

QM206 - 2022
PARCIAL I

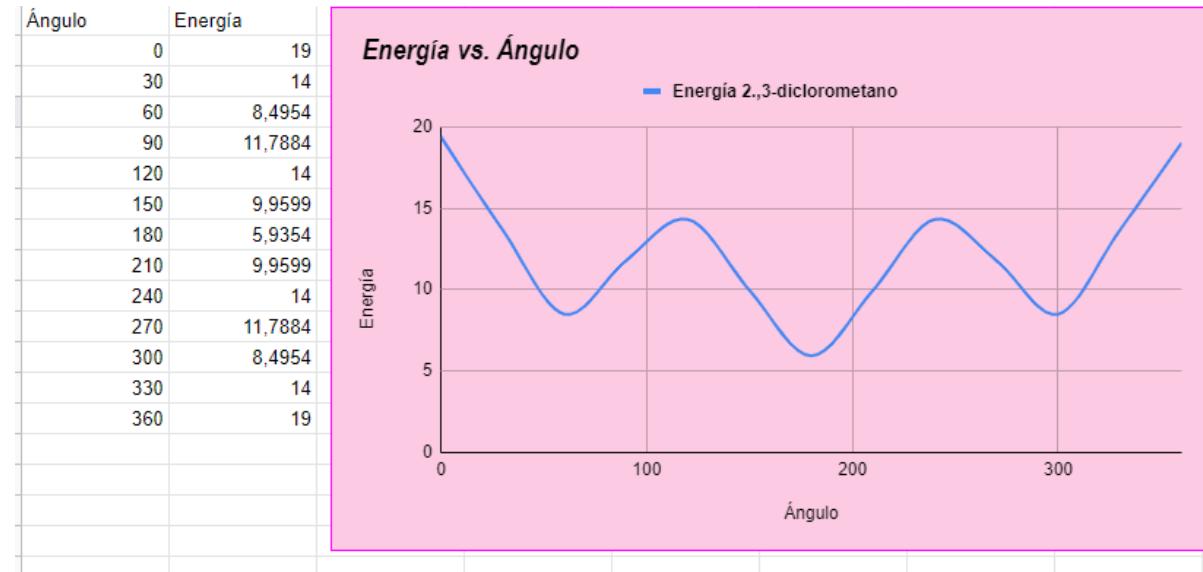
NOMBRE: Yaiseth Gaitán

4-823-571

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.

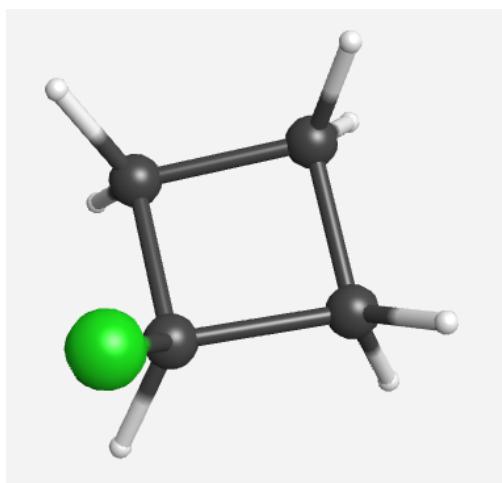
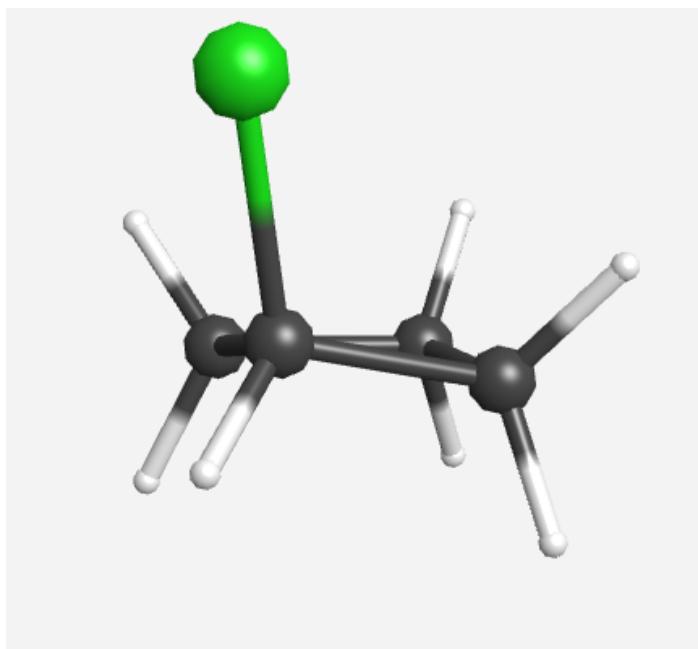
PROBLEMA 1: DIAGRAMA DE ENERGÍA

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

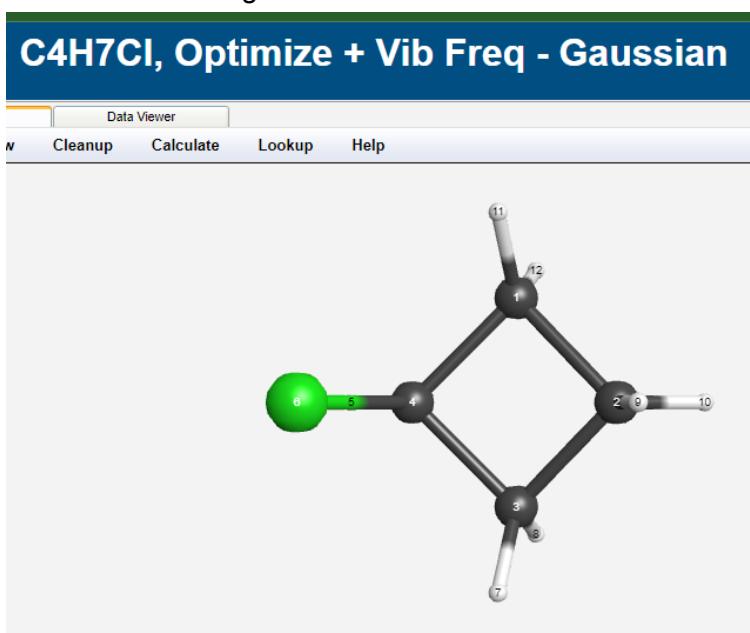


PROBLEMA 2: OPTIMIZACIÓN DE LA GEOMETRÍA

- Optimizar la geometría de la molécula de 1-clorociclobutano



- b) Encontrar las energías de los diferentes modos de vibración



						Show all
	Mode	Symmetry	Frequency (cm ⁻¹)	IR Intensity	Raman Intensity	Actions
1		A'	101.78 (112.3445)	1.0015	0.7212	
2		A''	311.77 (344.1201)	0.9071	2.6384	
3		A'	315.85 (348.6195)	3.8079	5.1545	
4		A'	555.17 (612.7728)	51.8615	23.2157	
5		A'	679.15 (749.6175)	13.6139	3.3343	
6		A''	730.87 (806.7016)	0.0426	0.0339	
7		A'	844.03 (931.5975)	3.0954	5.9689	
8		A''	858.15 (947.1862)	4.5556	7.7708	
9		A'	865.42 (955.2141)	2.0607	4.8849	
10		A''	899.46 (992.7832)	2.9399	11.9826	
11		A'	943.54 (1041.4341)	9.7534	26.9221	

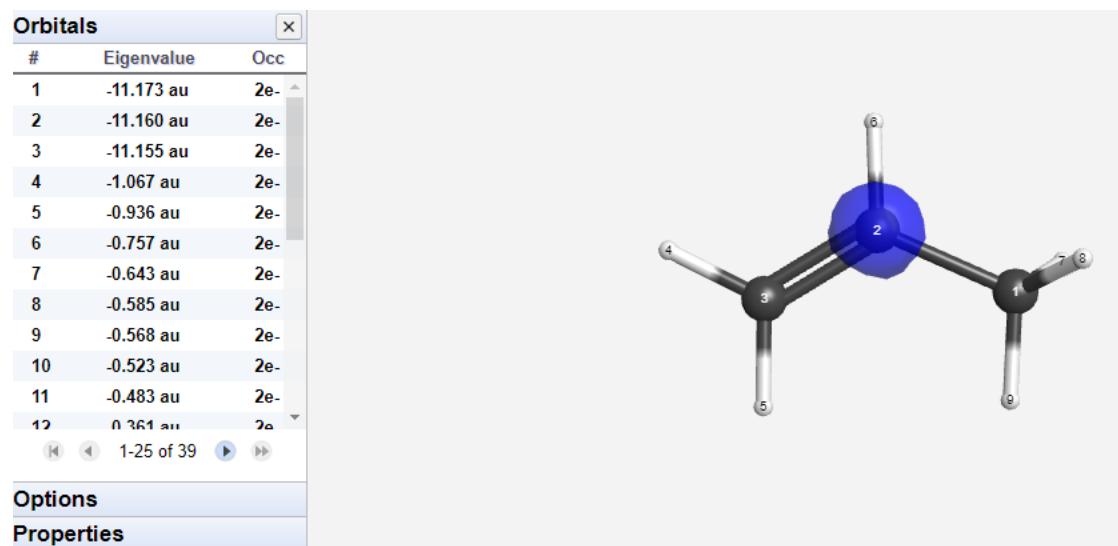
12	A'	1067.45 (1178.2033)	4.2038	6.6222		
13	A''	1075.88 (1187.5002)	0.0890	3.3945		
14	A''	1170.25 (1291.6659)	0.2922	2.9038		
15	A'	1185.84 (1308.8742)	16.2851	15.0842		
16	A''	1240.80 (1369.5417)	0.7716	11.4156		
17	A'	1256.96 (1387.3770)	43.1754	4.0340		
18	A''	1274.01 (1406.1954)	2.6038	0.1993		
19	A''	1286.07 (1419.5035)	0.7975	0.1285		
20	A'	1288.77 (1422.4823)	8.0154	2.5091		
21	A''	1466.76 (1618.9457)	10.0136	7.1947		
22	A'	1472.79 (1625.5916)	3.8891	20.8186		
23	A'	1495.13 (1650.2535)	1.4249	5.9498		
24	A''	2941.61 (3246.8148)	22.4317	25.7045		
25	A'	2944.57 (3250.0739)	12.2113	131.0920		
26	A'	2960.04 (3267.1523)	24.7061	109.6266		
27	A'	3005.53 (3317.3584)	6.8252	67.4663		
28	A''	3018.36 (3331.5187)	5.7132	63.1262		
29	A'	3023.93 (3337.6755)	11.8773	50.8215		
30	A'	3050.86 (3367.3978)	10.1235	90.6886		
Frequency Scale Factor				0.906		
Normal Mode Amplitude				1.0		
Animation Speed				50		
IR Spectrum						
Raman Spectrum						
Peak Width (cm ⁻¹)				40		

