

CHEM 304: π -Acceptor Ligands
Topic: Electron Count in Metal Nitrosyl Complexes

Name: _____ Roll No. _____ Submission date: _____

A group assignment adapted from:

A Thousand Manipulatable Inorganic Electron-Counting Problems from Crystallography
by George Lisensky, Beloit College

Over 80 interactive metal nitrosyl complexes have been selected and prepared for practice and discovery in electron counting problems. The structures can be displayed and manipulated without requiring software installation using a web browser with JavaScript and JSmol. The user can drag to rotate, shift-drag vertical to zoom, and shift-drag horizontal to turn the structure. The problems are numbered alphabetically with four structures in each problem for small group work (4 students/group). Each member could present their electron count for one of the four problems.

Sometimes a set designated by { } will contain more than one structure. In such cases the electron-count work is identical for all of them, for example {Co, Rh, Ir} or {Cl, Br, I} or {cis, trans} or {fac, mer}. Selected display options are retained while on a given page. The user can switch a given view to another representation (e.g. space-filling or ball&stick) or label atoms. One display option is to display the metal-metal distance but double-clicking can also be used to measure observed distances and angles between atoms.

The displayed structures are derived from crystallographic results. If the hydrogen atom positions were not reported, then hydrogen atoms have been added and their positions energyminimized. Any disorder is not shown. Counter ions may or may not be included; overall charge of the displayed portion is shown in the upper right of the JSmol window. Small deviations from ideal geometry may be due to crystal packing. See the link at the bottom of each page for the original references and cif files.

Later pages use ligands from earlier pages so examining the pages in order is helpful. The bottom of each page has links to all the other pages.

Metal Nitrosyl Complexes

Does observed geometry match 18-electron count predictions?

Nitrosyl is an interesting ligand since, depending on the M-N-O bond angle, it can be either a 1 or 3 neutral-ligand electron donor or either an NO⁺ or NO⁻ closed-shell-ligand electron donor. It really helps to be able to rotate the molecule to examine whether the NO is linear or bent. Counter ions are not shown.

Guidelines

- Students will be divided into groups, each group with 4 students, based on roll number or alphabetically based on their first name.
- Each group will be assigned one problem set, from A-U, <https://chem.beloit.edu/classes/structure/EAN/nitrosyl.html>.
- Each member will present their electron count for one of the four problems in each problem set.