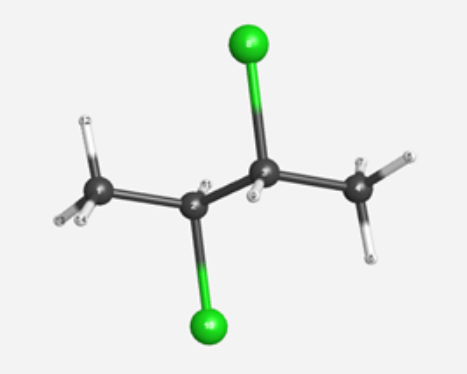
QM 206-2022
PARCIAL I

NOMBRE: MARÍA CECILIA CÓRDOBA BURBANO CÉDULA: 4-819-2142

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



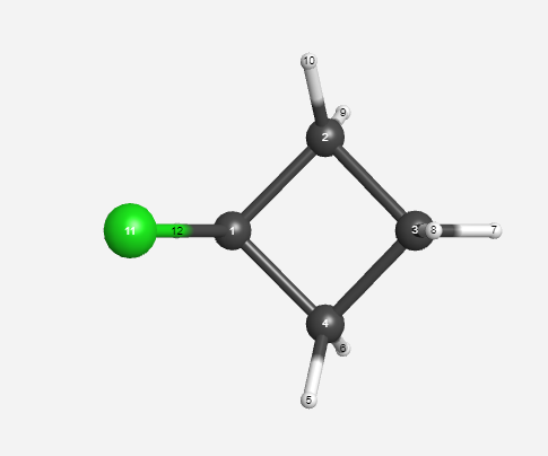
2,3-diclorobutano optimizado

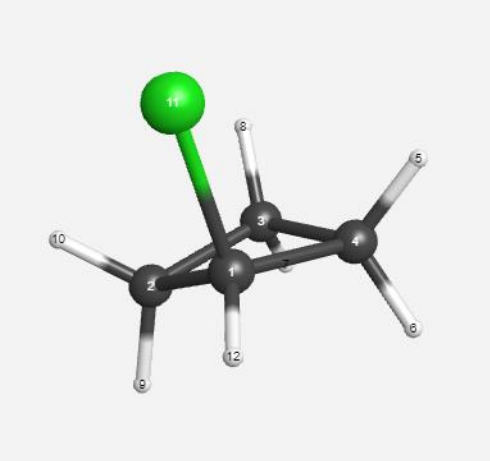
TABLA DE DATOS	
ÁNGULO °	ENERGÍA kcal/mol
0°	37
30°	27
60°	18.2
90°	22.7
120°	24.6
150°	19.04
180°	14.2
210°	19.04
240°	24.6
270°	22.7
300°	18.2
330°	26.9
360°	37.4

https://github.com/mariace2503/Parcial-N-1-Mar-a-C-rdoba/blob/main/2%2C3-Diclorobutano.png

PROBLEMA 2: OPTIMIZACIÓN DE LA GEOMETRÍA

a) **Optimizar la geometría de la molécula de 1-clorociclobutano**
b) **Encontrar las energías de los diferentes modos de vibración**





GEOMETRÍA DE 1-CLOROCICLOBUTANO OPTIMIZADA

Vibrational Modes

Show all

Mode	Symmetry	Frequency (cm^{-1})	IR Intensity	Raman Intensity	Actions
1	A	101.91 (112.4844)	1.0004	0.7204	
2	A	311.82 (344.1680)	0.9077	2.6369	
3	A	315.86 (348.6298)	3.8100	5.1506	
4	A	555.07 (612.6551)	51.9062	23.2272	
5	A	679.09 (749.5526)	13.6468	3.3393	
6	A	730.89 (806.7176)	0.0420	0.0342	
7	A	843.91 (931.4724)	3.0689	5.9824	
8	A	857.90 (946.9057)	4.5615	7.7830	
9	A	865.49 (955.2866)	2.0577	4.8818	
10	A	899.49 (992.8177)	2.9436	11.9716	
11	A	943.57 (1041.4652)	9.7555	26.9021	