PROBLEMA 3: ORBITALES MOLECULARES

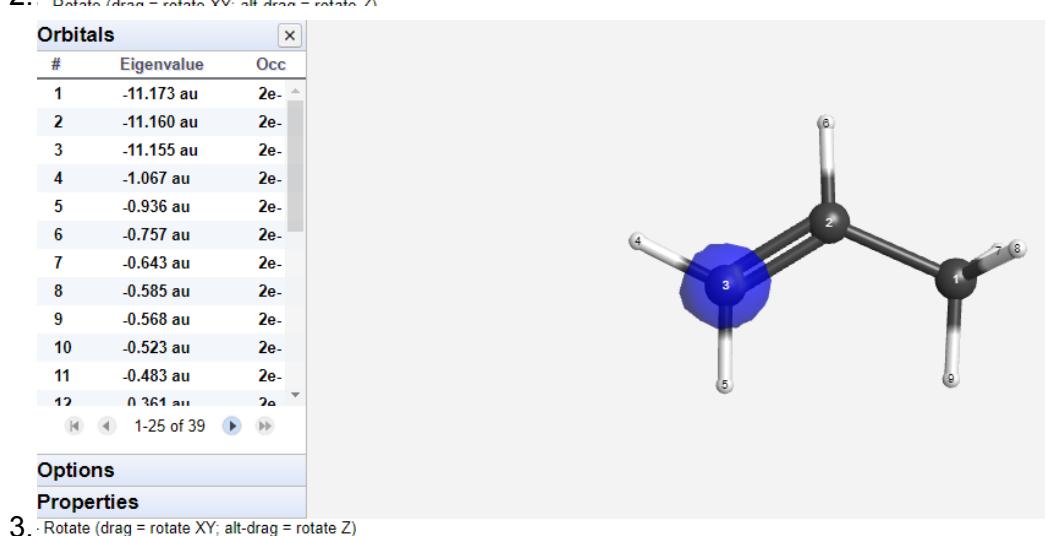
- a) Construya un diagrama de energía para los orbitales moleculares del propileno. Para cada nivel de energía presente la imagen con la estructura del OM correspondiente

1.

1.



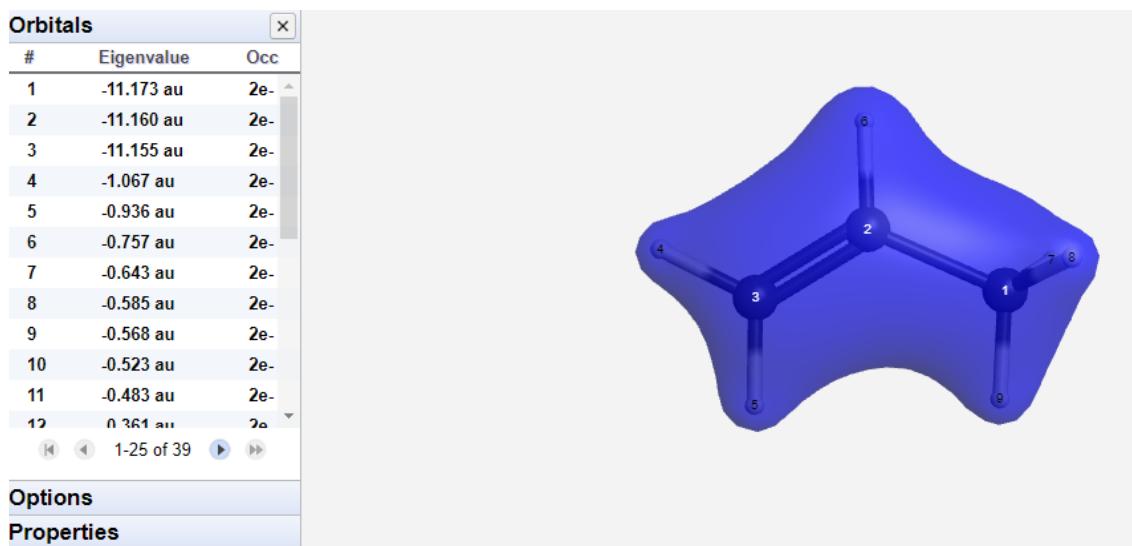
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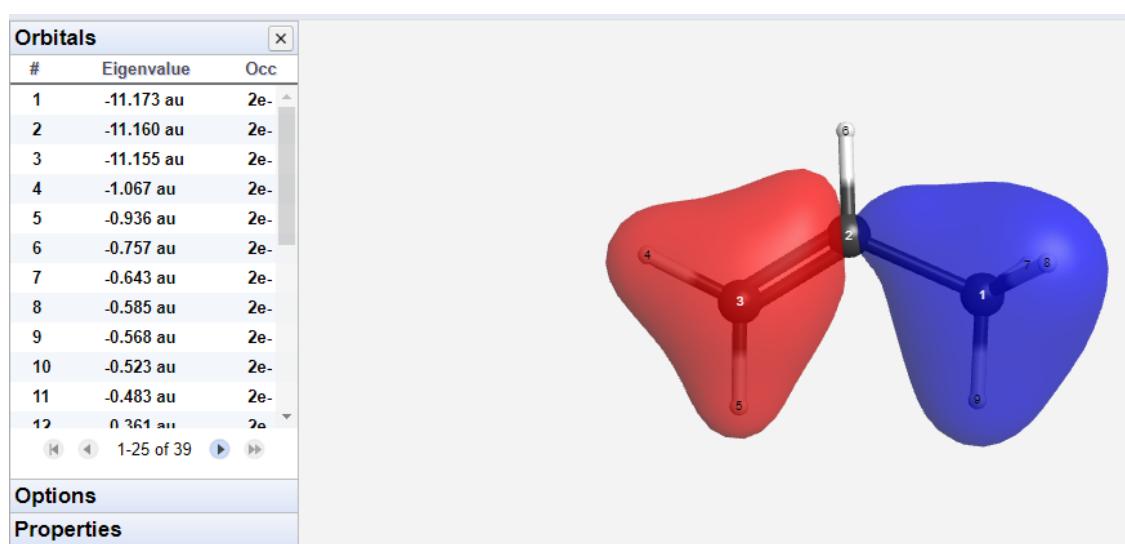
3.

Rotate (drag = rotate XY; alt-drag = rotate Z)

