

Recipe 2.1.4. Creating a ionizable molecule

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1. Problem

You want to create a molecule with ionizable group(s).

2. Solution

```
Molecule acetate =  
    IonizableMolecule.newInstance(ChemicalFacade  
        .getMolecule("CH3COOH"), new IonizableGroup.Builder(4.74,  
            NeutralMoleculeType.ACID).build());  
  
// get the average charge at specific pH  
Assert.assertEquals(-0.5, acetate.getAvgCharge(4.74));  
Assert.assertEquals(-0.99, acetate.getAvgCharge(8));  
  
// get the number of ionizable group  
Assert.assertEquals(1, acetate.getPkaNumber());
```

3. Discussion

4. See Also