Figure S1. Optimized ground state geometries of various structures that were obtained while exploring various dissociation routes of doubly ionized chloromethane along with their zero-point corrected optimized energies. Energy values are in *Hartree* and *EE* indicates electronic energy.

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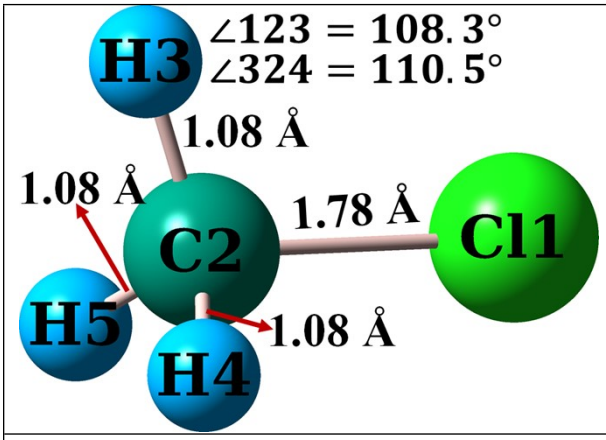
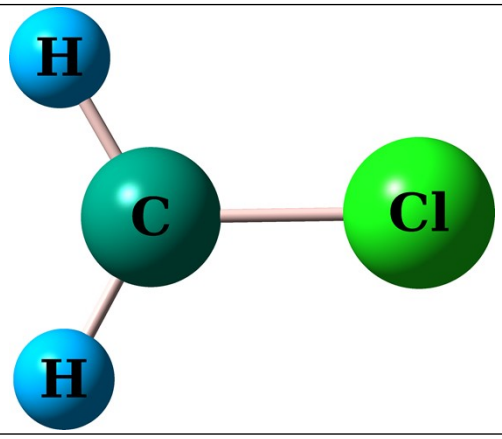
<tr><td> 
</td><td> 
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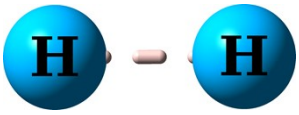
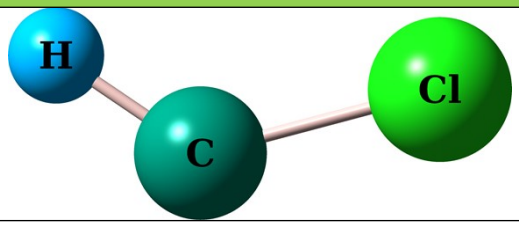
<tr><td> 
</td><td> 
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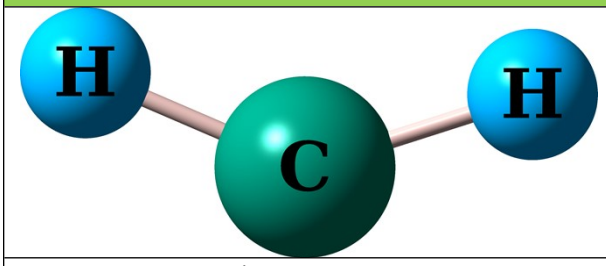
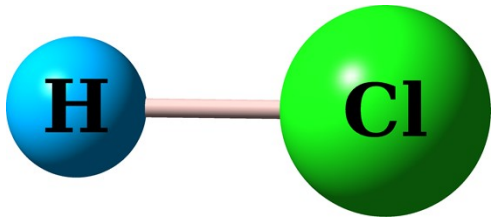
<tr><td> 
</td><td> 
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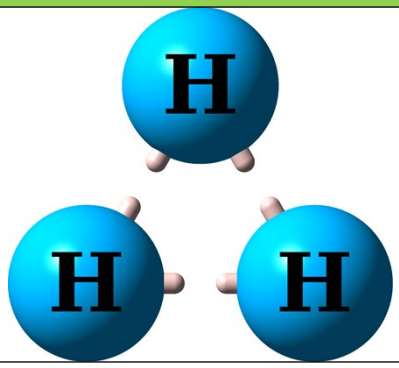
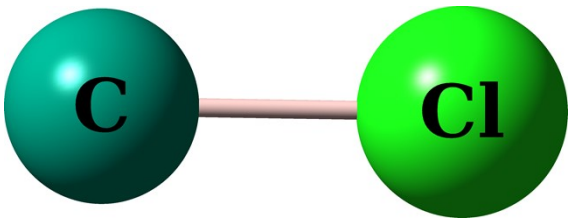
<tr><td> 
</td><td> 
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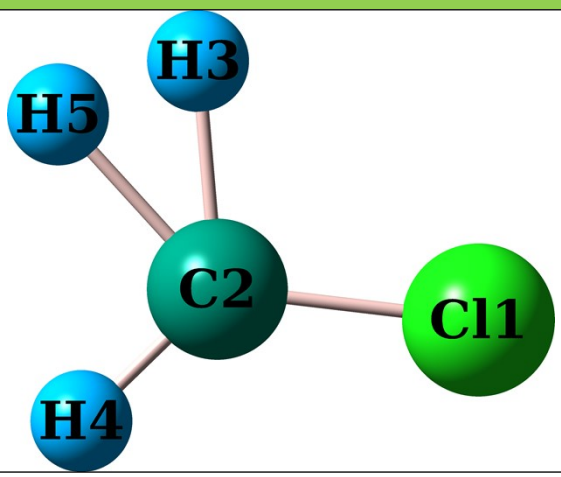

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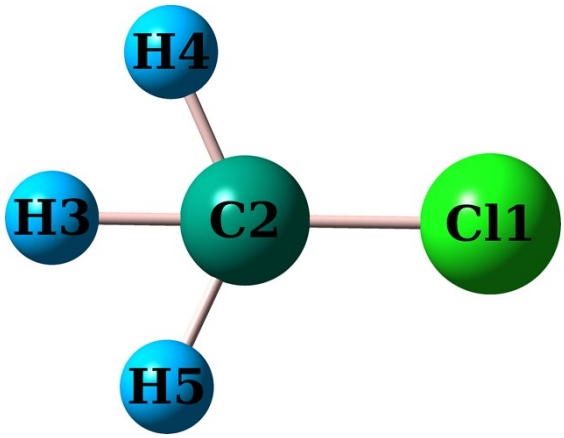
(Structure A)



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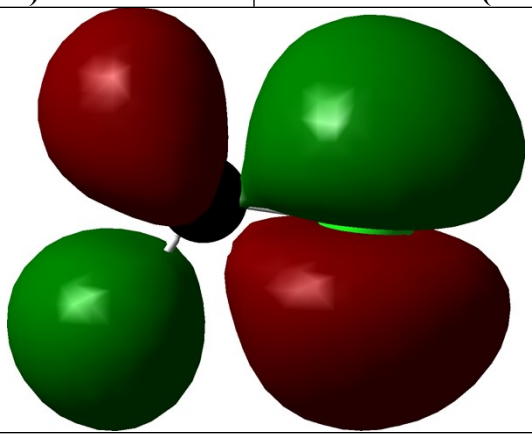
(Structure B)



HOMO of CH_3Cl^{++}

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