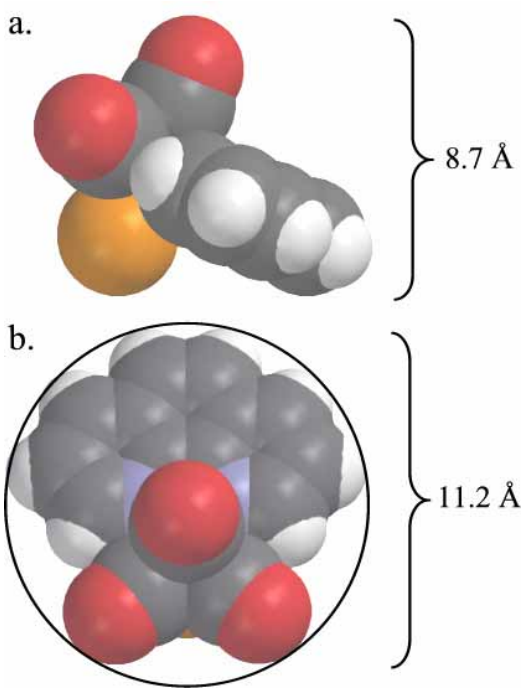
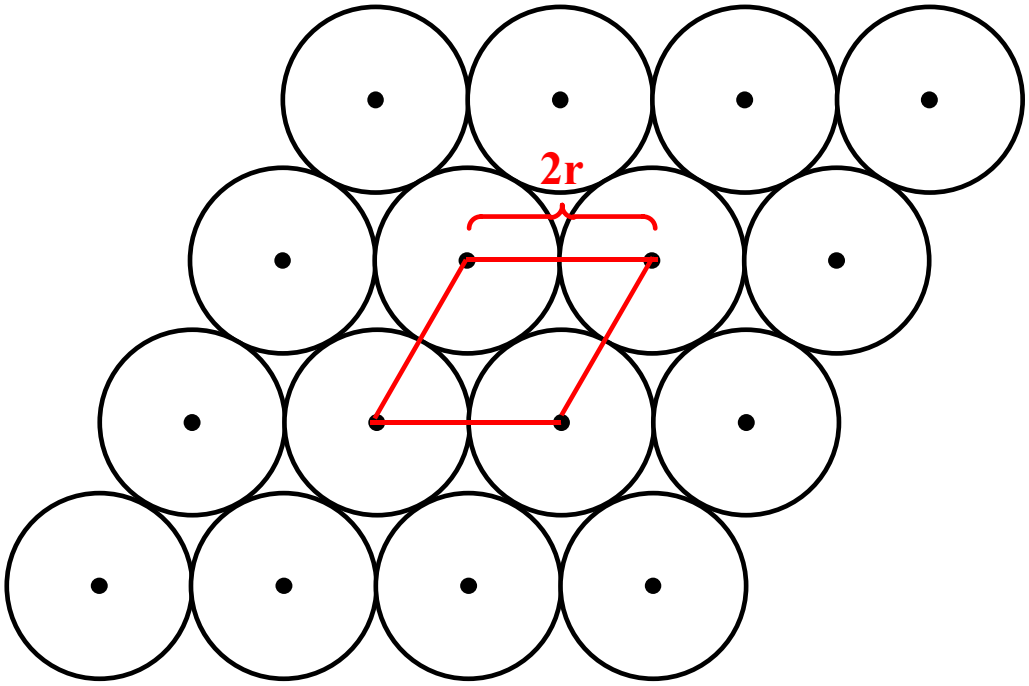


Figure 1. Space filling model for Re(phen)$(CO)_3$Cl presenting: a. the minimum distance in which the complex can be oriented; b. top view of the molecule presenting its circular projection in the ab plane.



Scheme 1. Ideal two dimensional arrangement of Re(phen)$(CO)_3$Cl complexes in van der Waals contact.

1. The area of the parallelogram denoted by the red segments is $P = (2r) \times (r\sqrt{3}) = 2r^2\sqrt{3}$.

2. The area of the circle that represent the cross sectional area of Re(phen)$(CO)_3$Cl in the ZrP plane is $\text{Re(phen)(CO)}_3\text{Cl} = \pi r^2$

3. The percent of area occupied by Re(phen)$(CO)_3$Cl in the parallelogram:

$$\text{Re(phen)(CO)}_3\text{Cl}\,\% = \frac{\pi r^2}{2r^2\sqrt{3}} \times 100 = 90.7\%$$

4. Being r = 5.6 Å and the cross sectional area of a ZrP formula unit = 24 $Å^2$, then the amount of Re(phen)$(CO)_3$Cl per ZrP is **0.221**.