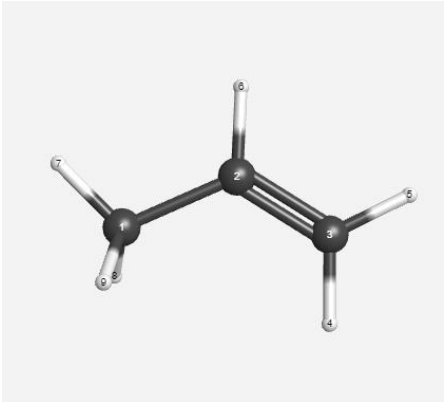
12	A	1067.43 (1178.1779)	4.2087	6.6259		
13	A	1075.87 (1187.4970)	0.0898	3.4035		
14	A	1170.18 (1291.5843)	0.2947	2.9049		
15	A	1185.74 (1308.7680)	16.3053	15.0990		
16	A	1240.75 (1369.4764)	0.7623	11.4133		
17	A	1256.89 (1387.2946)	43.1615	4.0319		
18	A	1273.90 (1406.0653)	2.6285	0.1958		
19	A	1285.91 (1419.3249)	0.7771	0.1207		
20	A	1288.72 (1422.4317)	8.0440	2.5125		
21	A	1466.74 (1618.9227)	10.0072	7.2138		
22	A	1472.74 (1625.5380)	3.8954	20.7925		
23	A	1495.06 (1650.1757)	1.4224	5.9466		
24	A	2941.80 (3247.0146)	22.4169	25.6103		
25	A	2944.75 (3250.2743)	12.2096	131.1008		
26	A	2960.42 (3267.5714)	24.8066	110.0607		
27	A	3005.83 (3317.6949)	6.5652	67.0980		
28	A	3018.41 (3331.5758)	5.6976	63.1267		
29	A	3024.13 (3337.8875)	12.0247	50.8463		
30	A	3051.18 (3367.7538)	10.1182	90.7045		

Frequency Scale Factor	0.906
Normal Mode Amplitude	1.0
Animation Speed	50
IR Spectrum	
Raman Spectrum	
Peak Width (cm^{-1})	40

https://github.com/mariace2503/Parcial-N-1-Mar-a-C-rdoba/blob/main/1-clorociclobutano.png

PROBLEMA 3: ORBITALES MOLECULARES

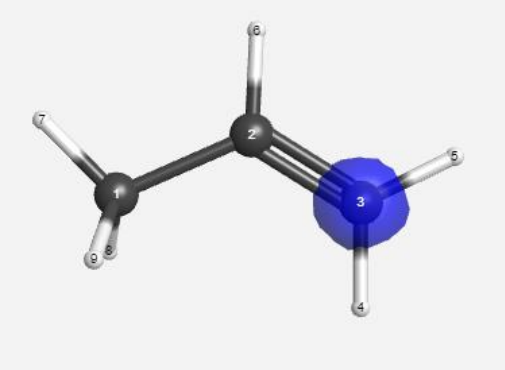
a) Construya un diagrama de energía para los orbitales moleculares del propileno. Para cada nivel de energía presente la imagen con la estructura del OM correspondiente.



MOLECULA DE PROPILENO OPTIMIZADA

ORBITAL N°1= -11.173 au

ORBITAL N°2= -11.159 au



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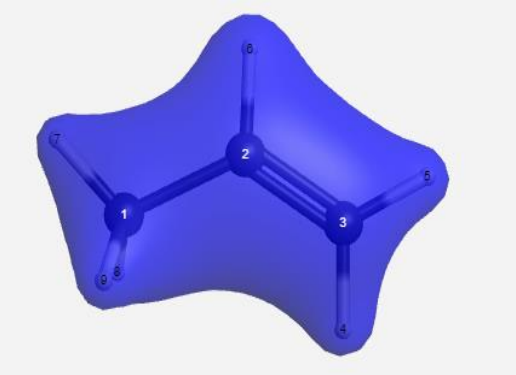