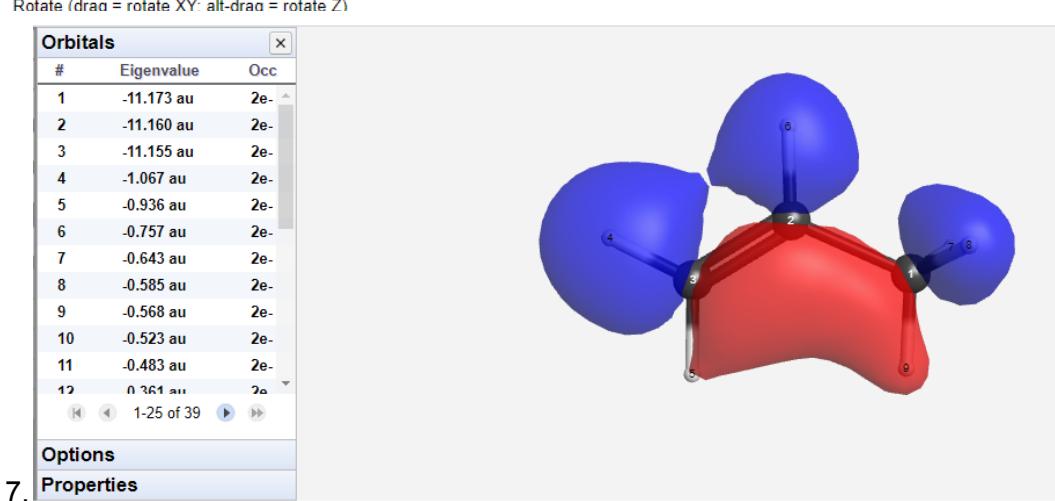
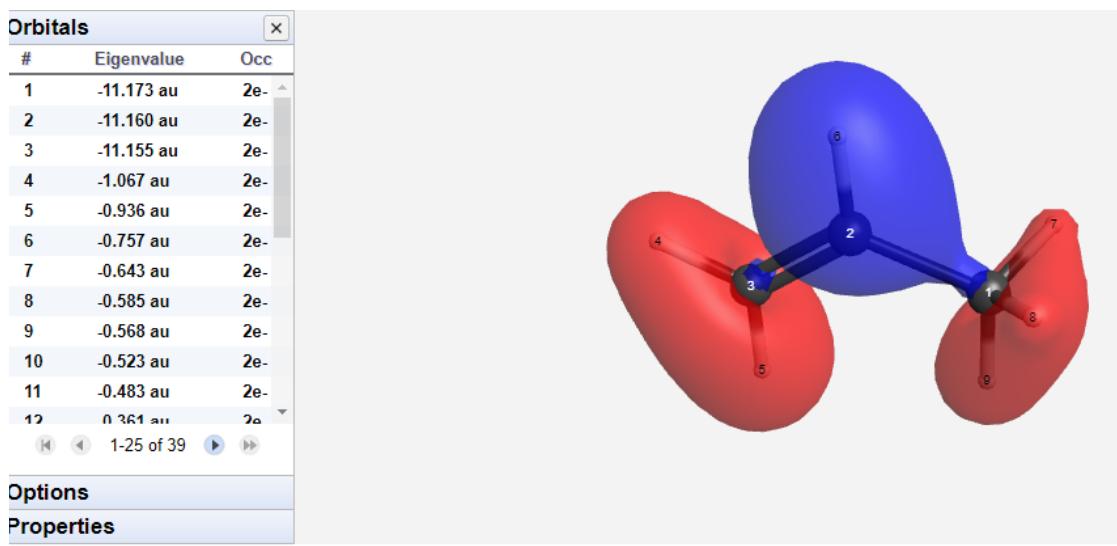
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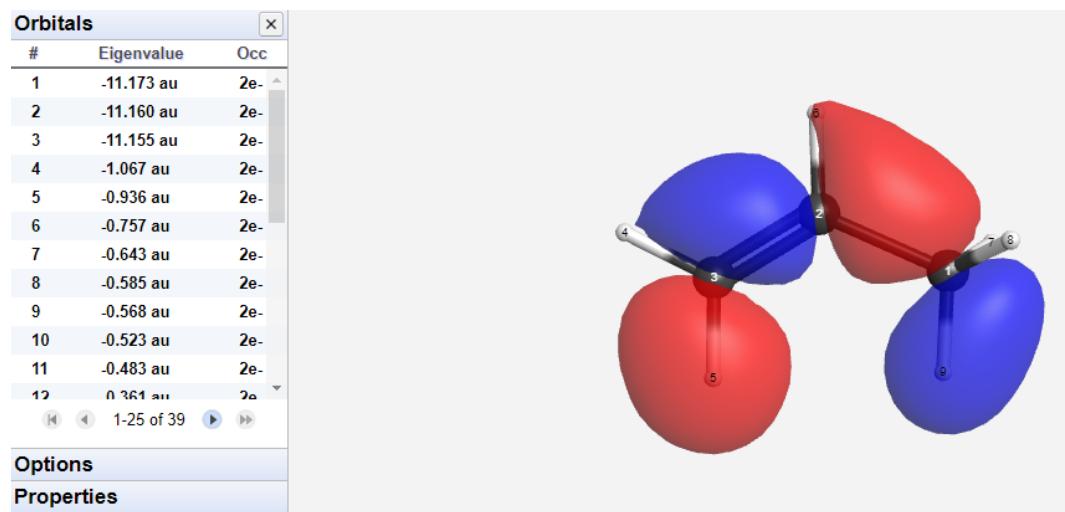


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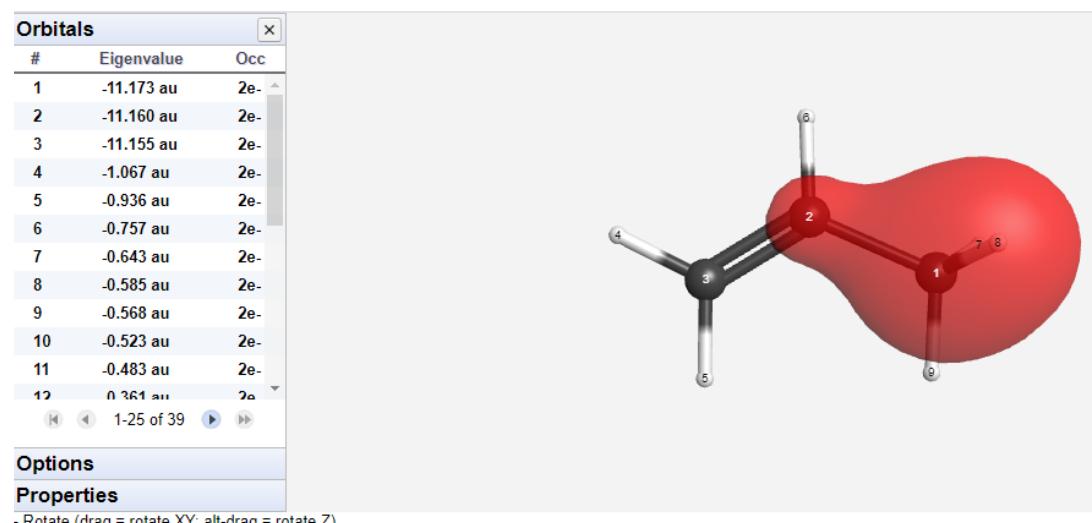


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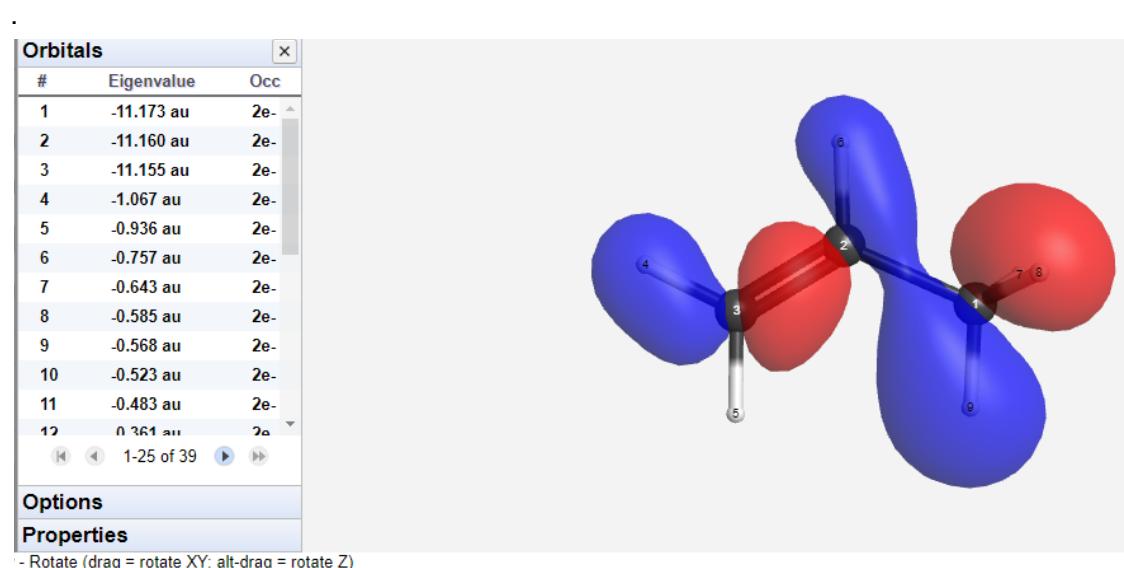




