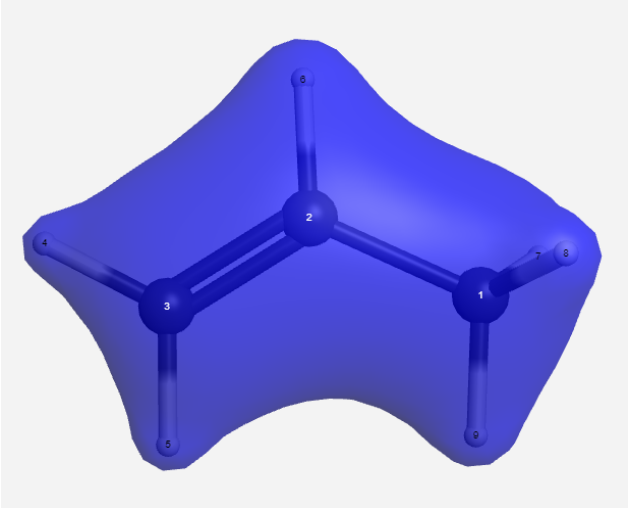
PROBLEMA 3: ORBITALES MOLECULARES

a) Construya un diagrama de energía para los orbitales moleculares del propileno. Para cada nivel de energía presente la imagen con la estructura del OM correspondiente

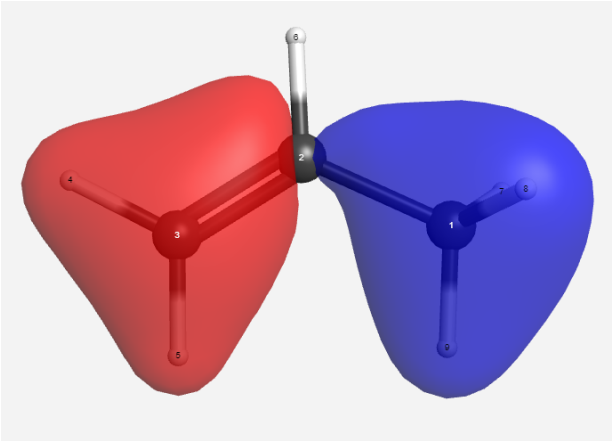
Molecular Orbitals

Show all

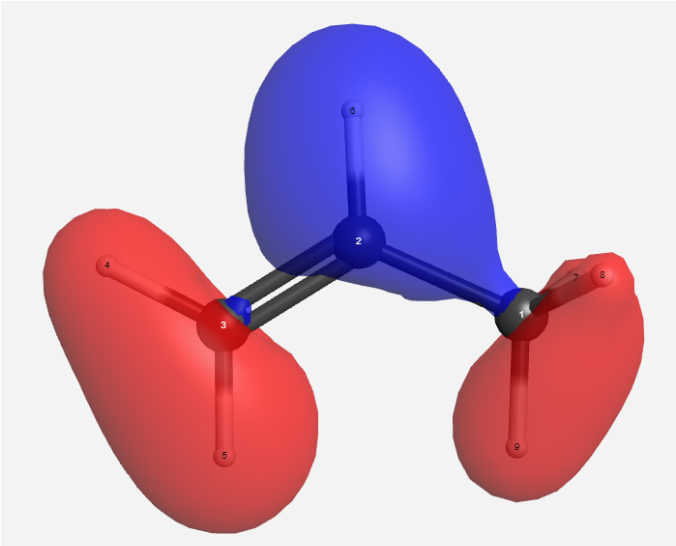
Orbital	Symmetry	Occupancy	Spin	Energy (au)	Actions
				> -1.30286	
4	-	2	-	-1.00644	
5	-	2	-	-0.87781	
6	-	2	-	-0.70545	
7	-	2	-	-0.58906	
8	-	2	-	-0.53181	
9	-	2	-	-0.53101	
10	-	2	-	-0.46939	
11	-	2	-	-0.44136	
12	-	2	-	-0.30286	
13	-	0	-	0.32069	
14	-	0	-	0.5998	
15	-	0	-	0.65992	
16	-	0	-	0.67543	