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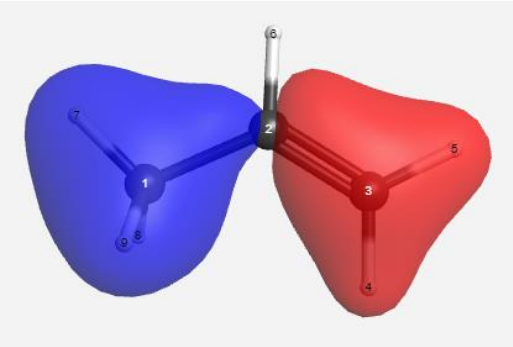

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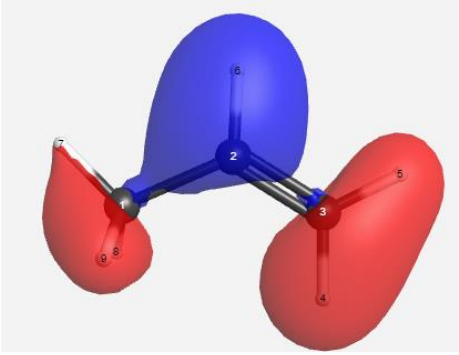

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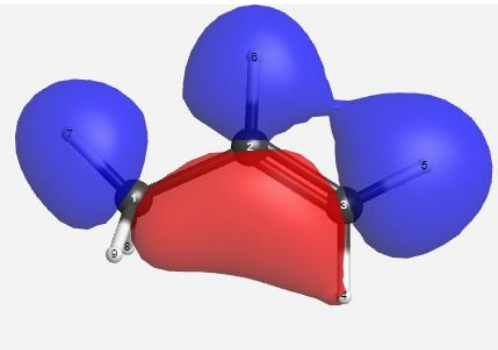

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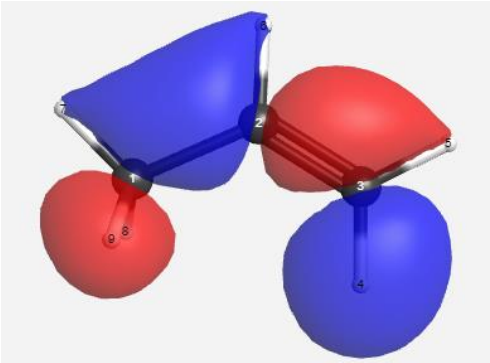

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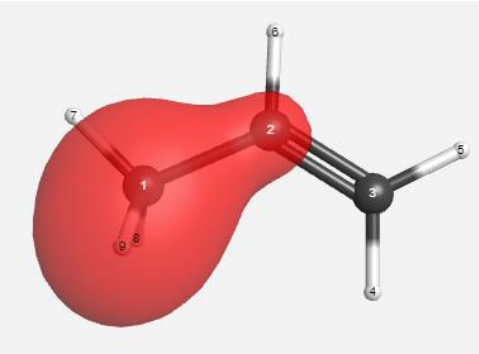

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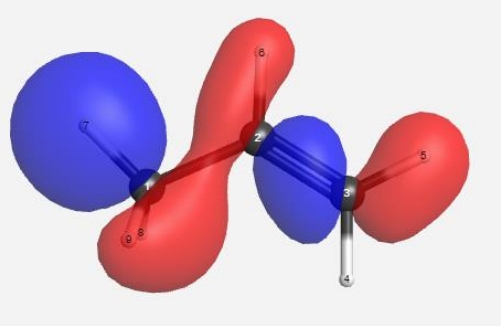

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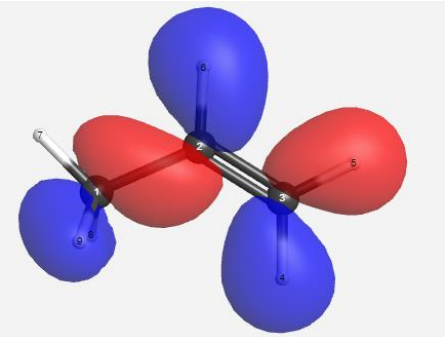

