QM206 - 2022
PARCIAL I

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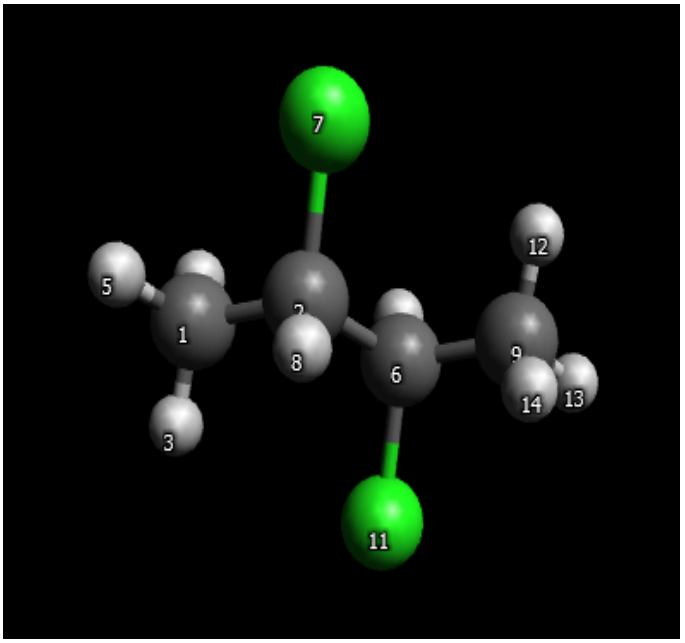
Realizar los siguientes cálculos utilizando los softwares utilizados en clases. Debe complementar sus cálculos con las imágenes correspondientes y anexar el enlace Github de los archivos generados.

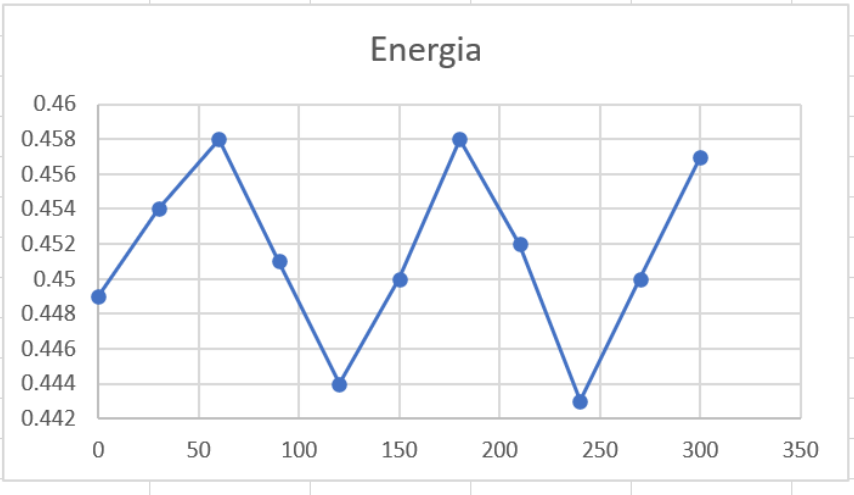
PROBLEMA 1: DIAGRAMA DE ENERGÍA

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



energía vs angulo

Angulo	Energia
0	0.449
30	0.454
60	0.458
90	0.451
120	0.444
150	0.45
180	0.458
210	0.452
240	0.443
270	0.45
300	0.457



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

Vibrational Modes

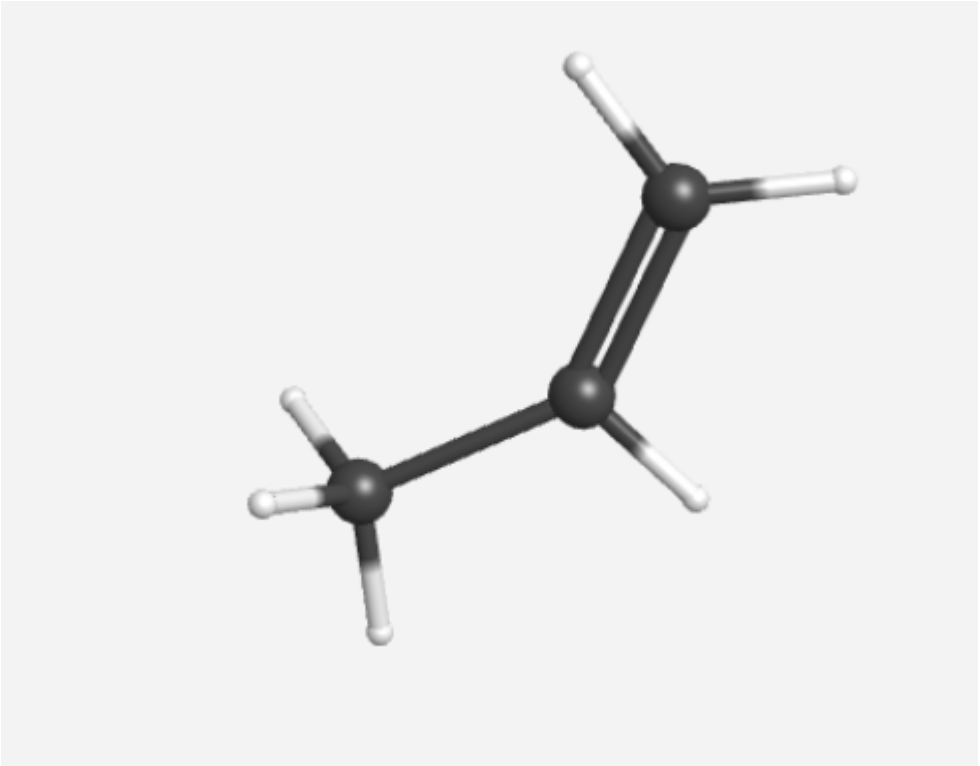
Show all

Mode	Symmetry	Frequency (cm^{-1})	IR Intensity	Raman Intensity	Actions
1	A	-143.55 (-175.7040)	0.5223	0.6785	
2	A	169.10 (206.9734)	1.1231	3.0150	
3	A	286.24 (350.3560)	7.3426	7.8133	
4	A	517.51 (633.4219)	2.6194	5.4783	
5	A	708.34 (866.9964)	47.7724	2.2225	
6	A	731.61 (895.4844)	20.2254	8.0998	
7	A	789.42 (966.2438)	12.4249	4.0160	
8	A	913.97 (1118.6891)	5.1124	0.5701	
9	A	940.67 (1151.3752)	10.1770	0.7179	
10	A	970.81 (1188.2629)	0.0217	3.0806	

11	A	1028.06 (1258.3402)	18.9603	10.1859		
12	A	1081.11 (1323.2692)	30.2371	8.9419		
13	A	1089.80 (1333.9028)	0.7502	4.3253		
14	A	1176.50 (1440.0195)	26.3300	5.5513		
15	A	1204.61 (1474.4347)	9.5497	10.8541		
16	A	1261.72 (1544.3334)	18.7690	1.2391		
17	A	1284.17 (1571.8090)	1.2403	0.4156		
18	A	1340.31 (1640.5269)	14.2790	13.9042		
19	A	1387.05 (1697.7344)	1.3237	32.5396		
20	A	1439.43 (1761.8428)	74.3840	2.7904		
21	A	1478.89 (1810.1468)	0.0135	15.1565		
22	A	1522.45 (1863.4627)	4.0912	12.7815		
23	A	1555.94 (1904.4524)	6.4311	35.6431		
24	A	2660.89 (3256.8993)	111.7134	3.1496		
25	A	2674.71 (3273.8248)	14.1120	163.0236		
26	A	2710.14 (3317.1872)	49.1087	52.4360		
27	A	2715.10 (3323.2605)	0.3179	55.4759		
28	A	2721.47 (3331.0559)	12.0269	58.5434		
29	A	2796.76 (3423.2038)	17.8109	46.8046		
30	A	2852.77 (3491.7616)	1.1500	40.6812		