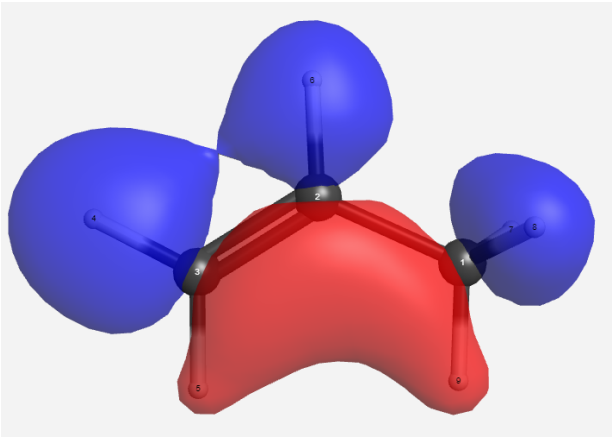
Orbital 4



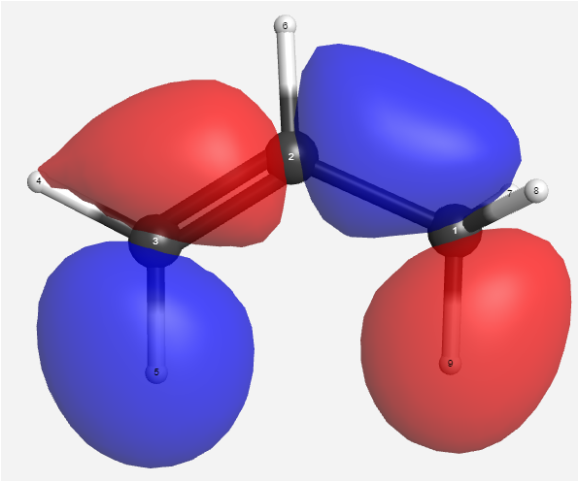
Orbital 5



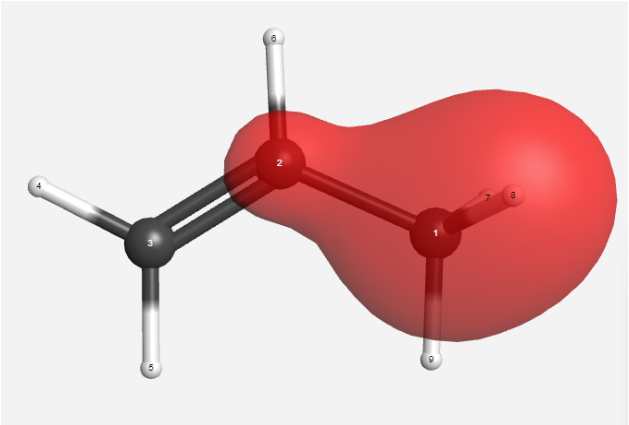
Orbital 6



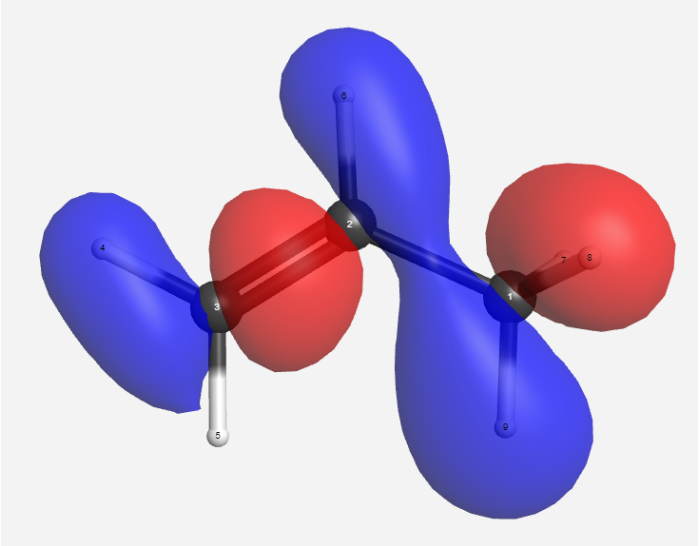