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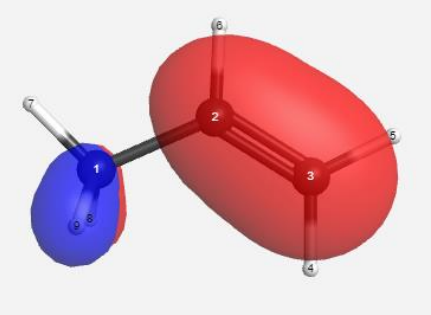

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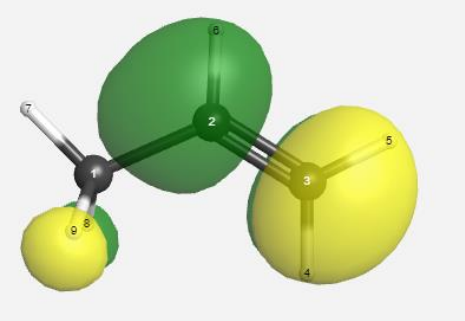

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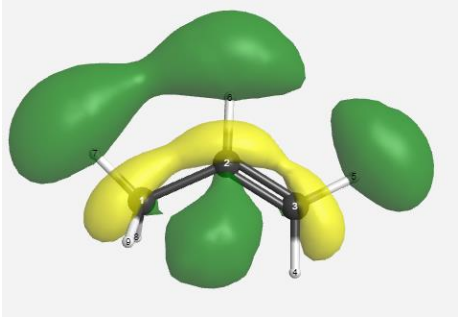

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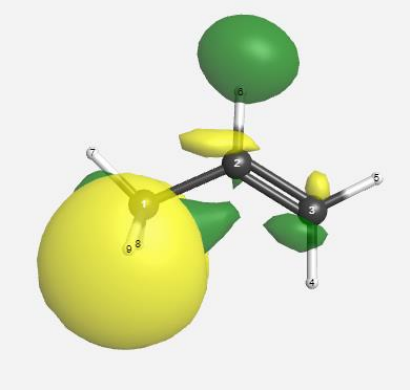

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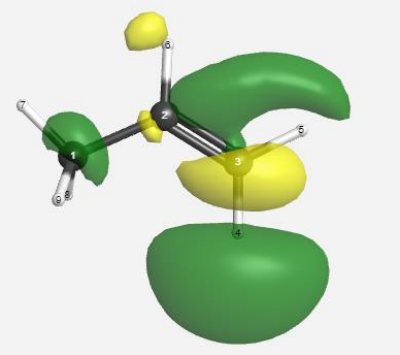

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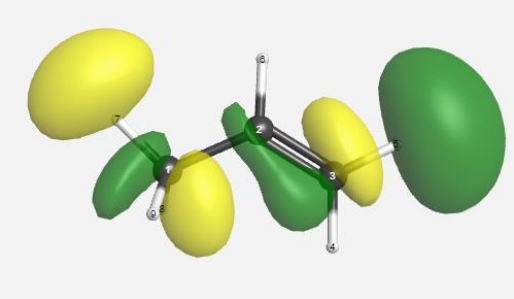

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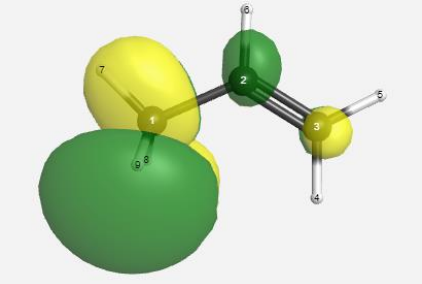

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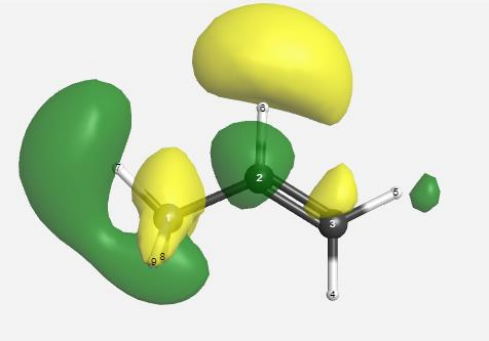

