Documentation

1. Filter by frequency range online: 12124 vibrations
2. Filter for anions, cations, radicals, dimers, trimers and tetramers: 10359 vibrations
3. Since dipole, quadrupole, and T melting are molecular properties and not properties of the vibrations, filter the vibrations to only have 1 vibration per molecule (the first one in the list): 777 molecules
4. Filter molecules based on their dipole moment (higher than 0.5):
   1. Good: pass the filter: 545
   2. No value: could not find dipole moment: 47
   3. Discarded: did not pass the filter: 185
   4. Joint: good and no value molecules: 592
5. Filter the joint molecules based on their quadrupole moment (higher than 0.5):
   1. Good: pass the filter: 458
   2. No value: could not find dipole moment: 65
   3. Discarded: did not pass the filter: 69
6. Complete list of dipole and quadrupole values for the remaining molecules by hand and re running the existing code
   1. Run dipole search again with molecules that have no value
      1. Passing filter: 24
      2. Not passing filter: 3
      3. No dipole moment found: 20
   2. Run quadrupole search again with molecules of quadrupole that have no value
      1. Passing filter: 28
      2. Not passing filter: 2
      3. No dipole moment found: 35
7. Join the dipole moment values from the two runs and the quadrupole moment values of the two runs and complete remaining by hand
   1. Dipole good + dipole good v2: all molecules that passed the filter
   2. Check no values v2 dipole and add to the previous: filter by hand and add to good 🡪 dipole final
   3. Quadrupole good + quadrupole good v2: all molecules that passed quadrupole filter (dipole passed + dipole unknown)
   4. Check no values v2 quadrupole and add to the previous if they are present in the dipole list: webpage not work so some NaN values not included. Quadrupole good + the filter of quadrupole no value v2 are merged 🡪 quadrupole final
   5. Check quadrupole final to see if molecules have unknown dipole values are in the dipole final list, if they are keep if not remove 🡪 after quadrupole and dipole 🡪 503 molecules
8. Separate into 3 groups based on the number of atoms:
   1. 1-5 🡪 166
   2. 5-10 🡪 194
   3. More 10 🡪 143
9. Get the 1-5 and filter by melting temperature, reactivity, stability and how easy is to buy 🡪 49 molecules
10. Filter by experimental dipole moment: how far away the two dipole moments are and by the value of the rotational constan 🡪 16
11. Filter once more based on quadrupole so it is higher than 1 🡪 13