PROBLEMA 3: ORBITALES MOLECULARES

a) Construya un diagrama de energía para los orbitales moleculares del propileno.



b) 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
				> -1.31732	
4	-	2	-	-0.99554	
5	-	2	-	-0.91795	
6	-	2	-	-0.76049	
7	-	2	-	-0.6014	
8	-	2	-	-0.56851	
9	-	2	-	-0.56735	
10	-	2	-	-0.51024	
11	-	2	-	-0.47388	
12	-	2	-	-0.31732	
13	-	0	-	0.1431	
14	-	0	-	0.24235	
15	-	0	-	0.27483	
16	-	0	-	0.29109	
17	-	0	-	0.30509	
18	-	0	-	0.33121	
19	-	0	-	0.33488	
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22	-	0	-	0.67989	

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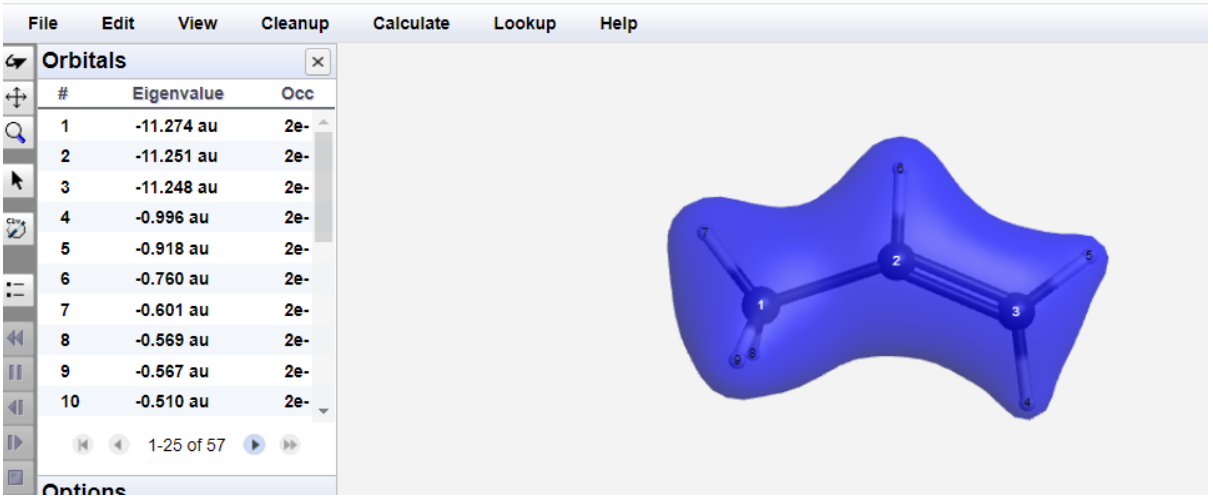
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9 -0.567 au 2e-
10 -0.510 au 2e-
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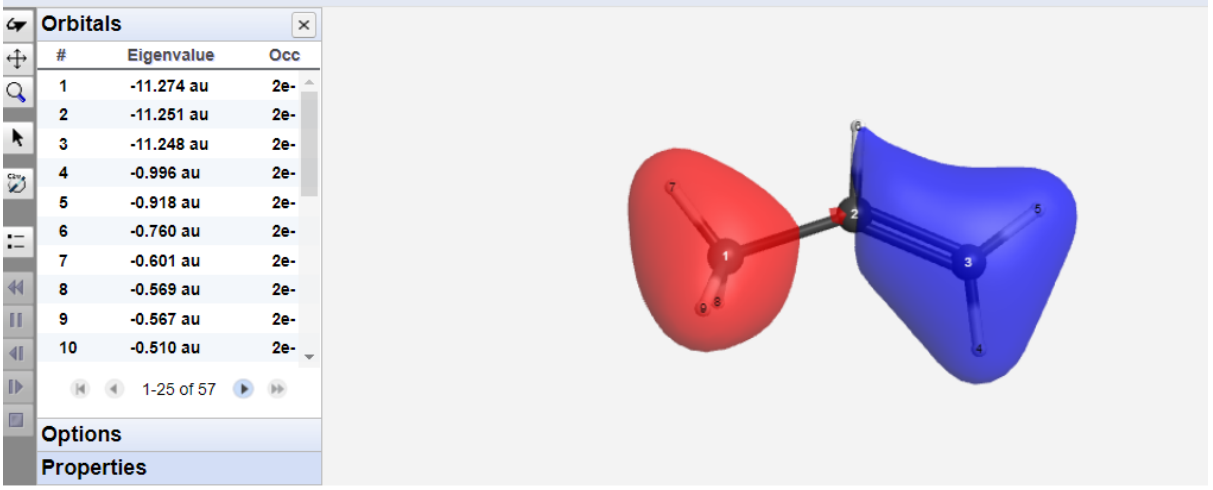
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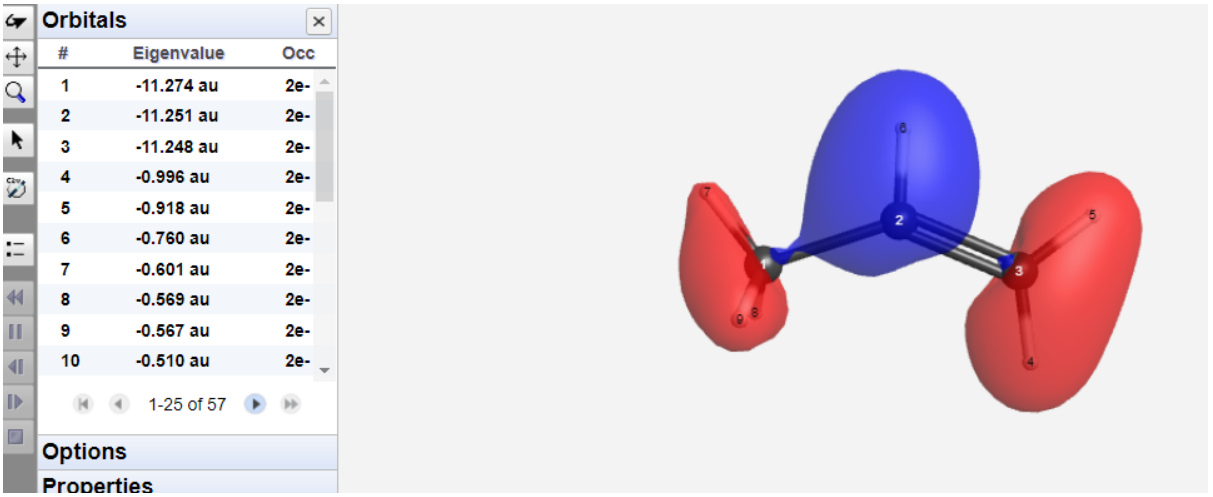