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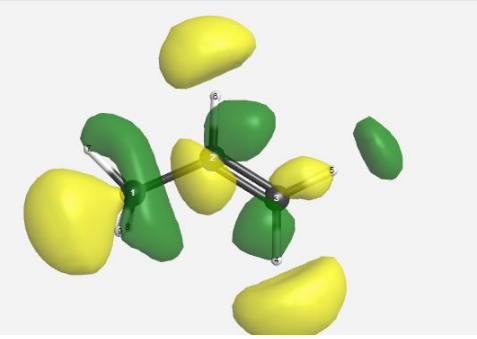

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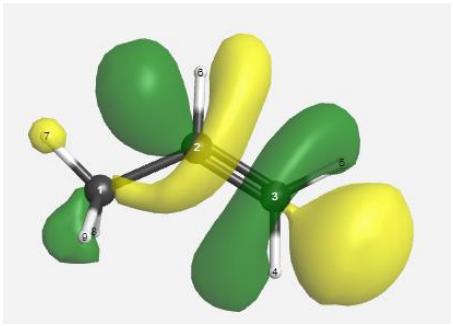

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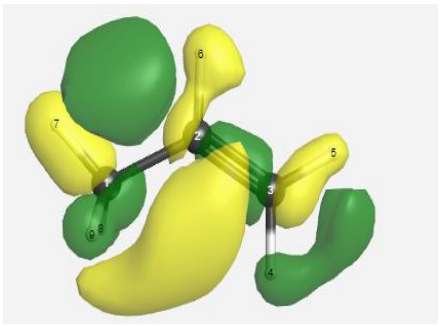

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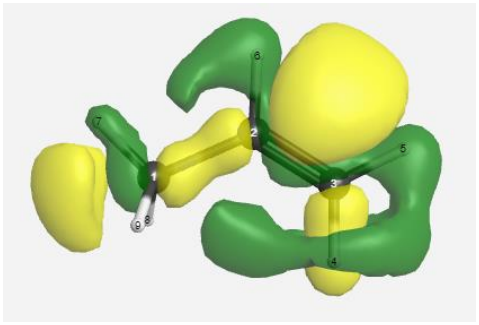

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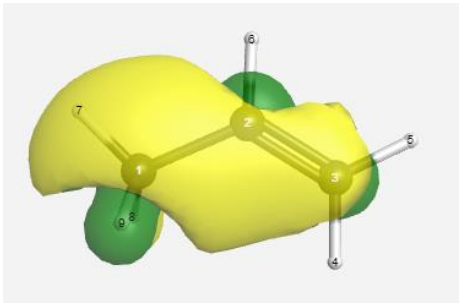

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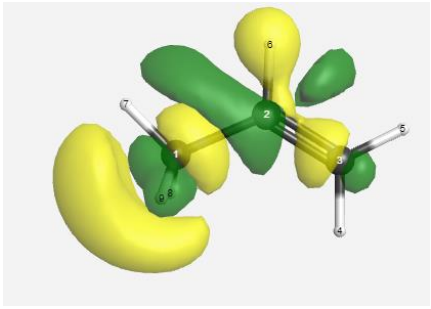

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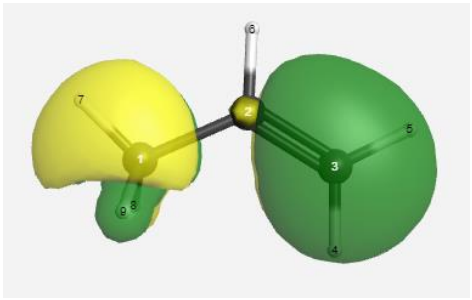

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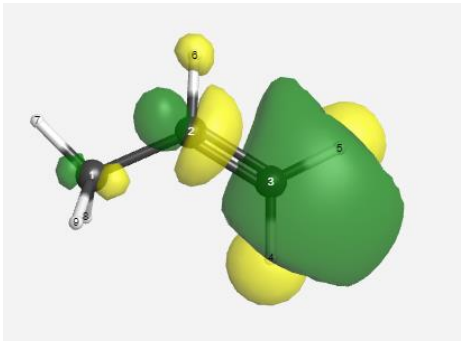

