coreip\_raw\_data.json

* This is the file containing revisions of the hackathon’s raw\_data.json
* Notes:
  + Metallo-organic Compounds:
    - To the best of my ability, metal-metal bond orders were assigned according to the 18-electron rule.
    - I tried to be consistent with the assignment of single/dative bonds, but they should be reviewed by a chemist. I know I have assigned carbon monoxides, halogens, and NO2 as single bonds, when they might be better classified as dative.
* Revisions seek to address the following:
  + Metallo-organic Compounds
    - Case 1: SMILE denotes ligands and metals disconnected.
      * Previous: [C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[C-]#[O+].[Mn]Br
      * Revised: [Mn](Br)(C#[O+])(C#[O+])(C#[O+])(C#[O+])(C#[O+])

cleaned\_graph\_data.json

* This is the file networkx-graphs generated from coreip\_raw\_data.json.