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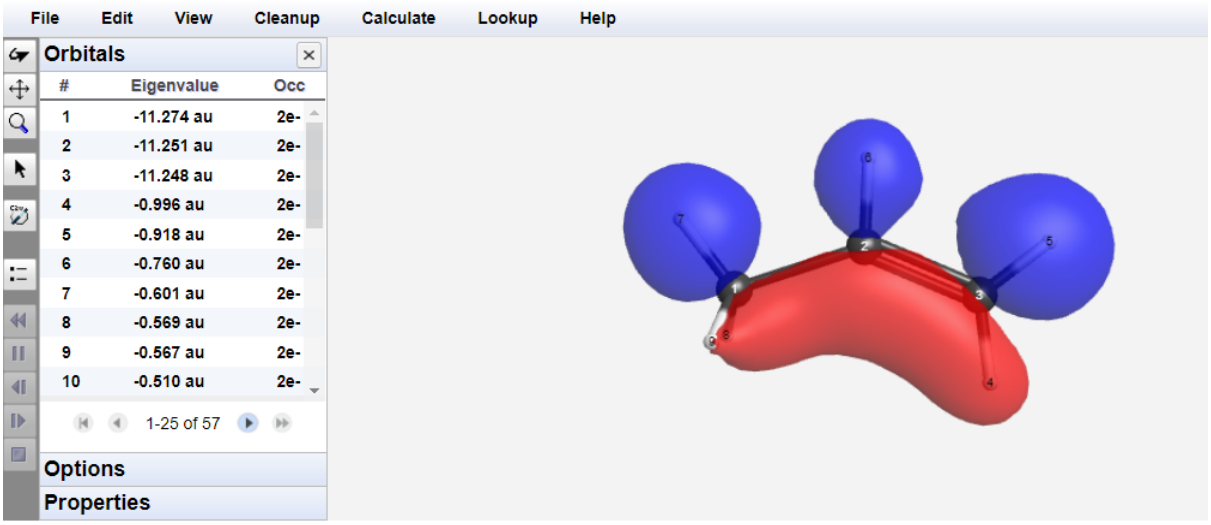
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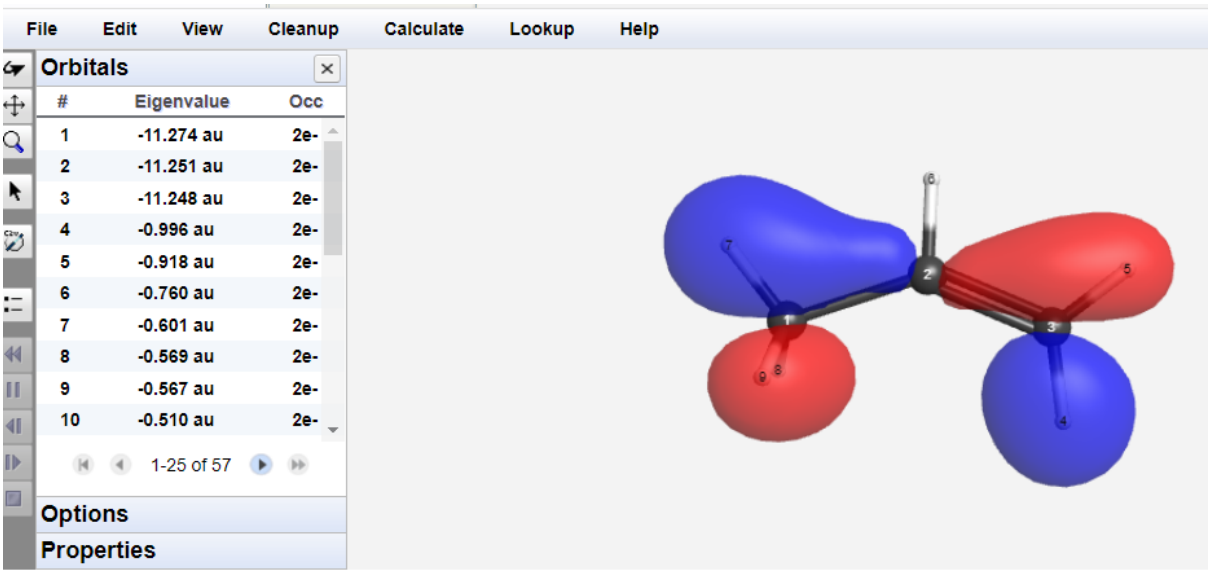
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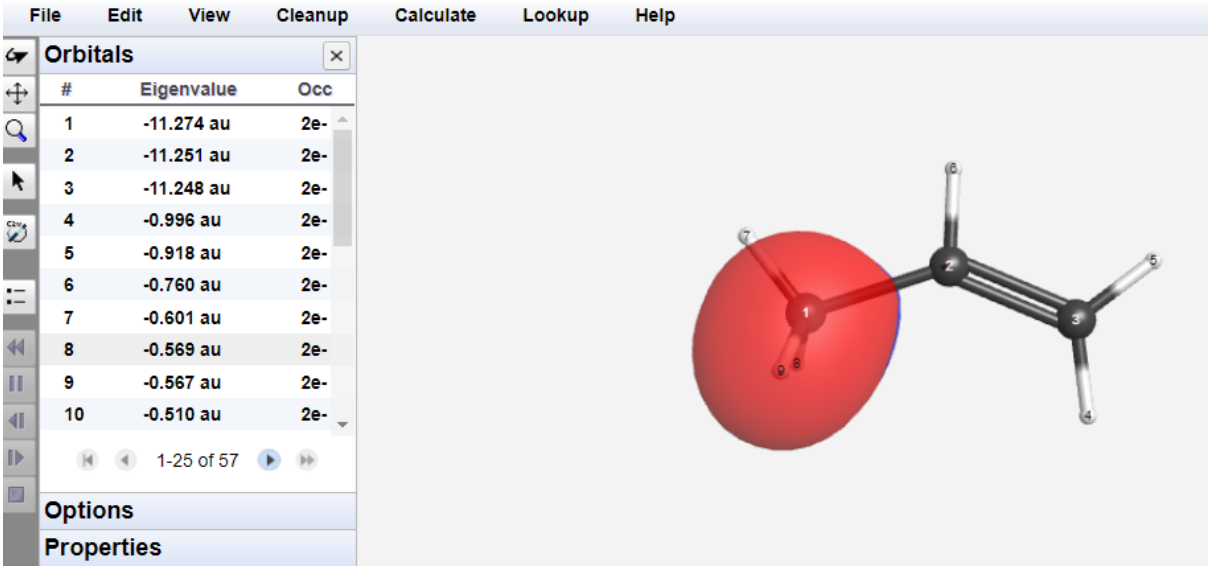
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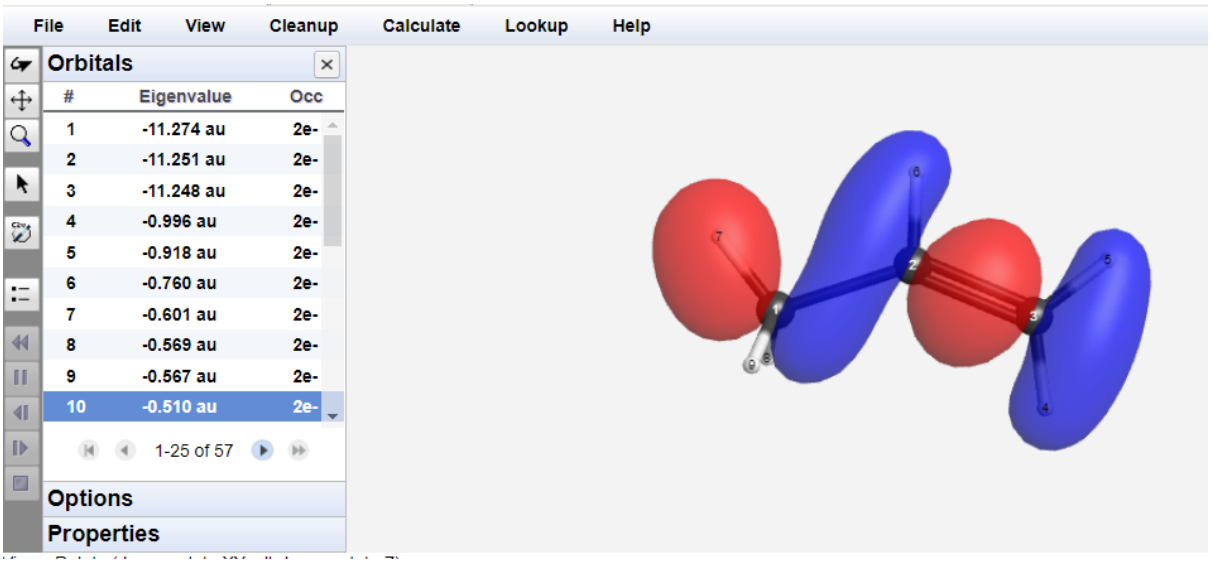
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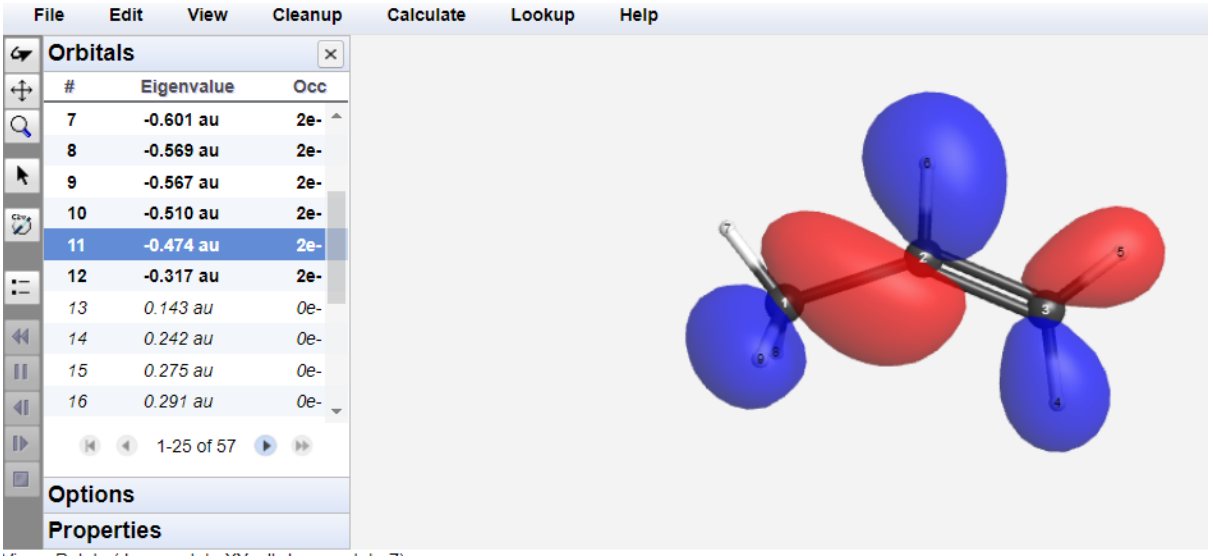