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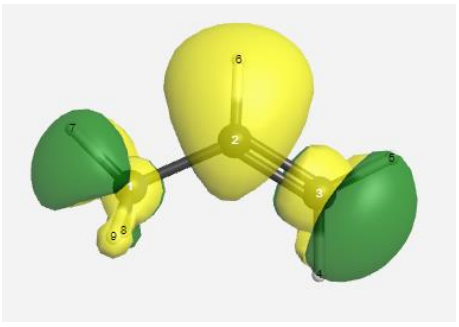

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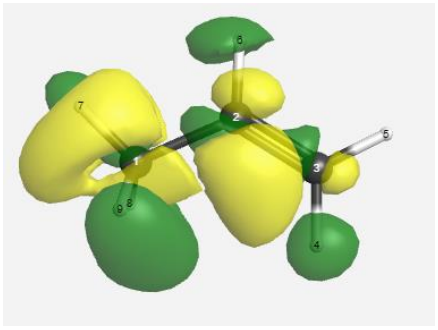

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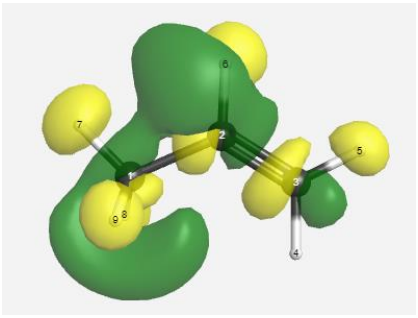

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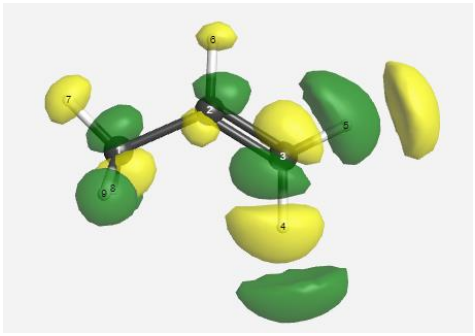

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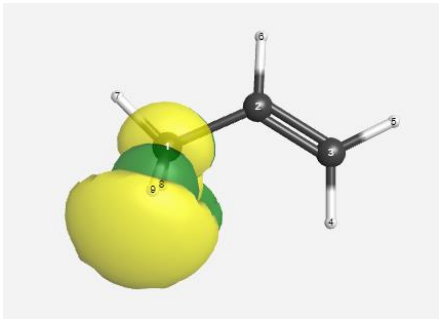

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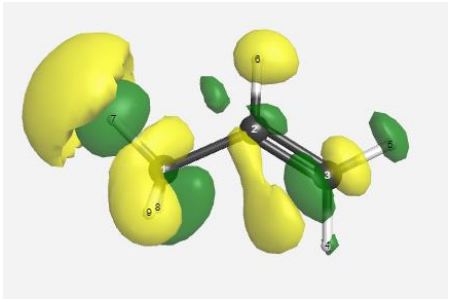

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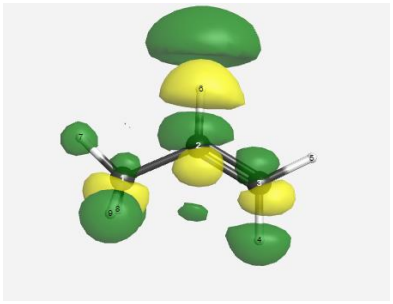

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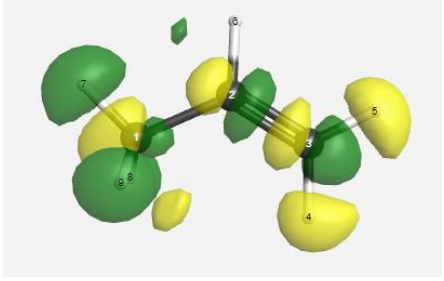

