**For our four reference complexes, draw the structures for each**

KSCN

K2Co(NCS)4

K2Hg(SCN)4

HgCo(SCN)4

**Using FT-IR data, determine the bonding mode of thiocyanate of the complexes marked unknown in the following table:**

From Baer, C.; Pike, J. *J. Chem. Ed.* **2010**, 87, 724.

IR stretching Frequencies due to SCN of both reference and unknown metal thiocyanates, ν cm-1

|  |  |  |
| --- | --- | --- |
| compound | C-N region2000-2200 cm-1 | C-S region700-850 cm-1 |
| References  |
| KSCN  | 2055 (s,br) | 746 (w, br) |
| K2Co(NCS)4  | 2086(s,br) | 819(w, br) |
| K2Hg(SCN)4  | 2108(s,sh) | 715(w, sh) |
| HgCo(SCN)4  | 2143(s,sh) | 790 (w, sh) |
| Unknowns |
| Mn(py)4(SCN)2 | 2060 (s,br) |  | 798(w, br) |
| Fe(py)4(SCN)2 | 2065(s,br) |  | 806(w, br) |
| Co(py)4(SCN)2 | 2074 (s,br) |  | 802(w, br) |
| Ni(py)4(SCN)2 | 2084(s,br) |  | 800(w, br) |
| Cu(py)2(SCN)2 | 2091(s,br) |  | 825(w, br) |
| Zn(py)2(SCN)2 | 2073(s,br) | 2099 (s,br) | 848(w, sh) |
| NH4[Ag(SCN)2] | 2122(s,sh) | 2097(s,sh) | 722 (w, sh) |

w= weak, m= medium, s=strong intensities; sh=sharp, br= broad shapes

**Data analysis using a quantitative comparison method (to be done in class)**

Using a spreadsheet, calculate the absolute difference of the stretching frequencies of the unknown compounds and each of the references. For each compound, sum the difference for the C-S and the C-N stretches of each reference; the smallest total supports the best bonding mode.