Orbital 7



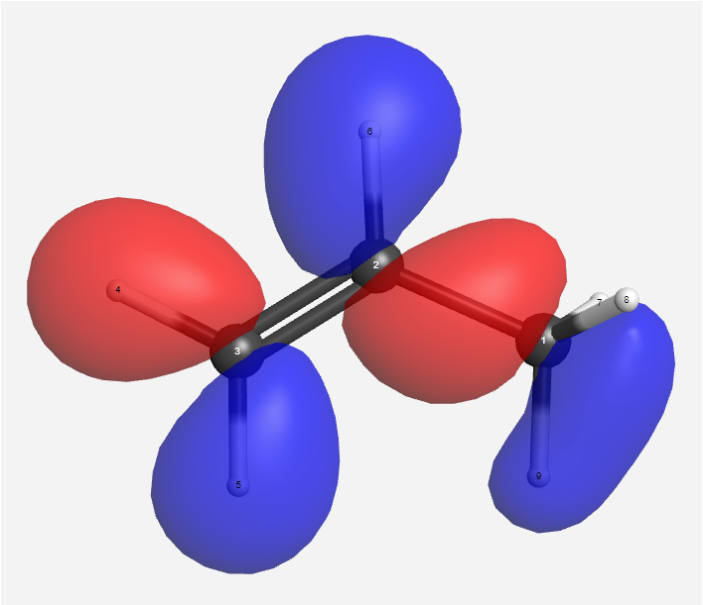
Orbital 8



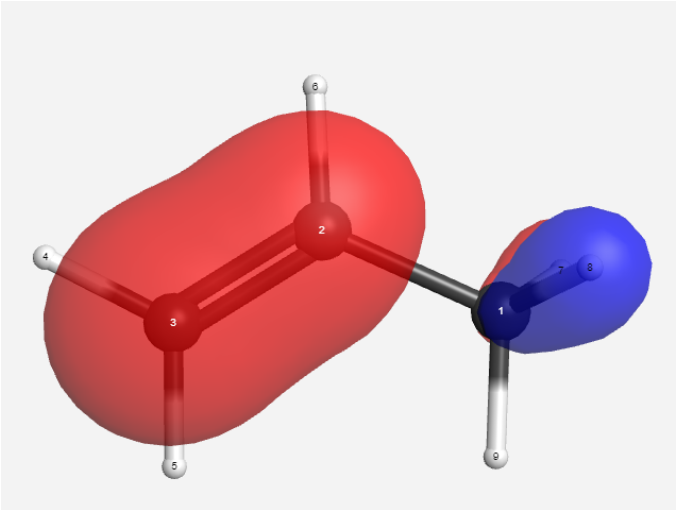
Orbital 9



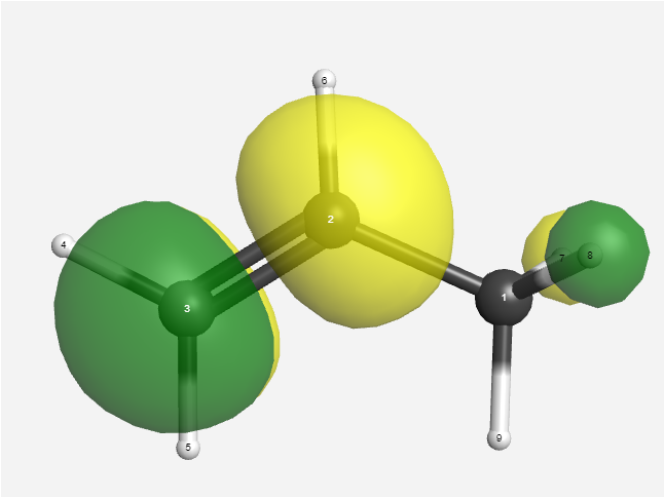
Orbital 10



Orbita 11