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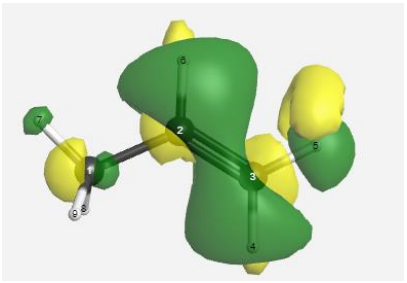

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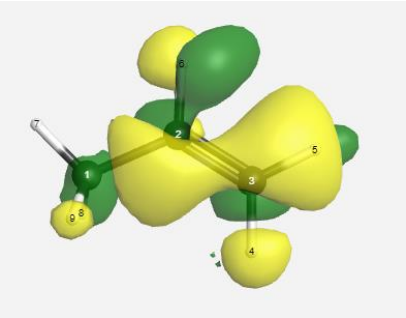

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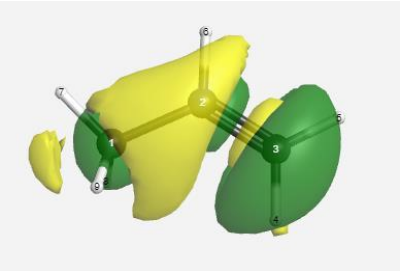

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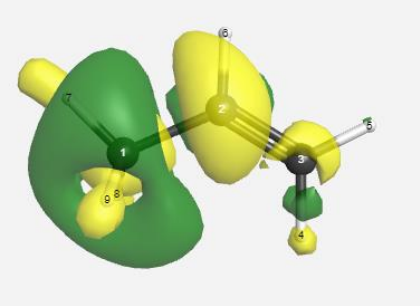

ORBITAL N° 39= 2.183 au

TABLA DE DATOS	
NÚMERO DE ORBITAL	ENERGÍA
1	-11
2	-11
3	-11.154
4	-1.604
5	-0.935
6	-0.755
7	-0.641
8	-0.585
9	-0.568
10	-0.522
11	-0.48
12	-0.36
13	0.186
14	0.281
15	0.311
16	0.311
17	0.368
18	0.375
19	0.497
20	0.571
21	0.859
22	0.933

23	0.962
24	1.012
25	1.044
26	1.12
27	1.124
28	1.219
29	1.234
30	1.341
31	1.347
32	1.365
33	1.394
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36	1.735
37	2.011
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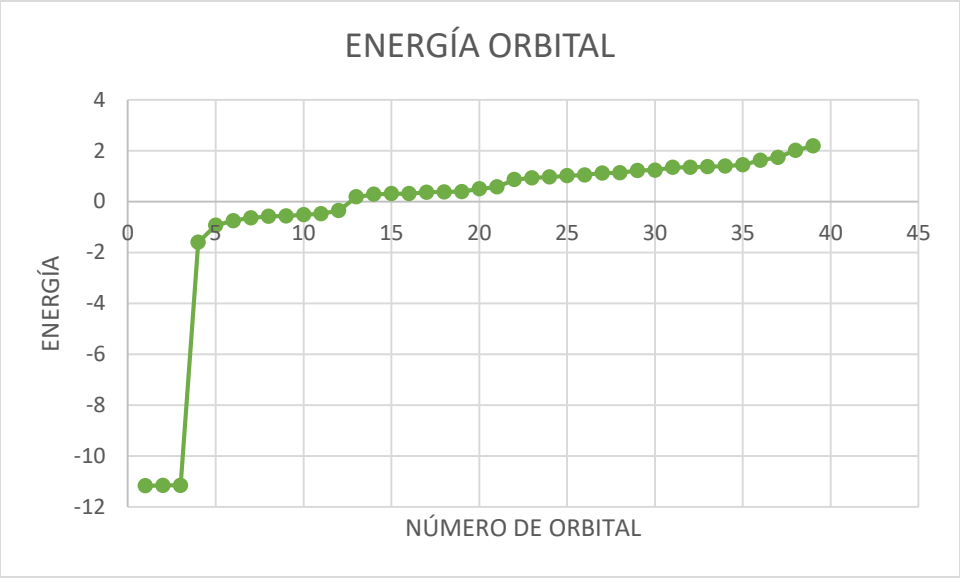
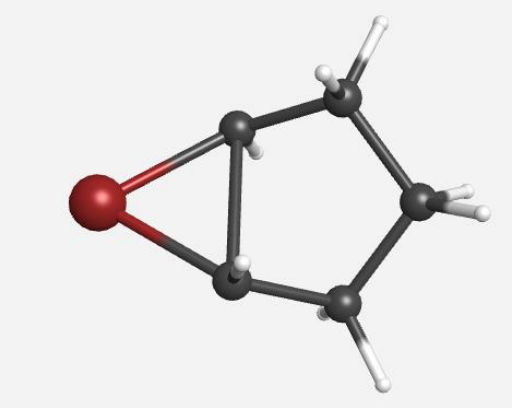
39	2.183