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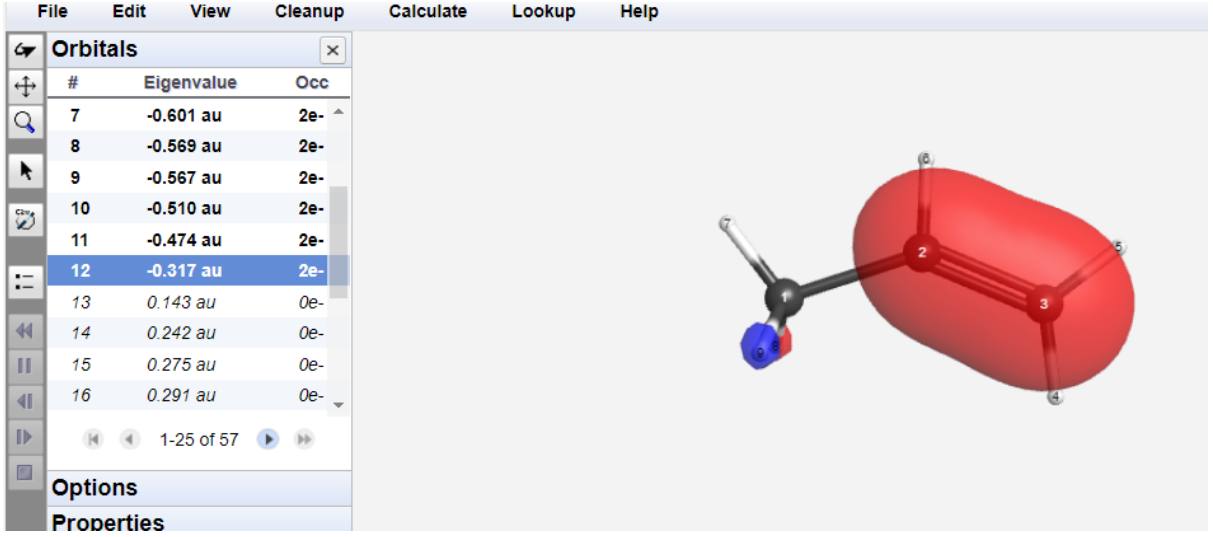
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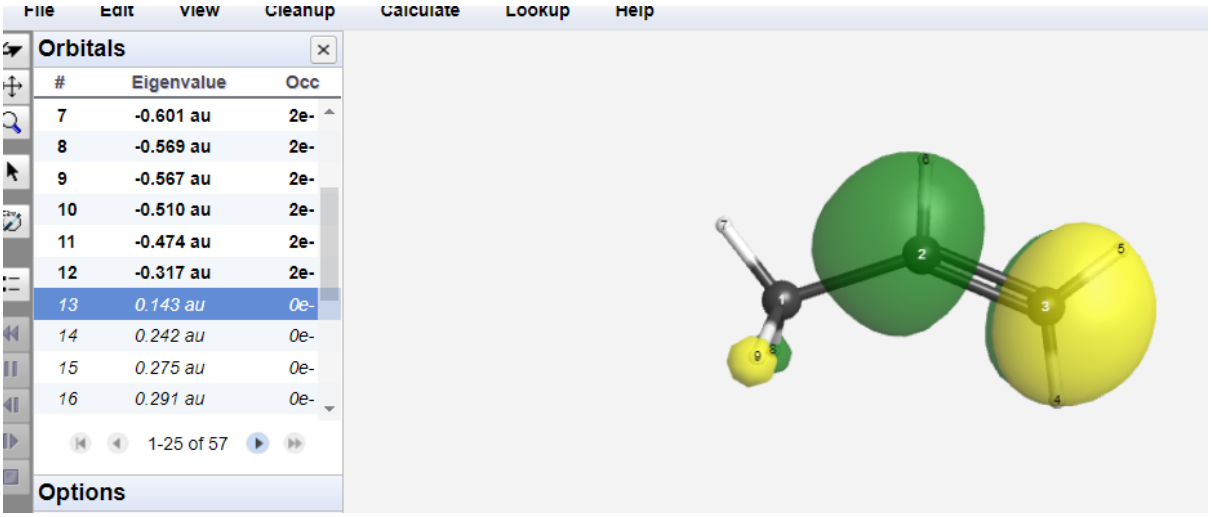
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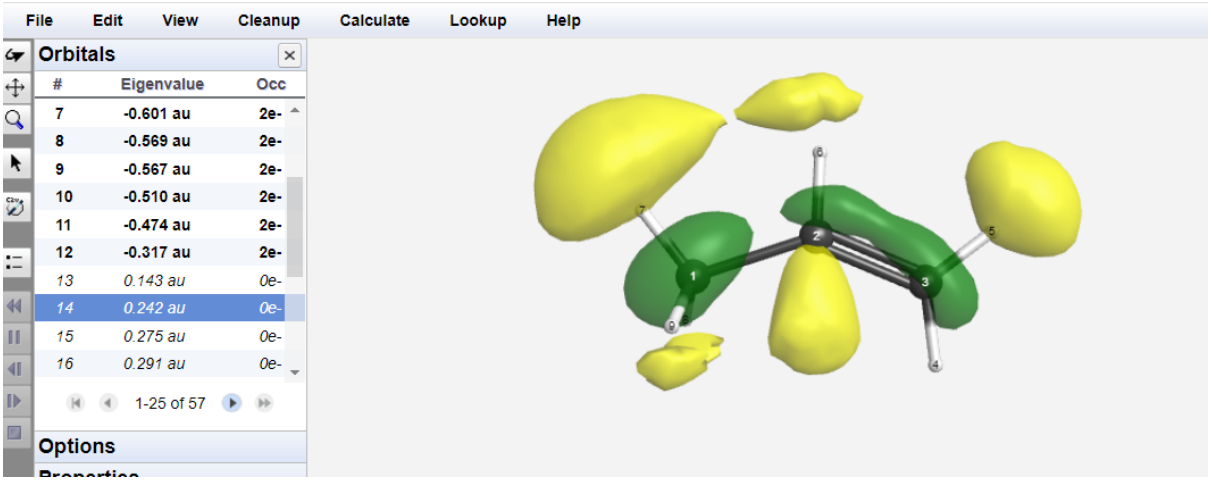
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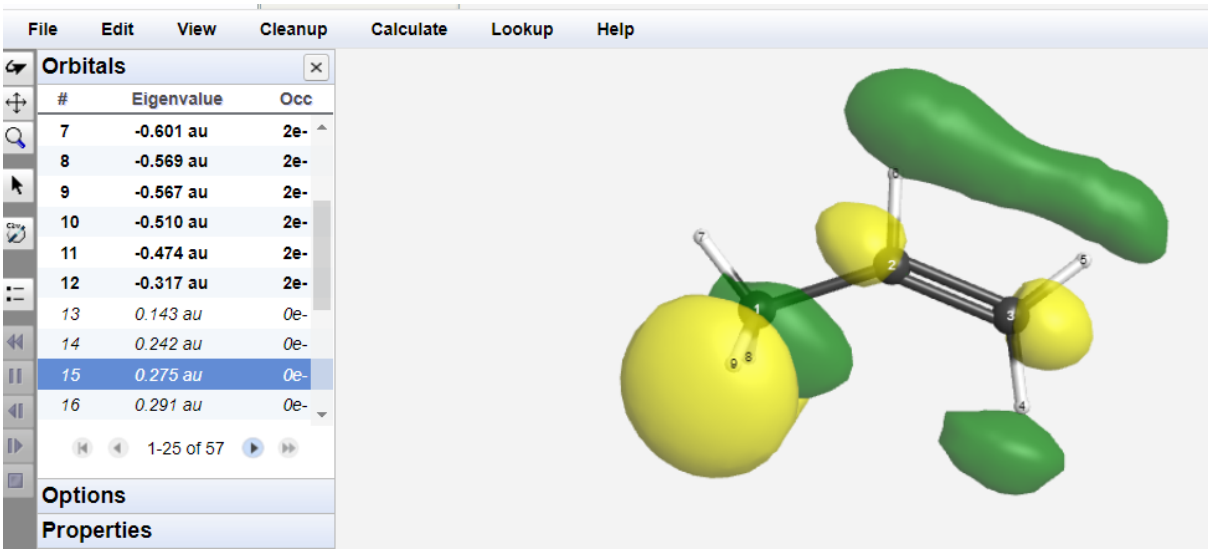
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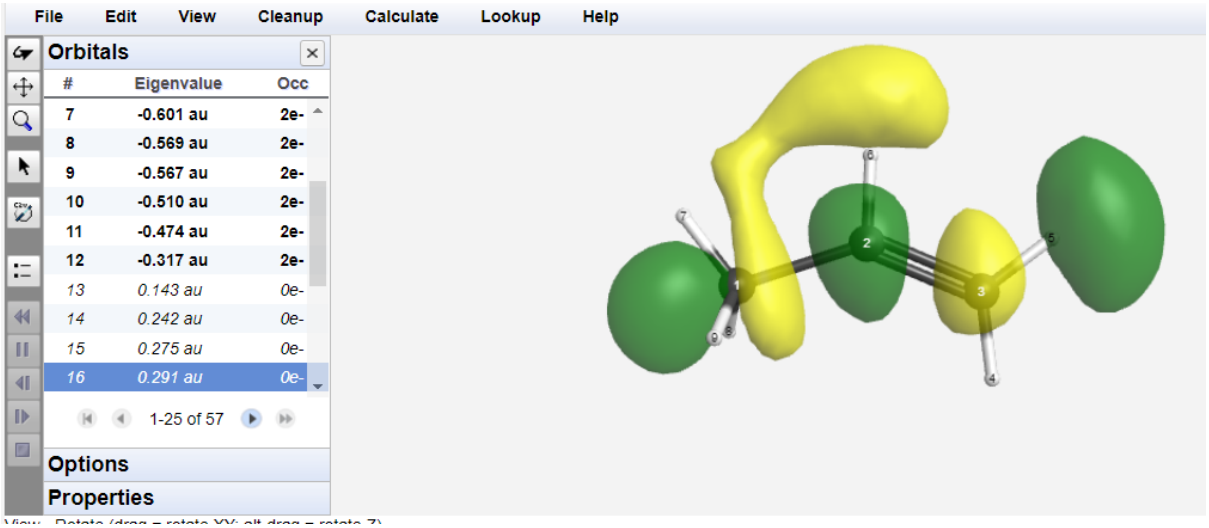