Orbita 12



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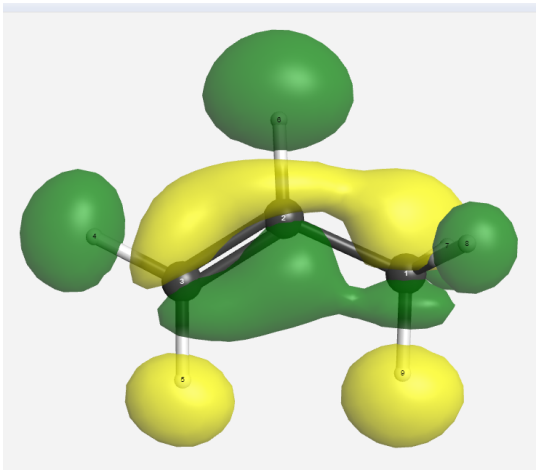
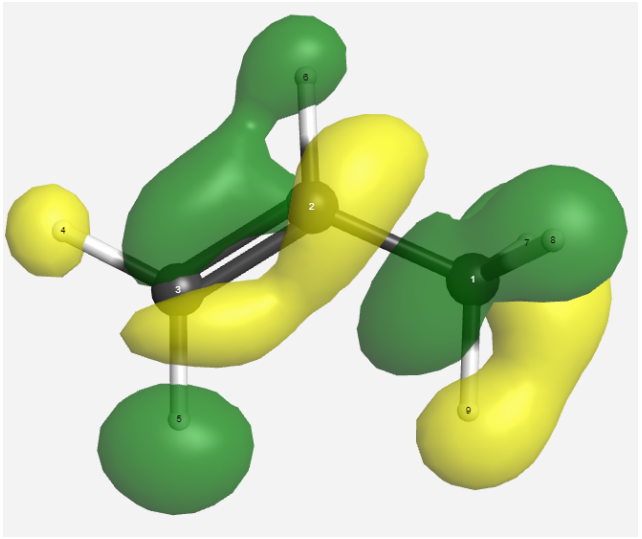
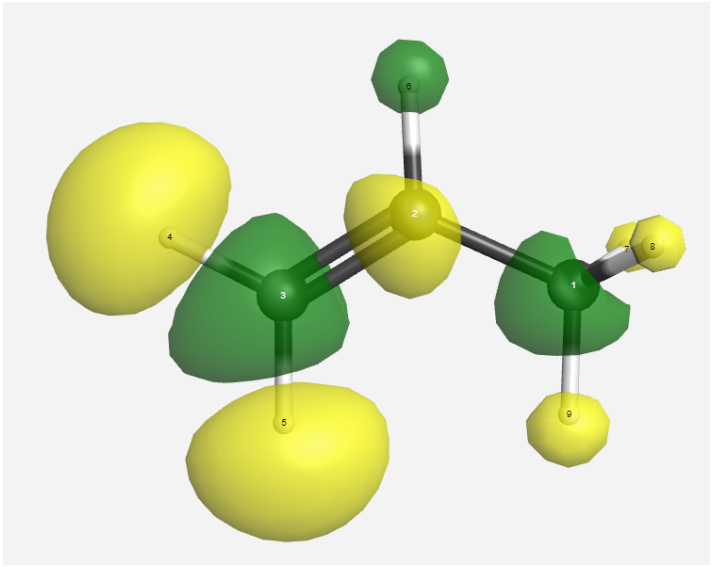