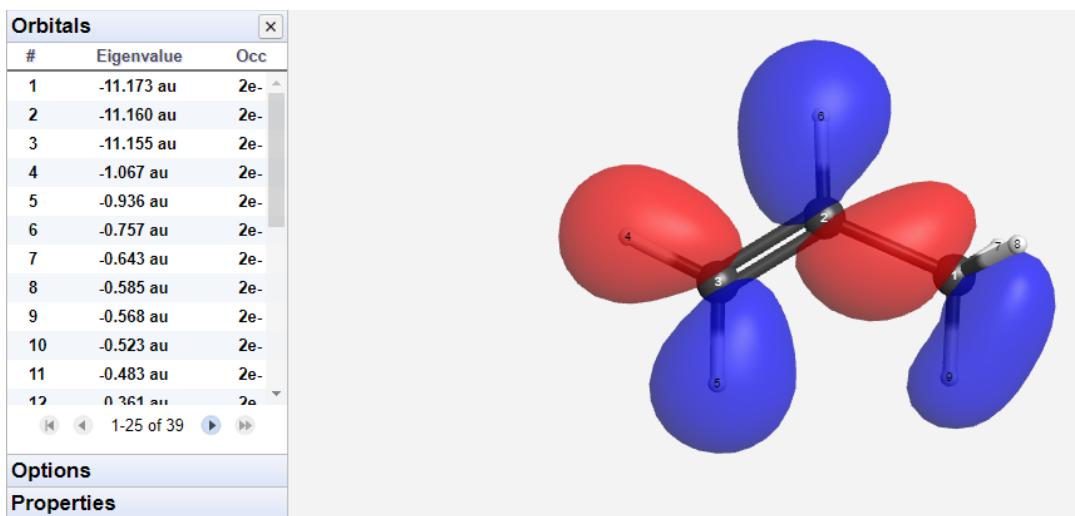
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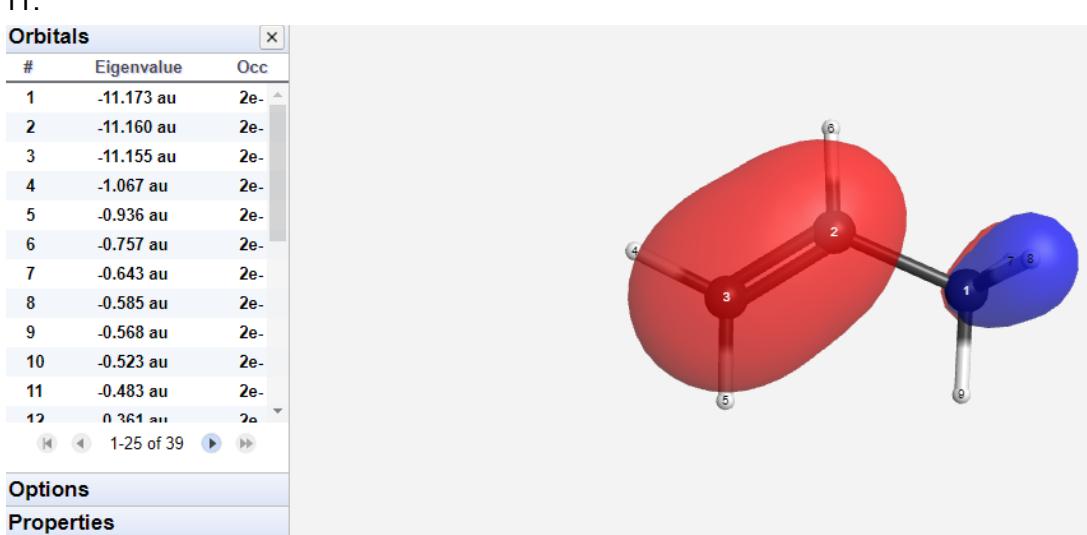
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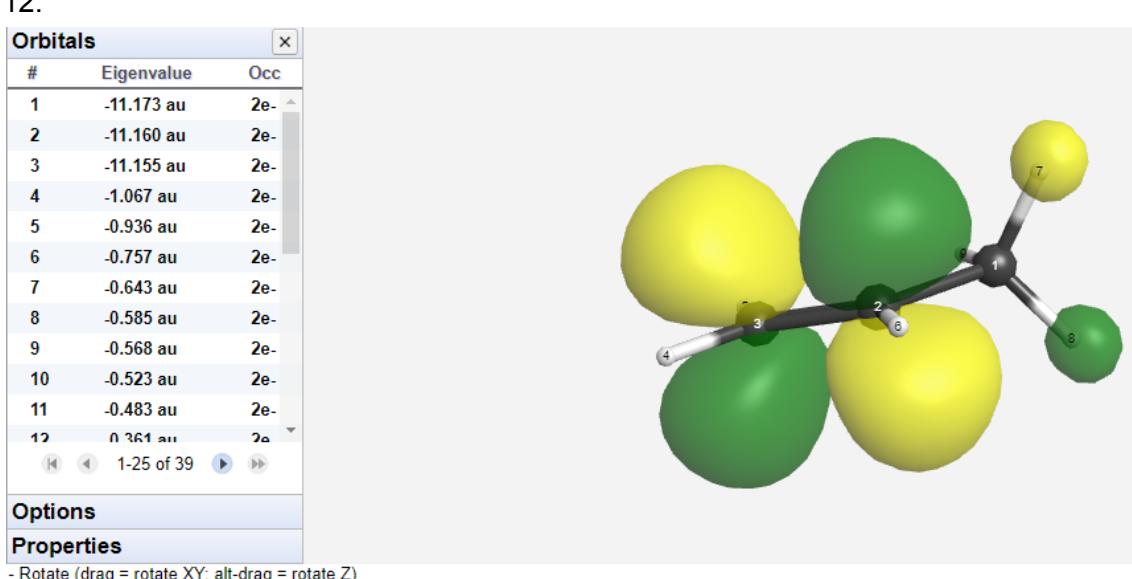
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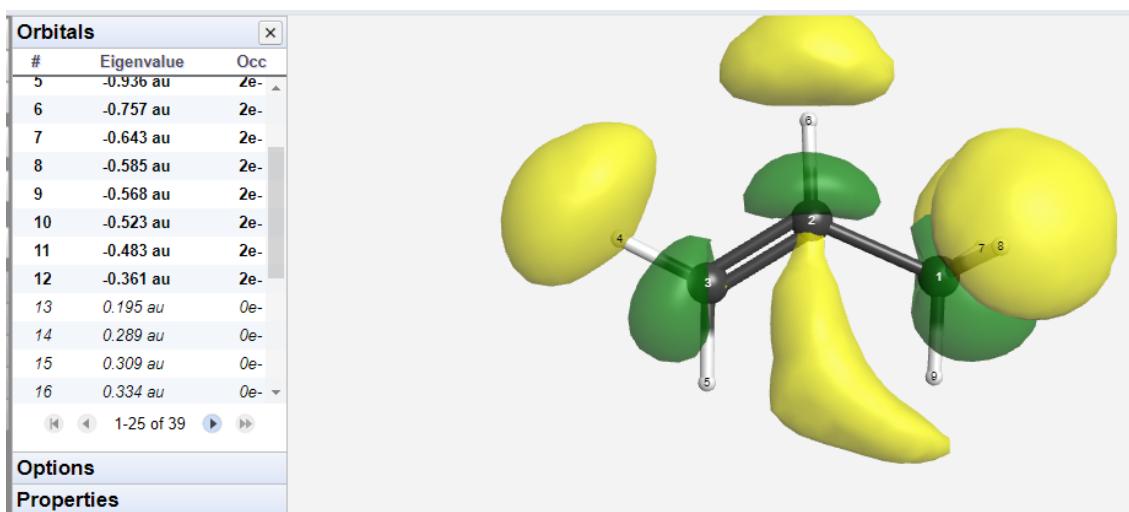
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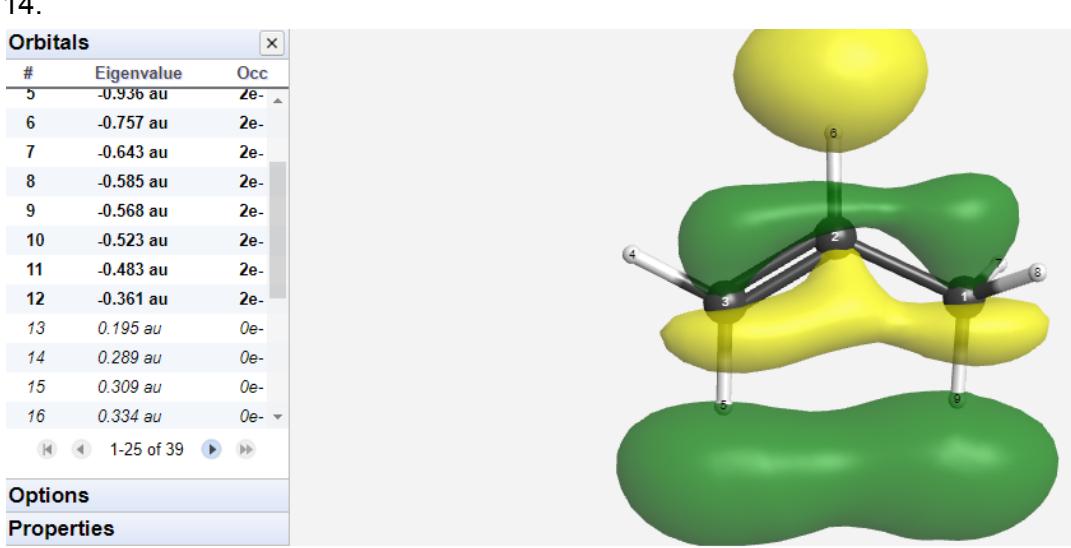
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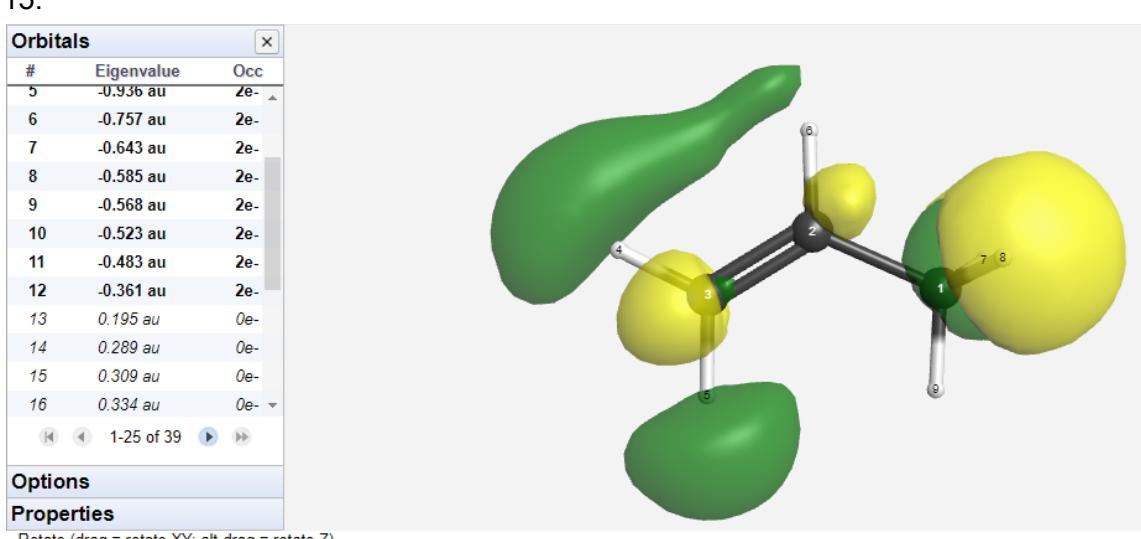
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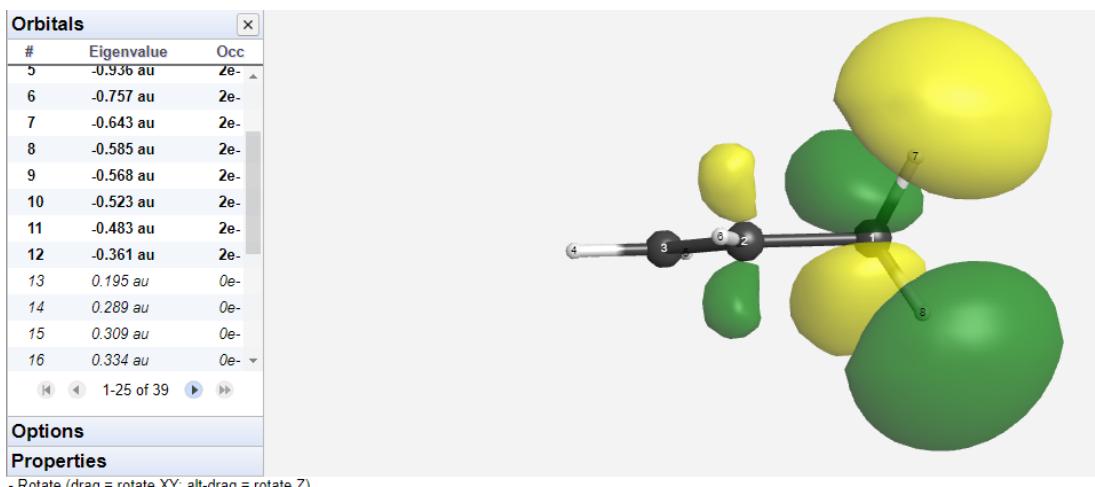
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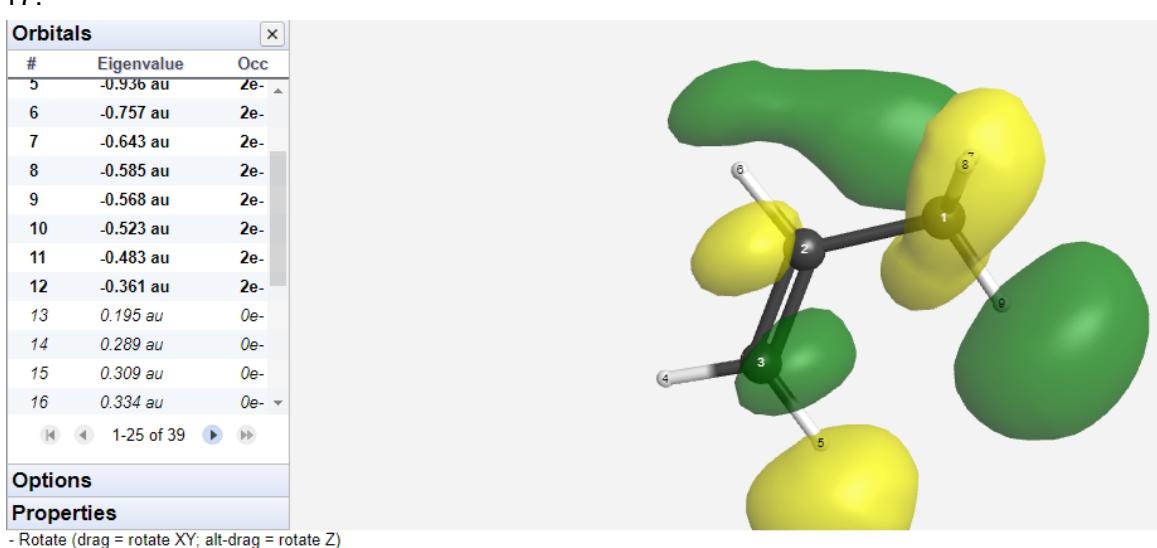
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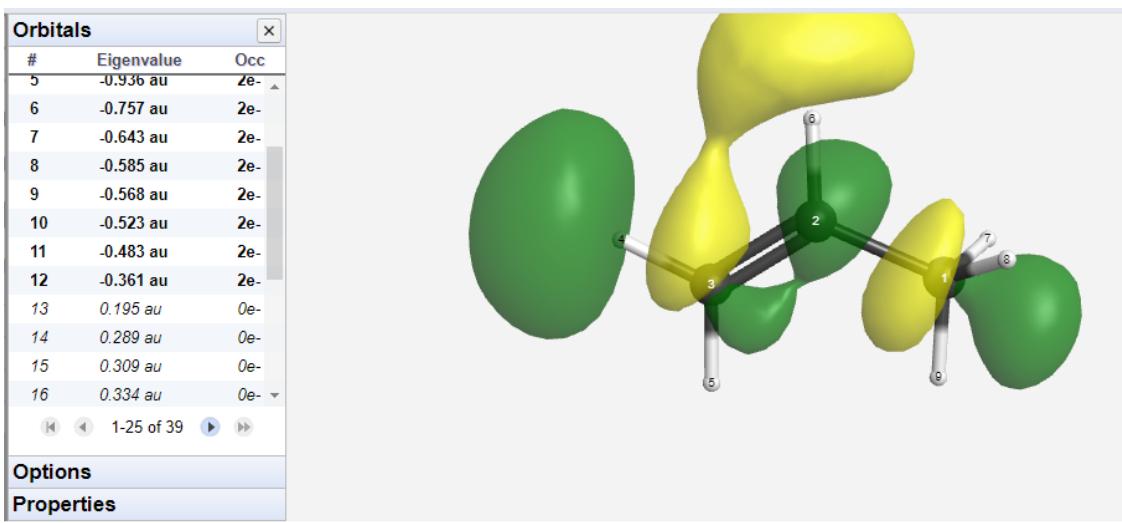
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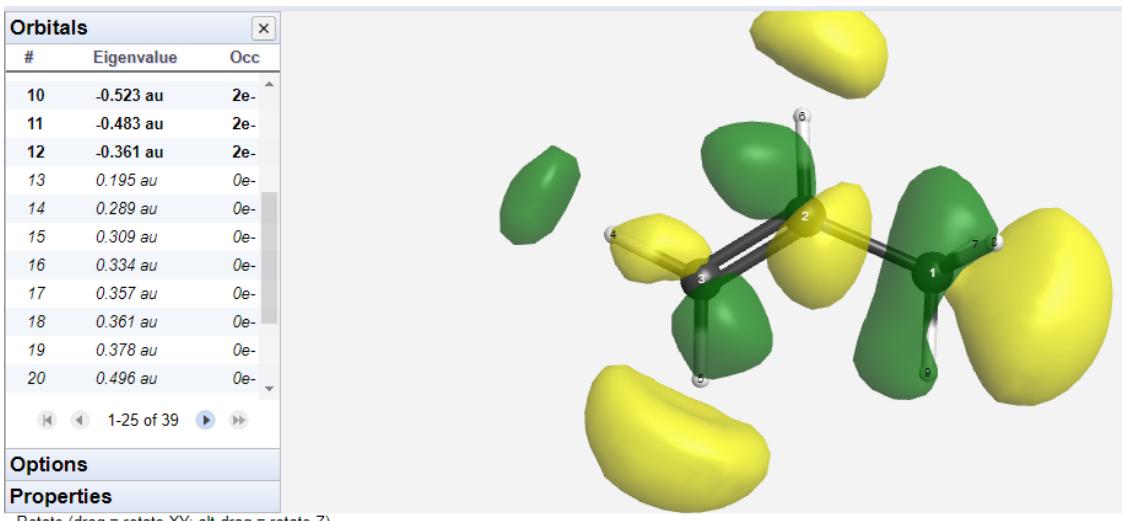
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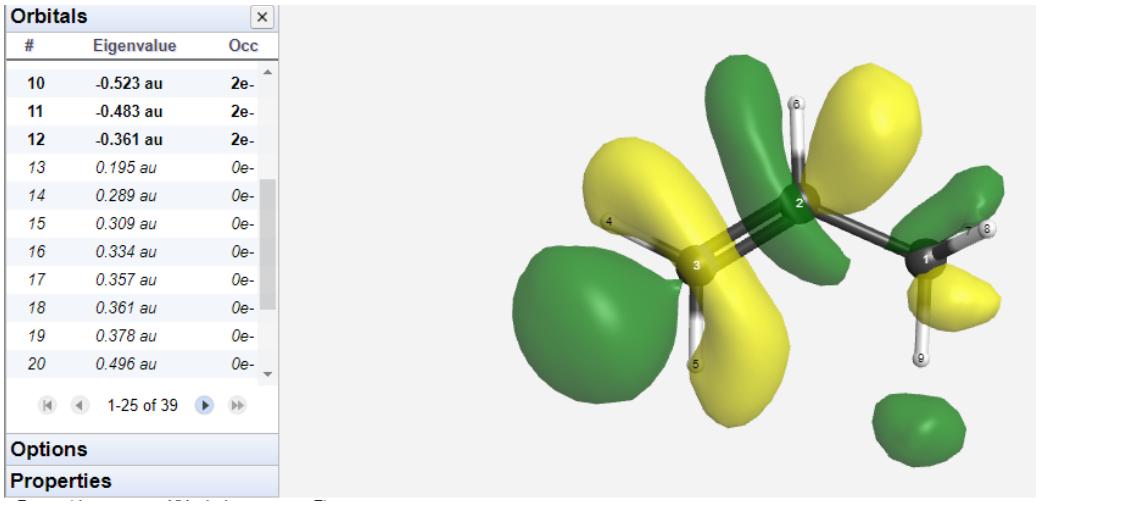
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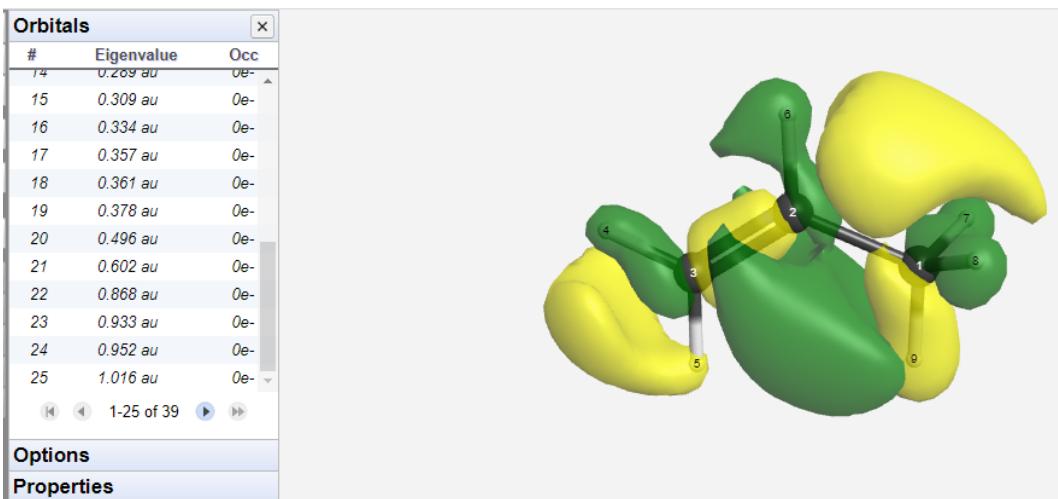
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20.