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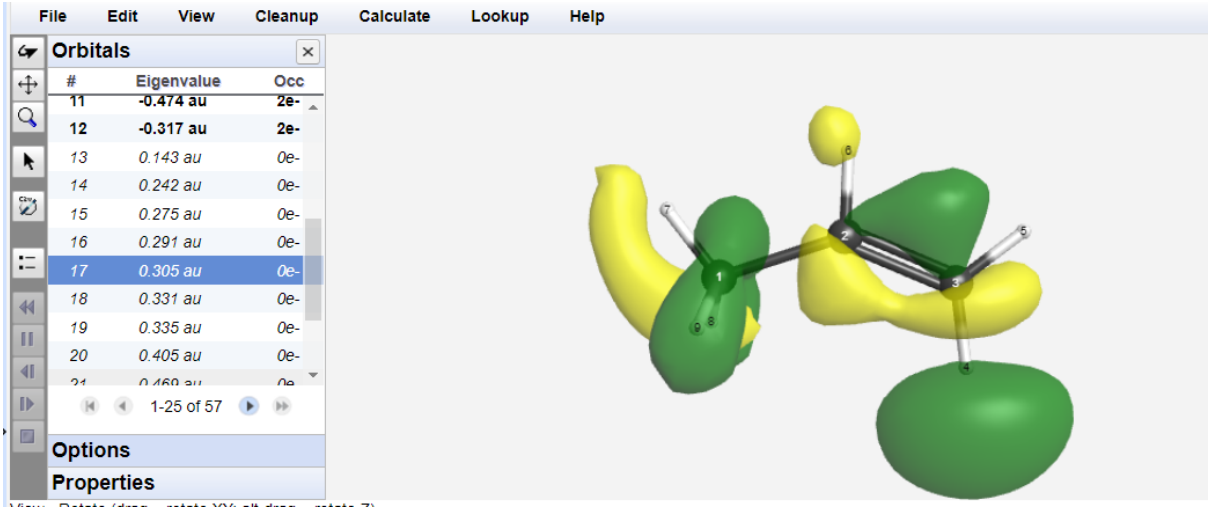
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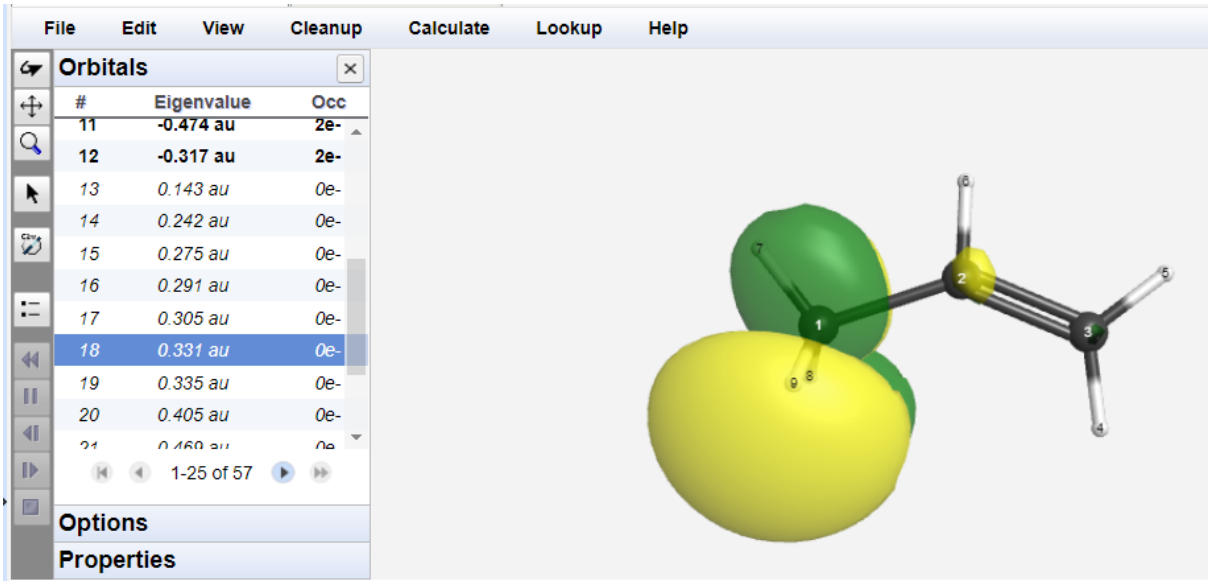
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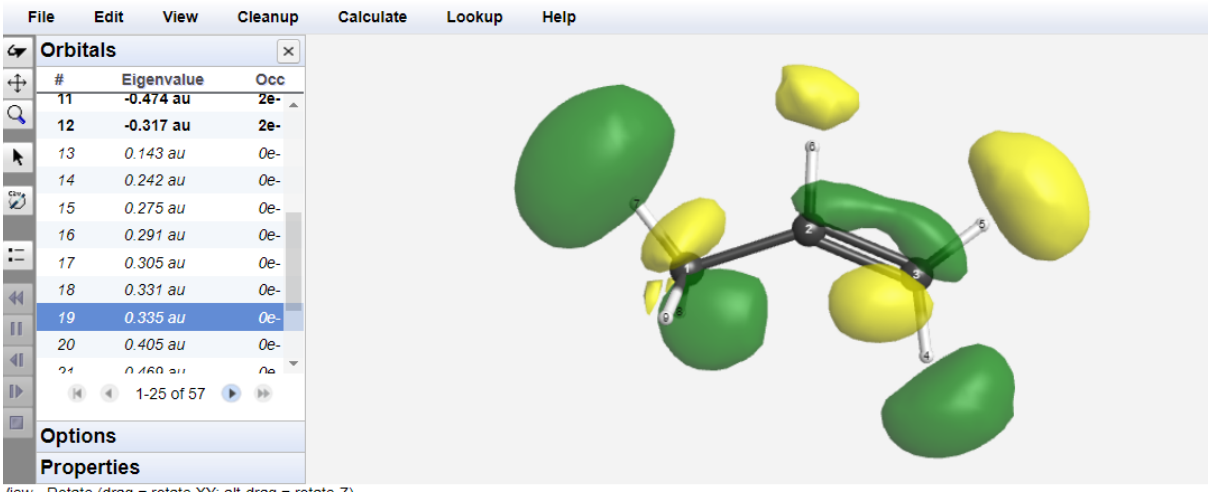
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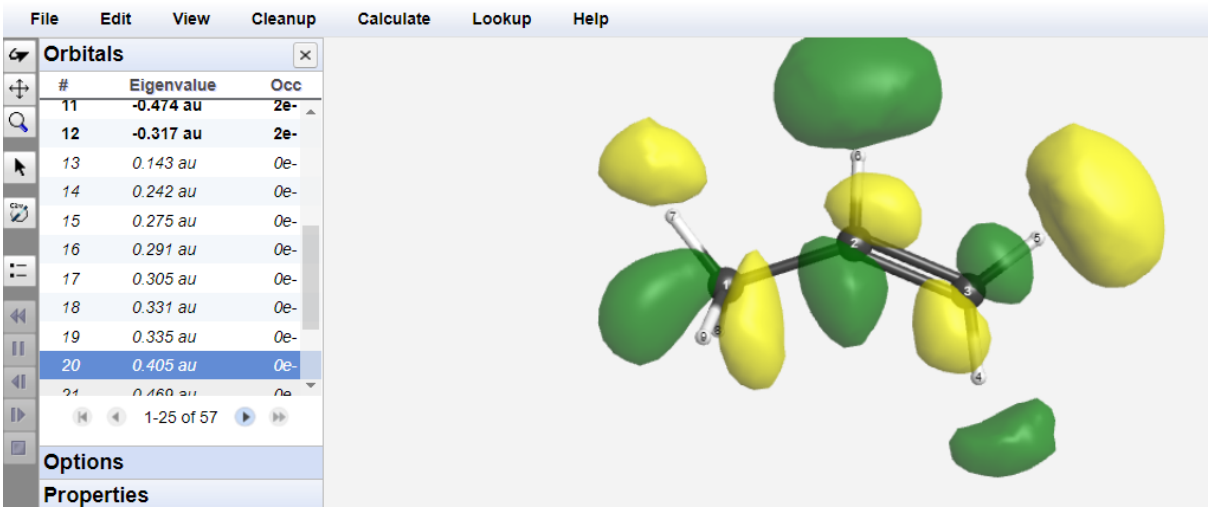
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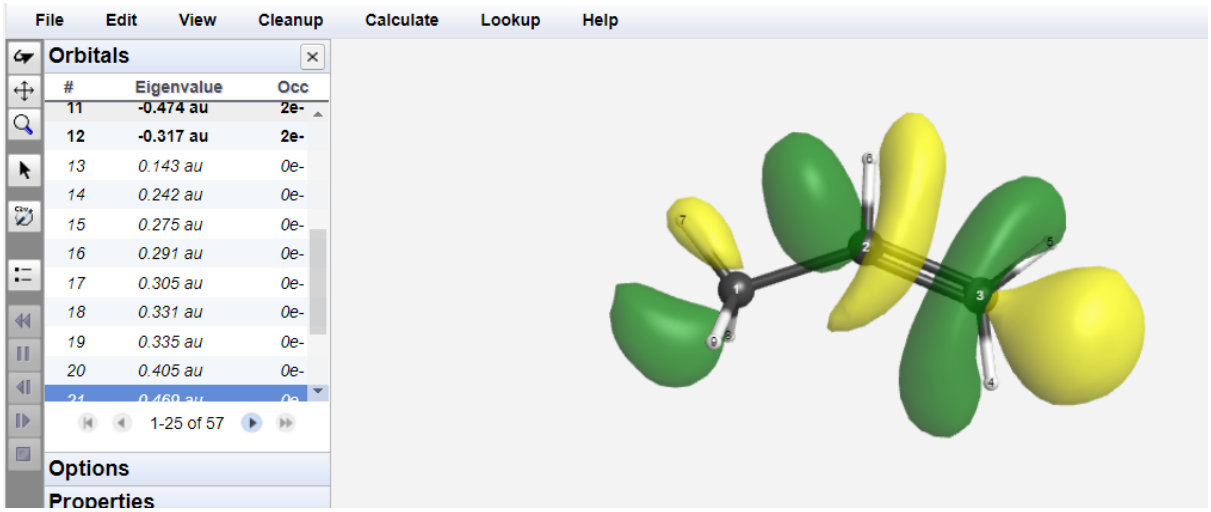