Orbital 14

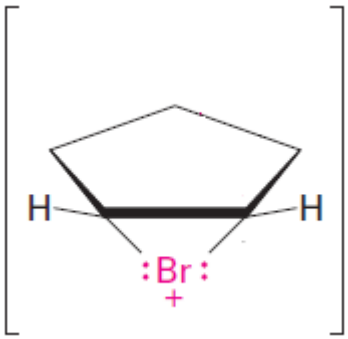


Orbita 15

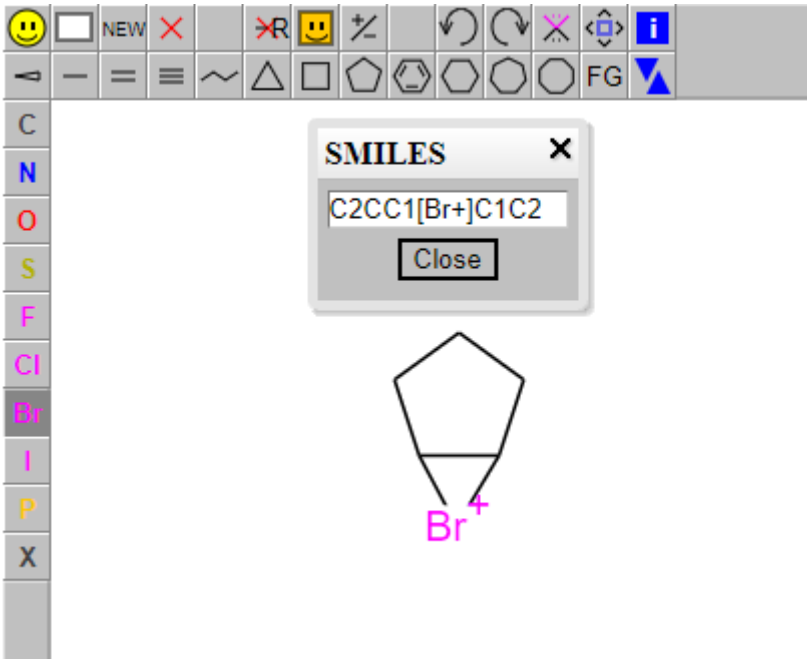


Orbita 16

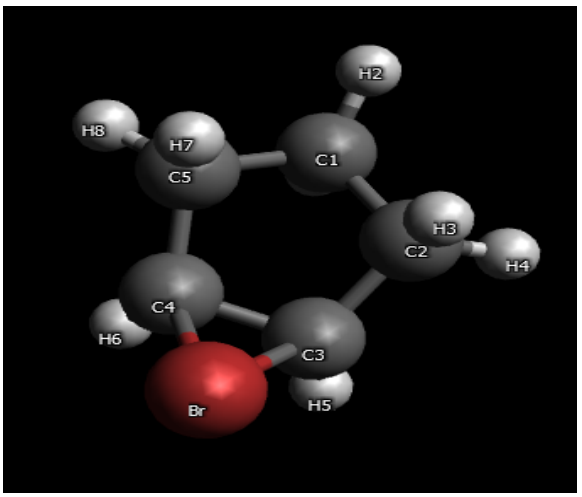
PROBLEMA 4: IÓN BROMONIO

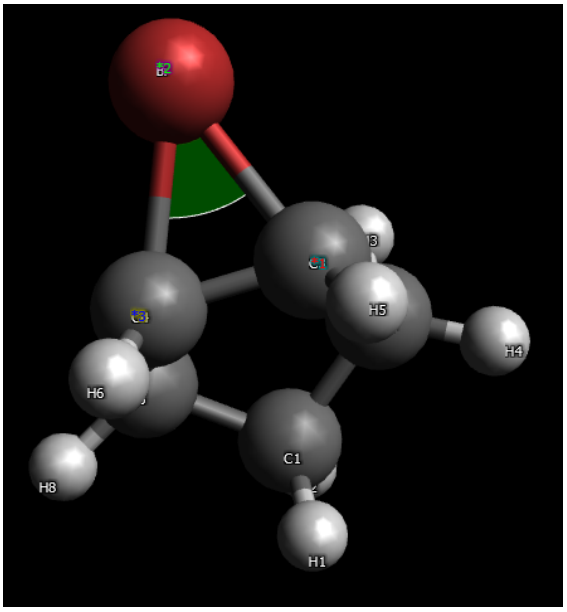


a) Determine la estructura del ión bromonio indicado. Señale los ángulos correspondientes y distancia de enlaces C-Br



Estructura





Distancia: 1.982 Â

Ángulo C-Br: 43.7º