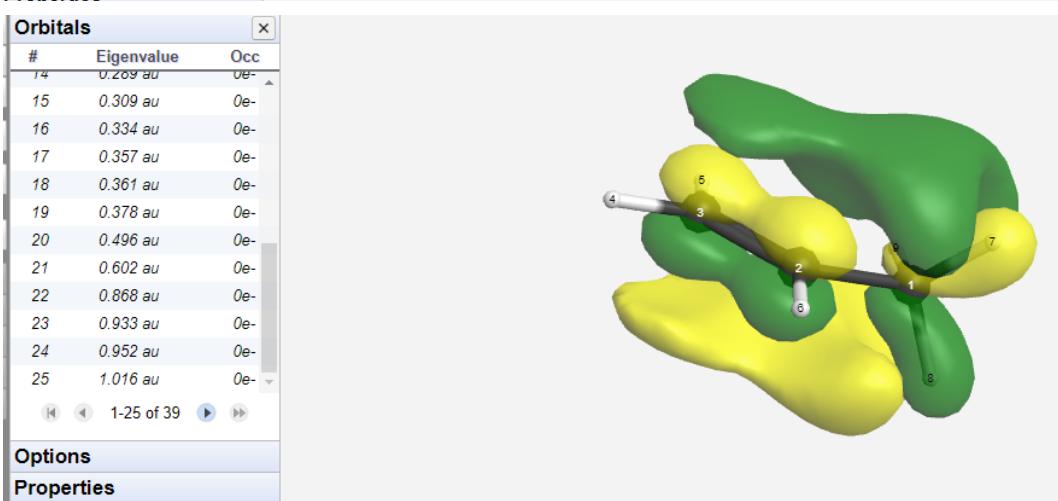
21.