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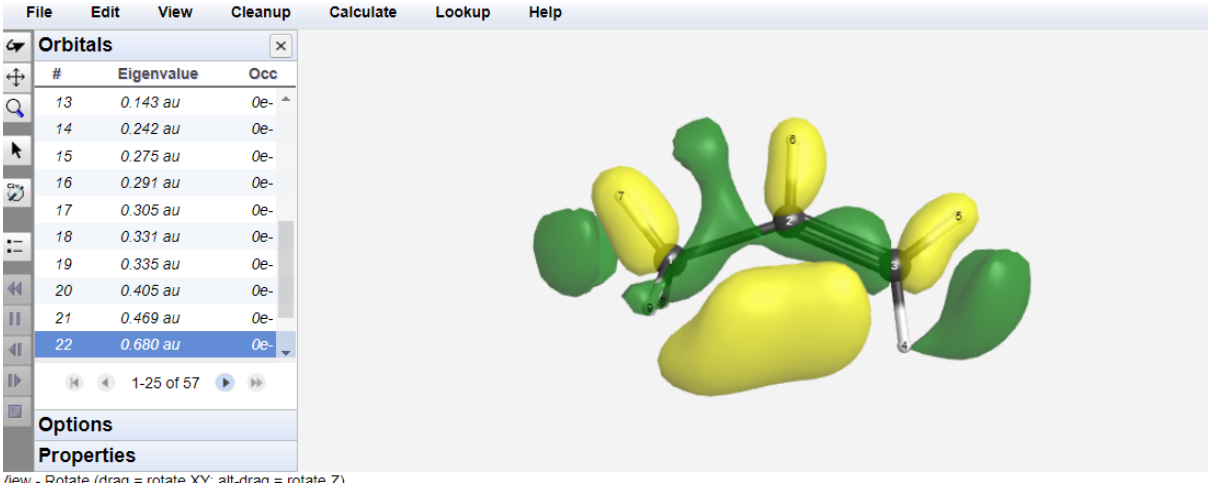
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Options
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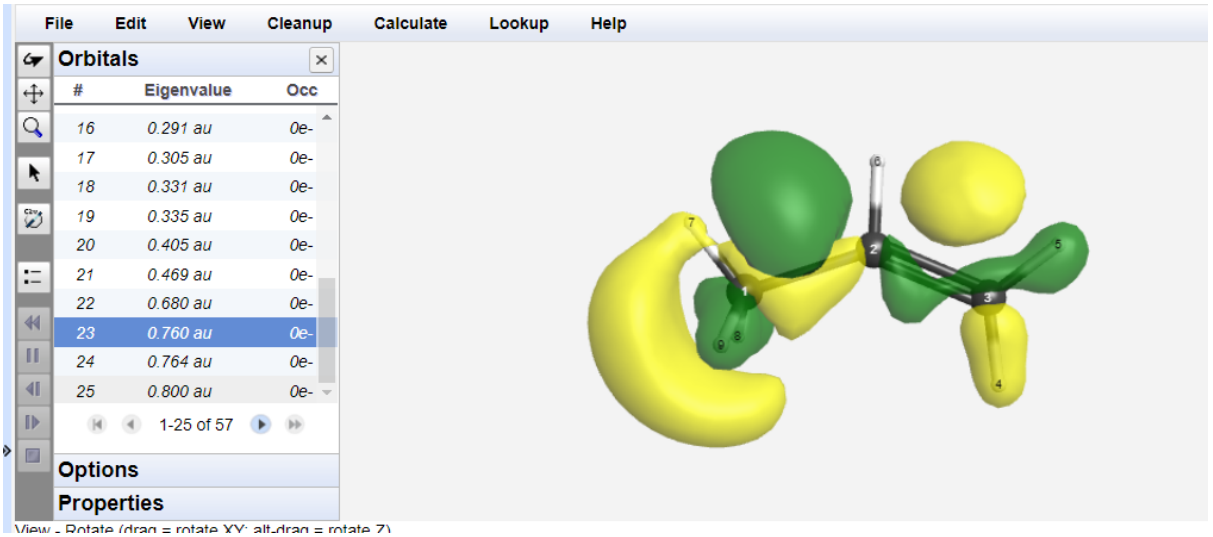
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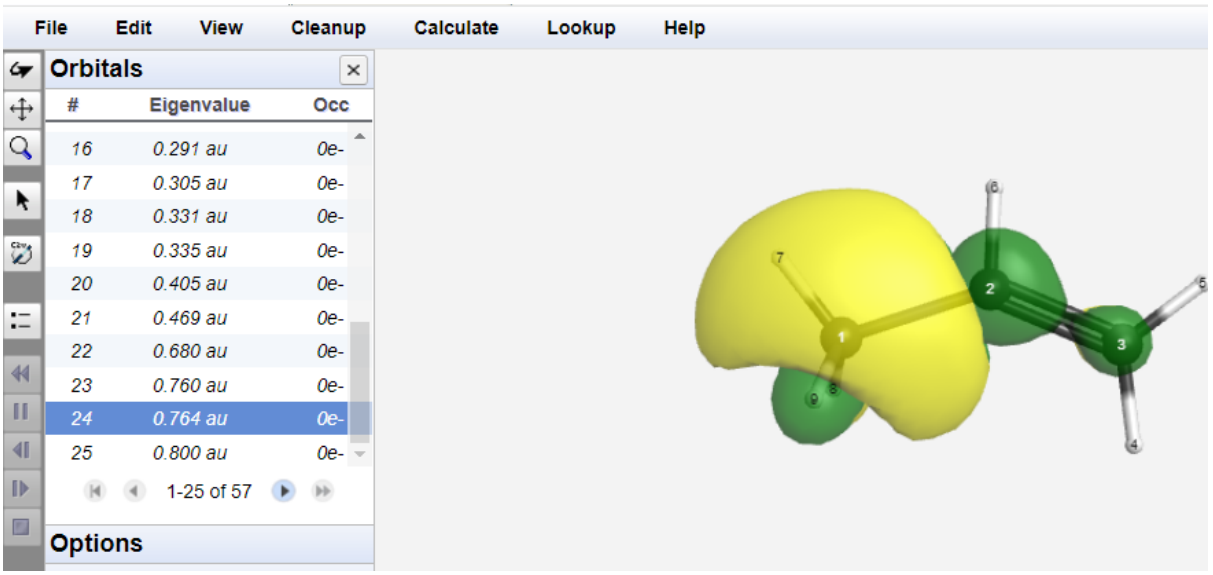
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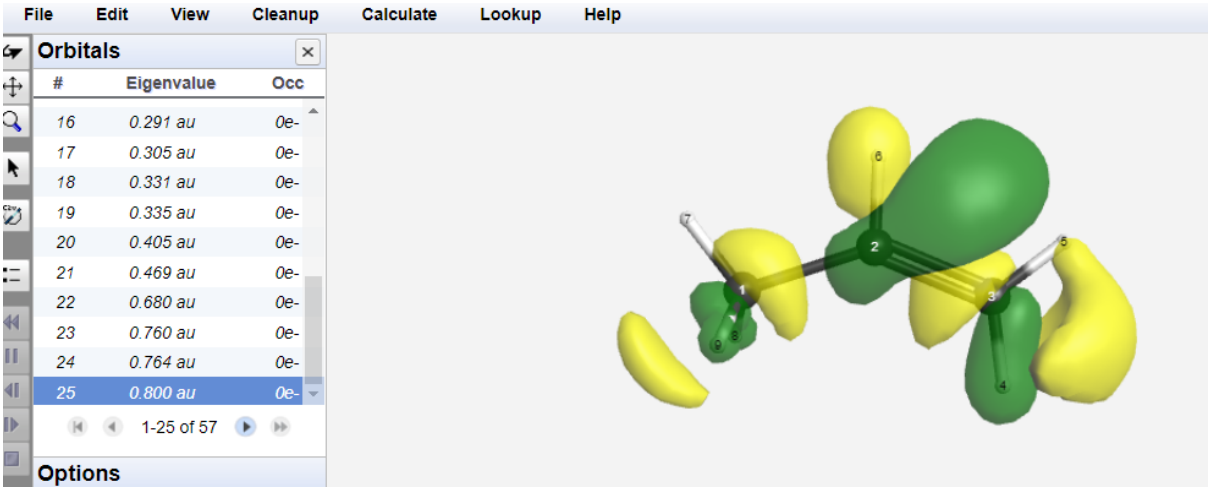
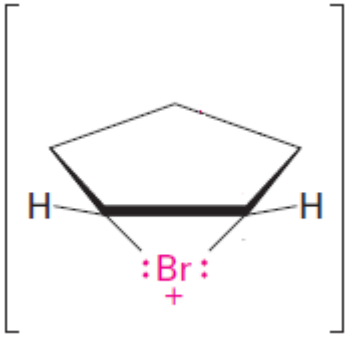
Options

