Mechanism of Berry pseudo-rotation in PF5

Bởi:

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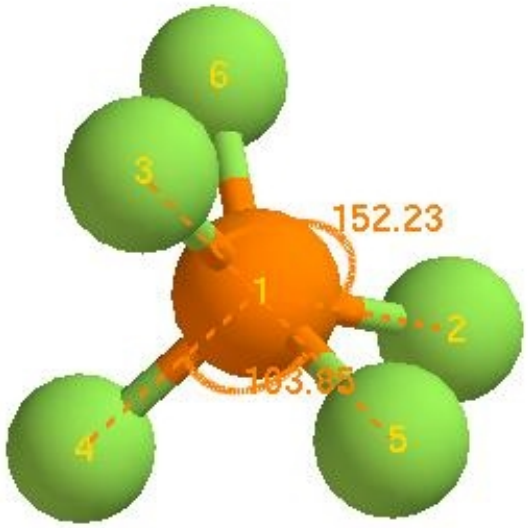
One of the unique properties of pentacoordinated compounds in inorganic chemistry is the pseudo-rotation where the axial and equatorial substituents in the triagonal bipyrimid configuration exchange their positions without breaking/forming any bond. This process is also known as Berry pseudo-rotation.

This experiment use PF5 to demonstrate the mechanism for this pseudo-rotation.

Procedure: Using tools in Avisto. You can down load Avisto and its tools from Astonis.

- Use MolDesign to create PH_5 and a guess structure for the transition state of the pseudo-rotation process.



Note that the angle (2,1,3) is about 150 degrees which is about 30 degrees bend from its original value of 180 degrees in PH_5 and the angle (4,1,5) = (4,1,6) = 104 degrees which are compressed from their original value of 120 degrees.

- Use Basic QChem Edu, Basic QChem, Mopac GUI Cloud or Pro, to search for the stable structure for PF5 and the transition state for Berry pseudo-rotation from the guess structure that you made. Record and compare the geometries of PF5 at the reactant and at the transition state.
- Using the same tool, perform vibrational analyses for both the reactant PF5 and the transition state that you found in step 2. Compare your calculated vibrational frequencies for PF5 with the experimental data below.

Mode	Experimental data[1] (cm-1)	Your data
A'1	640	
A'1	817	
A"2	575	
A"2	944	
E'	300	
E'	532	
E'	1026	
E"	514	

- Using the structure of the transition state found in step 2, perform the IRC calculation. Animate the structure changes along the reaction coordinate. What can you conclude regarding the mechanism for this pseudo-rotation?

References

1. Beattie, I.R; Livingston, K.M.S.; Reynolds, D.J. J. Chem. Phys. 1969, 51, 4269.