22. $\text{H}_2\text{C}=\text{CH}_2$ - Rotate (drag = rotate XY; alt-drag = rotate Z)



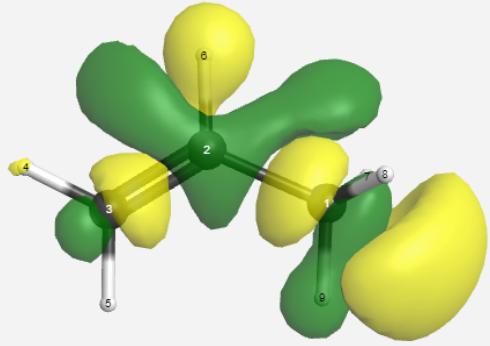
23. Properties



24.

Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

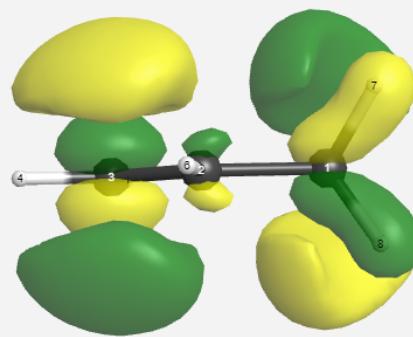
(◀ ▶ 1-25 of 39 ▶▶)



25.

Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

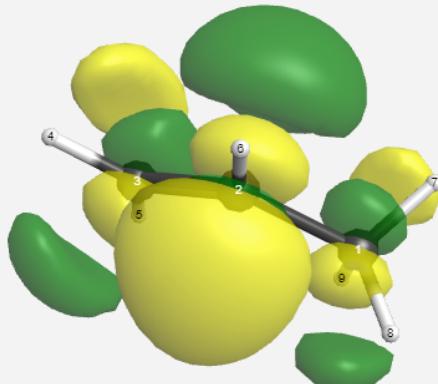
(◀ ▶ 1-25 of 39 ▶▶)



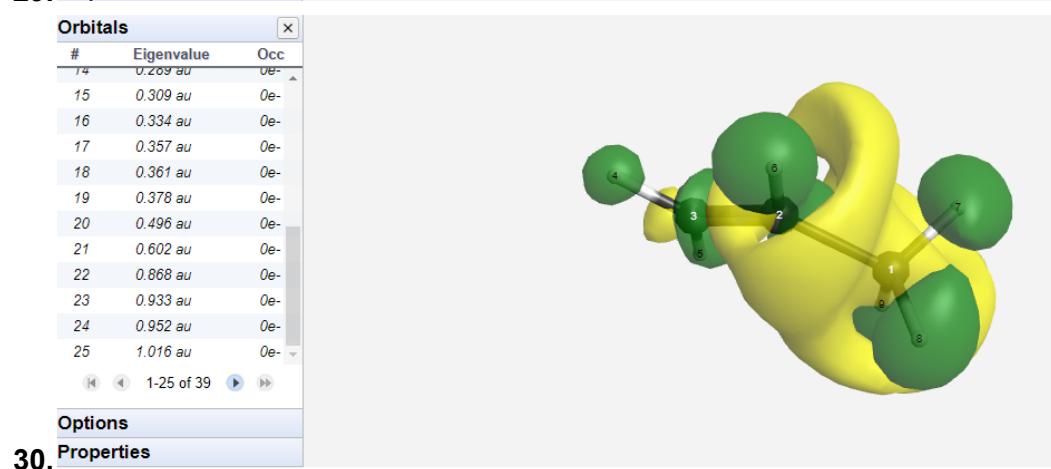
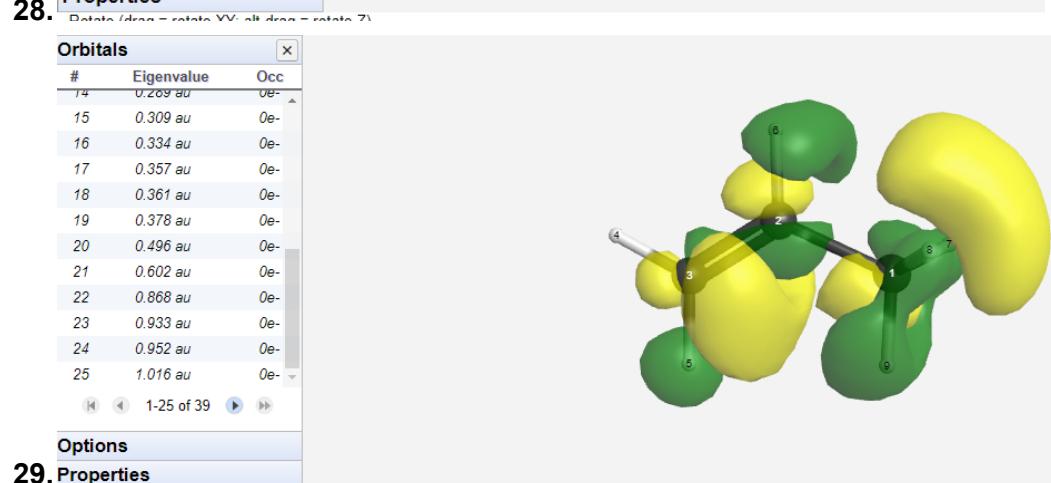
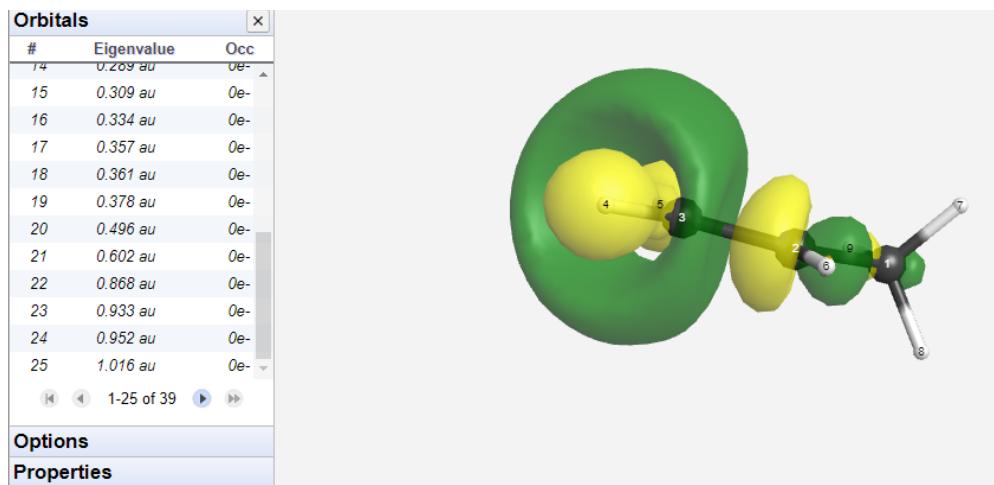
26.

Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

(◀ ▶ 1-25 of 39 ▶▶)

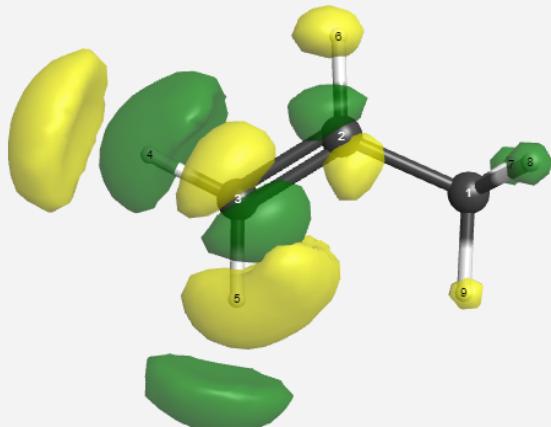


27.



Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

1-25 of 39



Options

31. Properties

Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

1-25 of 39

Options

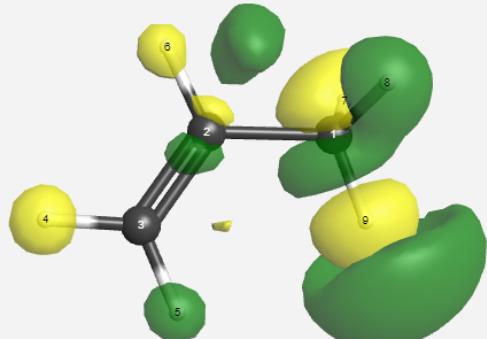
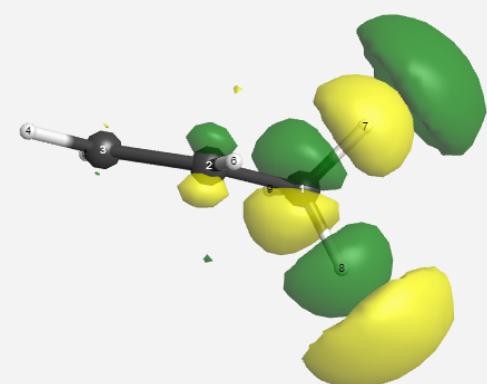
32. Properties

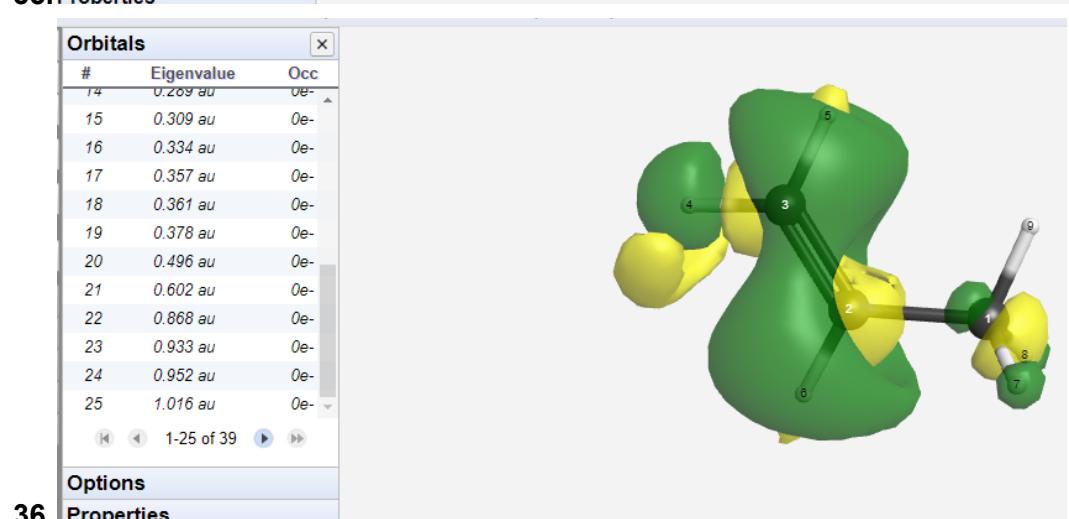
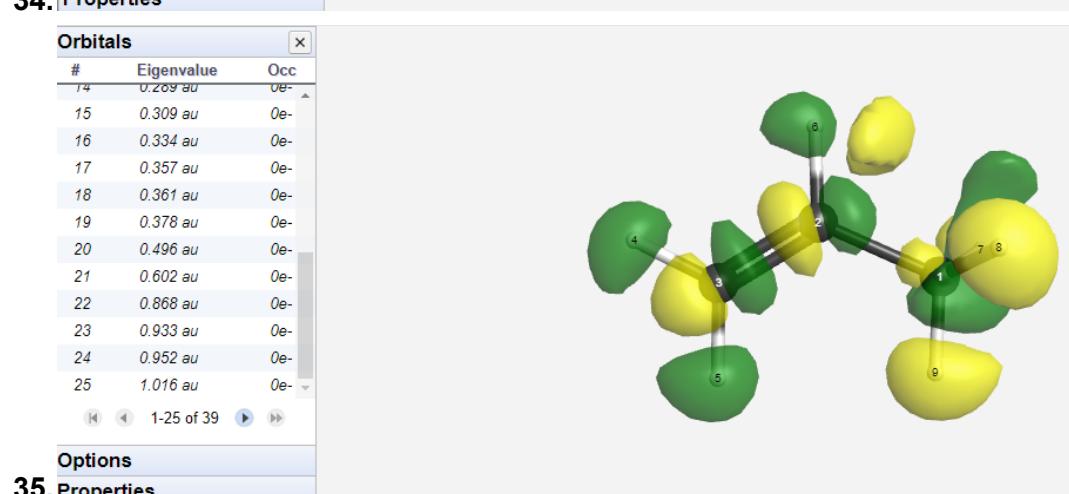
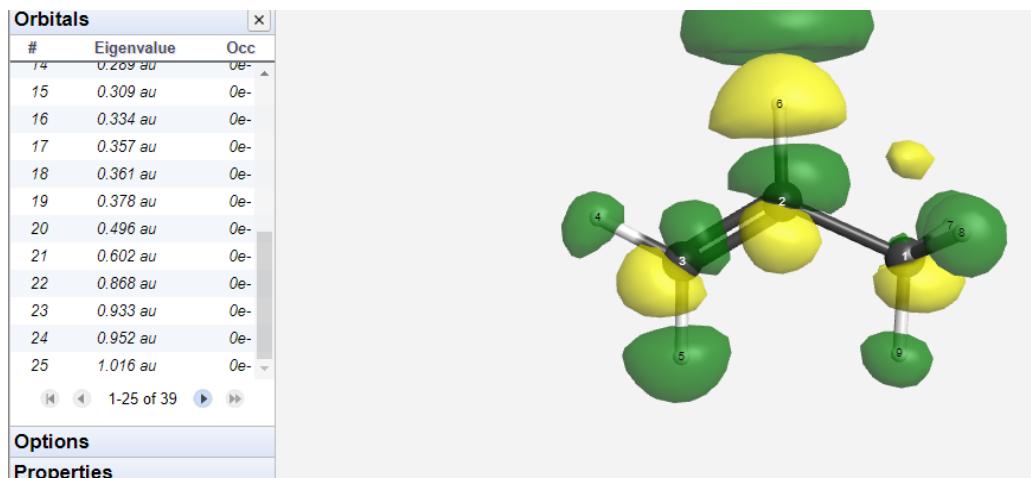
Orbitals		
#	Eigenvalue	Occ
14	0.209 au	0e-
15	0.309 au	0e-
16	0.334 au	0e-
17	0.357 au	0e-
18	0.361 au	0e-
19	0.378 au	0e-
20	0.496 au	0e-
21	0.602 au	0e-
22	0.868 au	0e-
23	0.933 au	0e-
24	0.952 au	0e-
25	1.016 au	0e-