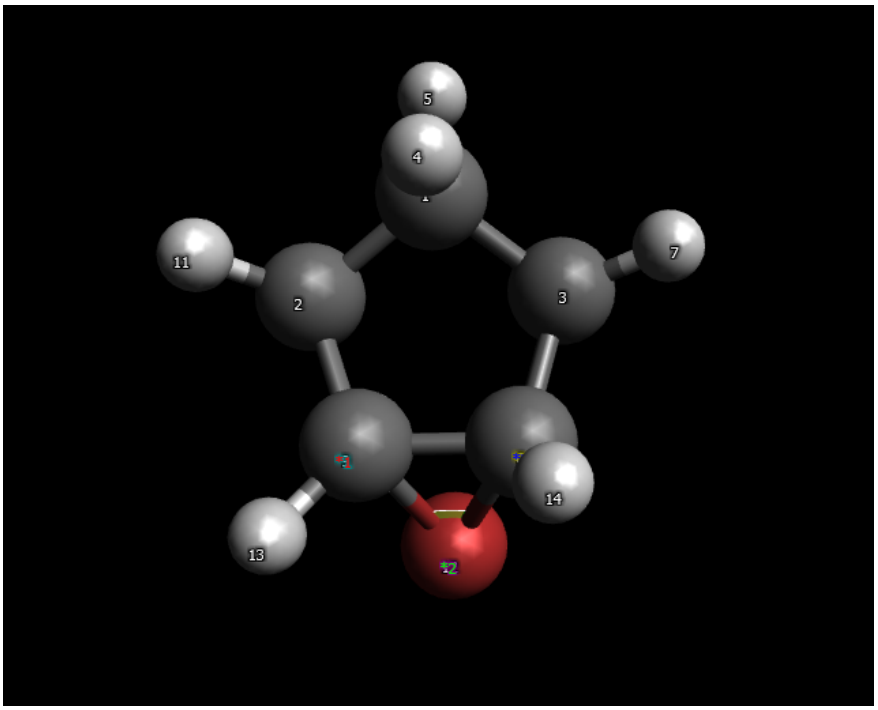
25-



PROBLEMA 4: IÓN BROMONIO



a) Determine la estructura del ión bromonio indicado.

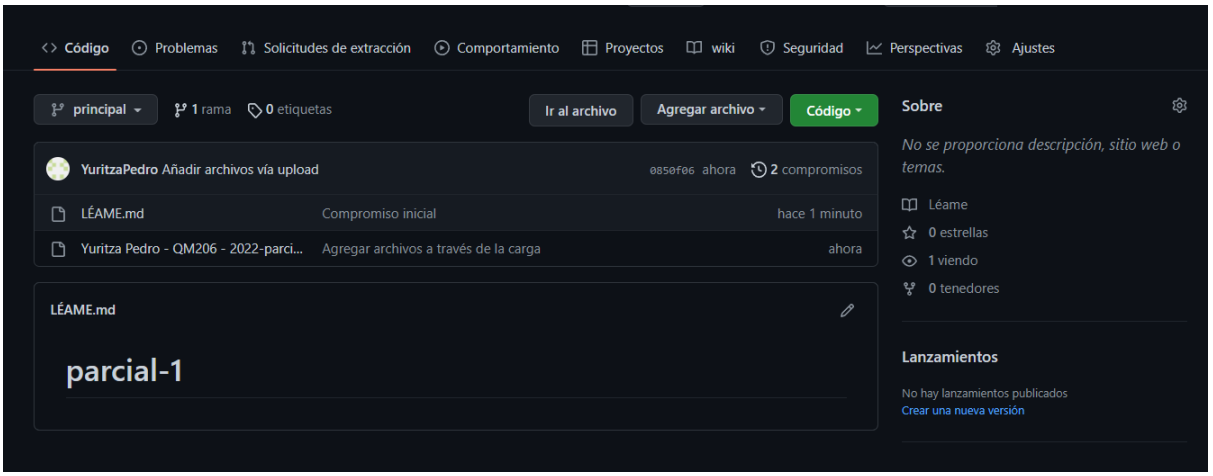


b) Señale los ángulos correspondientes y distancia de enlaces C-Br

Bond Properties

	Type	Start Atom	End Atom	Bond Order	Rotatable	Length (Å)
Bond 1	C-C	C1	C2	1	Yes	1.51405
Bond 2	C-C	C1	C3	1	Yes	1.50778
Bond 3	C-H	C1	H1	1	No	1.11498
Bond 4	C-H	C1	H2	1	No	1.11057
Bond 5	C-C	C3	C4	1	Yes	1.53354
Bond 6	C-H	C3	H3	1	No	1.11034
Bond 7	C-H	C3	H4	1	No	1.11356
Bond 8	C-C	C4	C5	1	No	1.46697
Bond 9	C-C	C5	C2	1	Yes	1.52642
Bond 10	C-H	C2	H5	1	No	1.1125
Bond 11	C-H	C2	H6	1	No	1.11057
Bond 12	C-Br	C5	Br	1	No	1.9864
Bond 13	C-H	C5	H7	1	No	1.11005
Bond 14	C-Br	C4	Br	1	No	1.97382
Bond 15	C-H	C4	H8	1	No	1.11068

parcial enviado en Github



https://github.com/YuritzaPedro/parcial-1/blob/main/Yuritza%20Pedro%20-%20QM206%20-%202022-parcial1.pdf