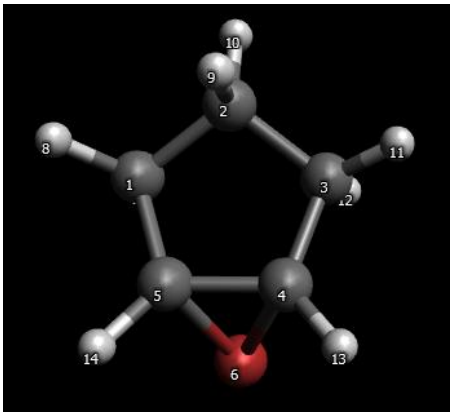


https://github.com/mariace2503/Parcial-N-1-Mar-a-C-rdoba/blob/main/Propileno.png

PROBLEMA N°4: ION BROMONIO

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





IÓN BROMONIO OPTIMIZADO

Bond 6	C-Br	C5	Br	1	No	1.98376
Bond 7	C-Br	C4	Br	1	No	1.97618

Angle Properties

	Type	Start Atom	Vertex	End Atom	Angle (°)
Angle 1	CCC	C2	C1	C5	102.3813
Angle 2	CCH	C2	C1	H1	111.6149
Angle 3	CCH	C2	C1	H2	109.9606
Angle 4	CCH	C5	C1	H1	110.3404
Angle 5	CCH	C5	C1	H2	113.2236
Angle 6	HCH	H1	C1	H2	109.2141
Angle 7	CCC	C1	C2	C3	104.1360
Angle 8	CCH	C1	C2	H3	106.5979
Angle 9	CCH	C1	C2	H4	115.4640
Angle 10	CCH	C3	C2	H3	106.6229
Angle 11	CCH	C3	C2	H4	115.4273
Angle 12	HCH	H3	C2	H4	107.9464
Angle 13	CCC	C2	C3	C4	102.5167
Angle 14	CCH	C2	C3	H5	109.9728
Angle 15	CCH	C2	C3	H6	111.5532
Angle 16	CCH	C4	C3	H5	113.2831
Angle 17	CCH	C4	C3	H6	110.1446
Angle 18	HCH	H5	C3	H6	109.2644
Angle 19	CCC	C3	C4	C5	107.7770
Angle 20	CCBr	C3	C4	Br	109.1815
Angle 21	CCH	C3	C4	H7	122.6648

Angle 22	CCBr	C5	C4	Br	68.6411
Angle 23	CCH	C5	C4	H7	128.2043
Angle 24	BrCH	Br	C4	H7	102.2694
Angle 25	CCC	C1	C5	C4	107.7323
Angle 26	CCBr	C1	C5	Br	108.6470
Angle 27	CCH	C1	C5	H8	122.3186
Angle 28	CCBr	C4	C5	Br	68.0880
Angle 29	CCH	C4	C5	H8	129.4397
Angle 30	BrCH	Br	C5	H8	99.8381
Angle 31	CBrC	C4	Br	C5	43.2709

https://github.com/mariace2503/Parcial-N-1-Mar-a-C-rdoba/blob/main/I%C3%B3n%20bromonio.png