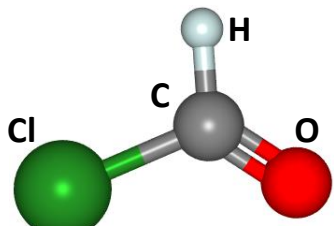


p4853 Use of student-specific molecules and their spectroscopic properties in physical chemistry courses. David E. Woon, University of Illinois at Urbana-Champaign.

Track 1

Select a random molecule.



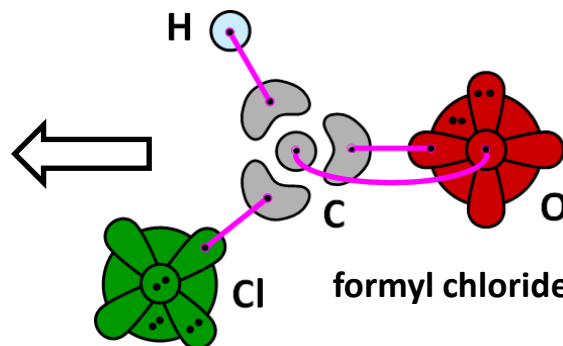
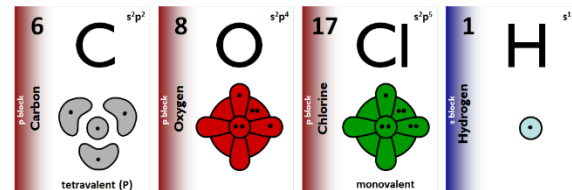
formyl chloride

Look up or calculate its spectroscopic properties.

```
molecule::::::::::HClCO
mol_weight:::::::::: 63.9716
point_group:::::::::: CS
symmetry_number:::: 1
linear(y/n):::::::::: n
rot_constant_A::::: 2.6197
rot_constant_B::::: 0.2011
rot_constant_C::::: 0.1868
N_vibmodes:::::::::: 6
mode01,degen::::: 445 1
mode02,degen::::: 717 1
mode03,degen::::: 947 1
mode04,degen:::::1322 1
mode05,degen:::::1846 1
mode06,degen:::::3052 1
```

Track 2

Select a set of atoms.



Build a valid molecule.

(glyph-based bonding)

Calculate: q^T , q^R , q^V , $\langle \epsilon \rangle_m$, $C_{V,m}$, S_m

Interested in implementation?
email: davidewoon@gmail.com



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