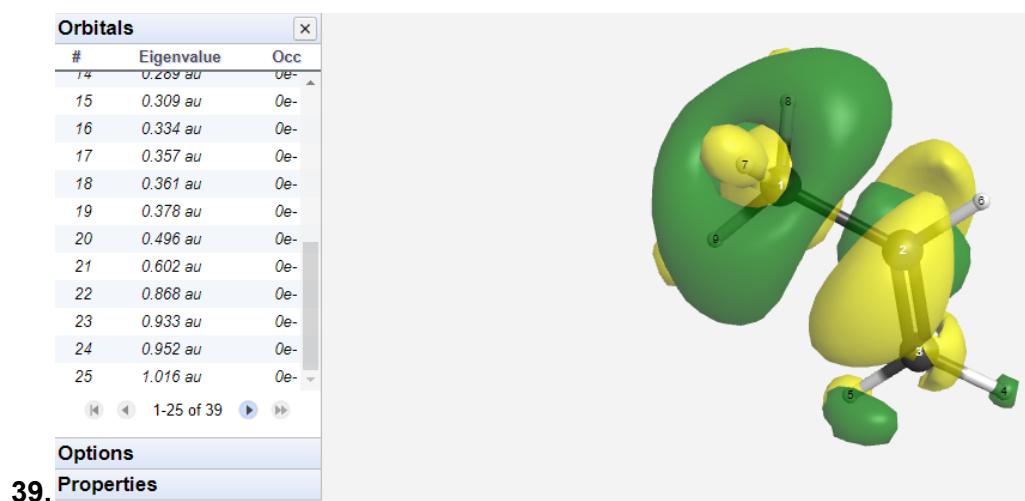
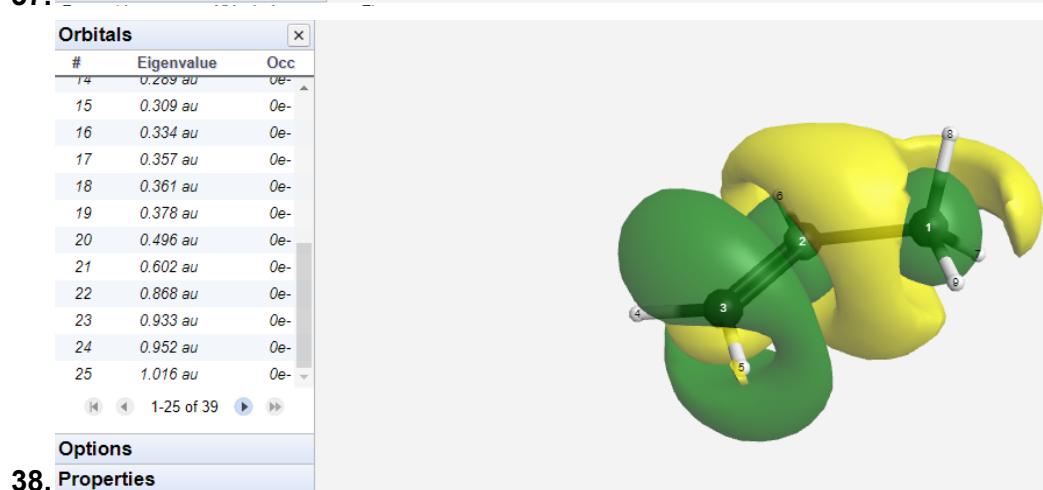
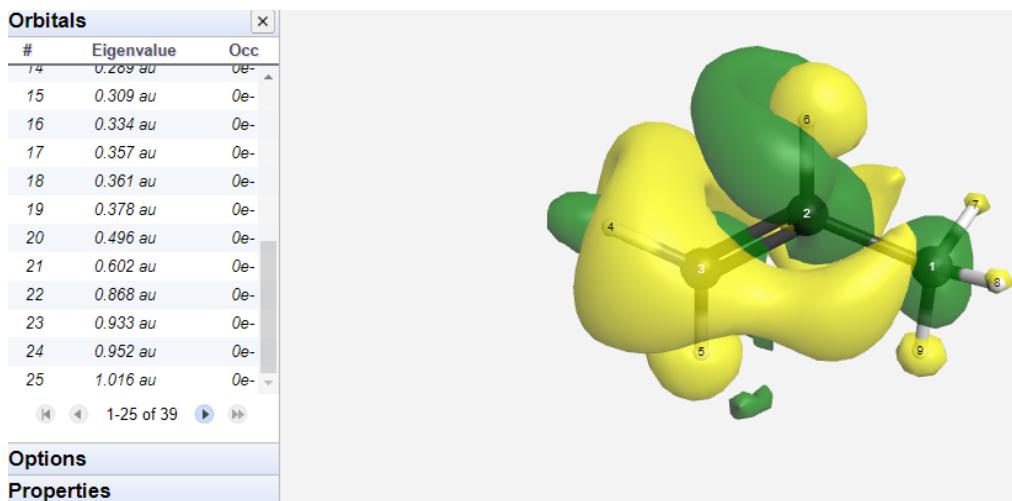
1-25 of 39

Options

33. Properties





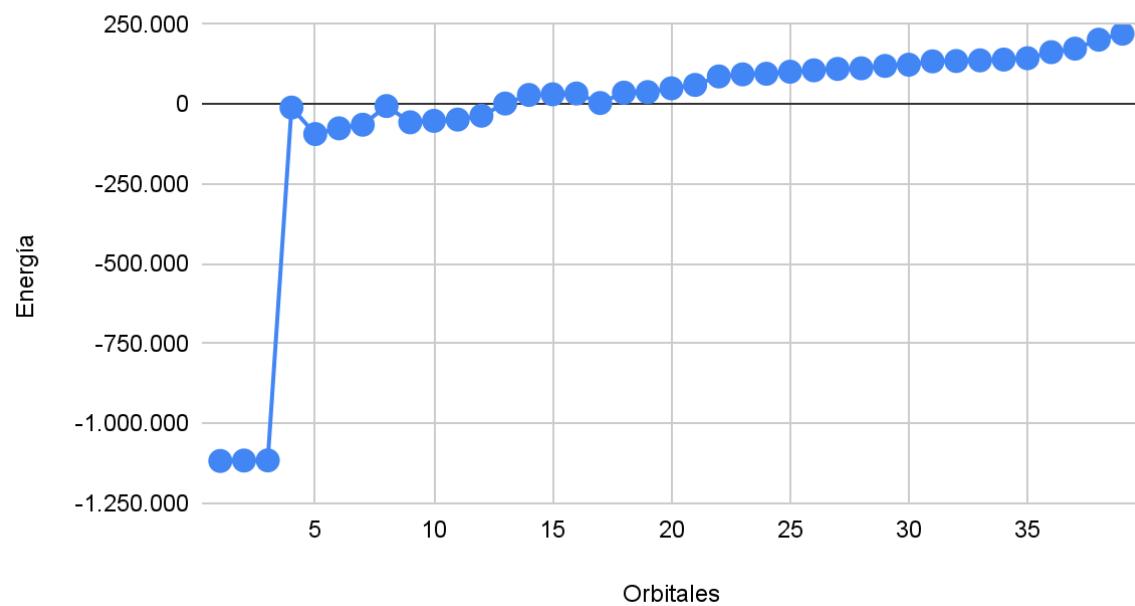


▼ Molecular Orbitals

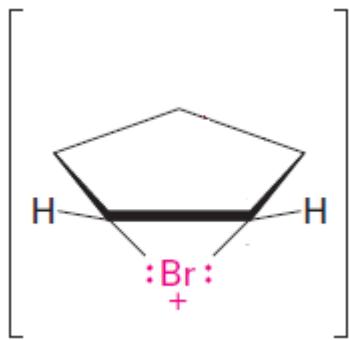
					Show all
Orbital	Symmetry	Occupancy	Spin	Energy (au)	Actions
1	-	2	-	-11.17342	
2	-	2	-	-11.15977	
3	-	2	-	-11.15543	
4	-	2	-	-1.0666	
5	-	2	-	-0.93565	
6	-	2	-	-0.75657	
7	-	2	-	-0.64315	
8	-	2	-	-0.5849	
9	-	2	-	-0.56807	
10	-	2	-	-0.52269	
11	-	2	-	-0.48287	
12	-	2	-	-0.36123	
13	-	0	-	0.1949	
14	-	0	-	0.28909	
15	-	0	-	0.30897	
16	-	0	-	0.33367	
17	-	0	-	0.3572	

18	-	0	-	0.36113		
19	-	0	-	0.37848		
20	-	0	-	0.49588		
21	-	0	-	0.60212		
22	-	0	-	0.86815		
23	-	0	-	0.93294		
24	-	0	-	0.95231		
25	-	0	-	1.01585		
26	-	0	-	1.05937		
27	-	0	-	1.10353		
28	-	0	-	1.12288		
29	-	0	-	1.19728		
30	-	0	-	1.23543		
31	-	0	-	1.34061		
32	-	0	-	1.35125		
33	-	0	-	1.37117		
34	-	0	-	1.39673		
35	-	0	-	1.43887		
36	-	0	-	1.62813		
37	-	0	-	1.73878		
38	-	0	-	2.01846		
39	-	0	-	2.20713		

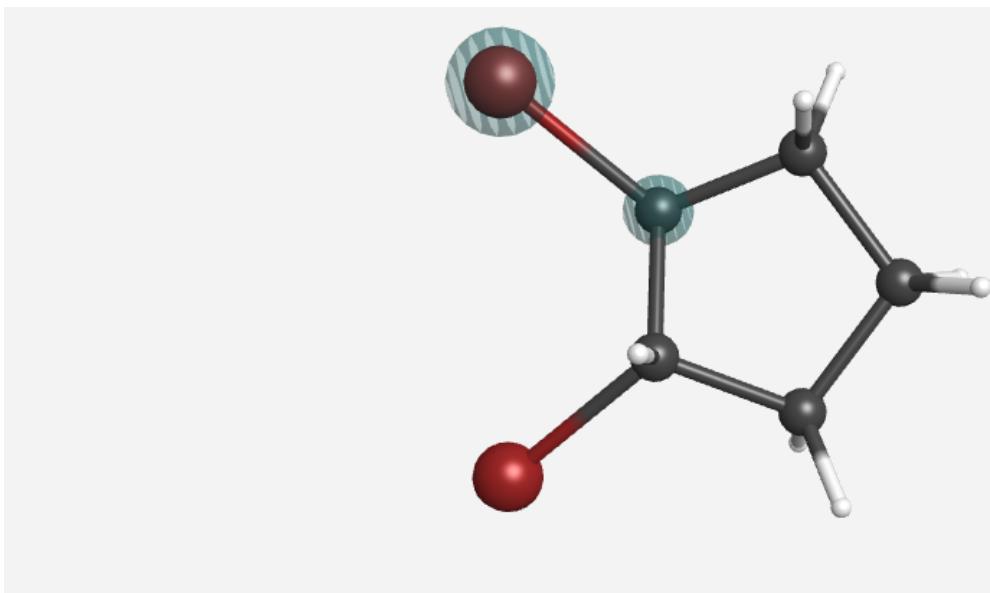
Energía de los orbitales



PROBLEMA 4: IÓN BROMONIO



- a) Determine la estructura del ión bromonio indicado. Señale los ángulos correspondientes y distancia de enlaces C-Br
C-Br longitud de enlace 1.960 Å



Bond Length: 1.960 Å

Angulo dihedrico C-Br

