**Aromatic inclusion within a neutral cavity-containing rectangular grid**

Please complete these guiding questions to *Chemical Communications* **1998**, *61*, 2735-2736. <https://doi.org/10.1039/A807738J>

This article discusses the synthesis and characterization of a supramolecular grid based upon coordination chemistry principles.

1. Consult this Chemistry Libre Text article on [principles of host-guest chemistry](https://chem.libretexts.org/Courses/Saint_Marys_College_Notre_Dame_IN/CHEM_431%3A_Inorganic_Chemistry_(Haas)/CHEM_431_Readings/09%3A_Acid-Base_and_Donor-Acceptor_Chemistry/9.05%3A_Intermolecular_Forces/9.5.01%3A_Host-Guest_Chemistry_and_-_stacking_interactions#:~:text=%CF%80%E2%88%92%CF%80%20interactions.-,In%20Host%2DGuest%20Chemistry%20a%20large%20molecule%20or%20network%20material,molecule%20in%20a%20binding%20pocket.&text=Host%2Dguest%20binding%20is%20analogous,many%20enzymes%20bind%20their%20substrates.).

(a) What type of interaction is used to bind the guest molecule to the host in host-guest chemistry?

(b) List the types of forces often used to induce binding of the guest in the host.

(c) What are three design principles used to favor host-guest binding?

2. (a) Draw the Lewis structures for the three reactants used for synthesis of rectangular supramolecular assembly **2**.

(b) Why did the authors use 2 equivalents of pyrazine relative to the other reactants?

(c) Which of the design principles from question 1(c) apply to the synthesis of supramolecular assembly **2**?

(d) Which types of interactions from question 1(b) are present between host and guest in supramolecular assembly **2**?

(e) What type of experimental evidence did the authors cite as evidence that the supramolecular assembly **2•pyz** was formed?

3. (a) Write the electron configuration of Co and Co2+.

(b) Is the terph ligand acting as a monodentate or bidentate ligand in supramolecular assembly **2**?

(c) Use the covalent bond classification (CBC) method to fill in the table below for the Co2+ complex in the middle of supramolecular assembly **2** as shown in Fig. 1.

|  |  |
| --- | --- |
|  | [Co(pyz)2(terph)2(H2O)2] |
| pyz CBC ligand classification |  |
| terph CBC ligand classification (see (b) above) |  |
| water ligand classification |  |
| MLlXxZz classification |  |
| Valence number |  |
| Ligand bond number |  |
| Electron count from ligands |  |
| Electron count from metal |  |
| Total electron count |  |
| dn count for metal |  |

(c) Go to the [Columbia University Parkin group website on CBC](http://www.columbia.edu/cu/chemistry/groups/parkin/mlxz.htm). Click on “MLX plots” on the list on the left and systematically click on the following links to answer the corresponding questions.

“MLXZ plots” for Co: What is the prevalence of Co complexes with the MLlXxZz classification determined in part (b)? What is the most common MLlXxZz classification for Co?

“Electron count distribution” for Co: What is the prevalence of Co complexes with the electron count determined in part (b)? What is the most common electron count for Co?

“Valence distribution” for Co: What is the prevalence of Co complexes with the valence number determined in part (b)? What is the most common valence distribution for Co?

“Ligand Bond Number” for Co: What is the prevalence of Co complexes with the ligand bond number determined in part (b)? What is the most common ligand bond number for Co?

4. Compare and contrast the views of supramolecular assembly **2** shown in Figures 1-3. Why did the authors include each of these perspectives?

5. Why did the authors cite reference 6?