Appendix

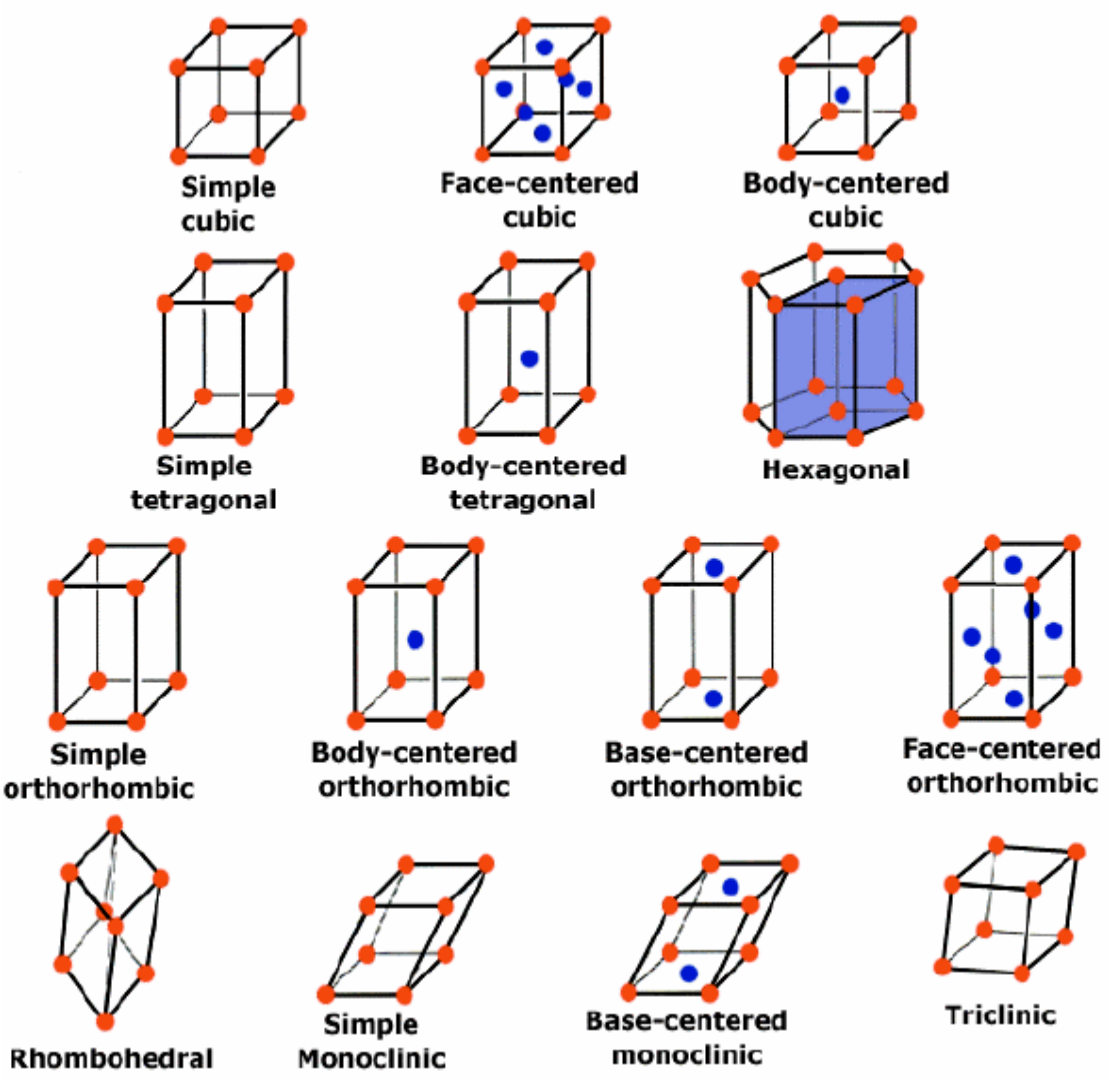

Figure 49 The Bravais lattices

Table 12 ^{13}C Chemical shifts for organometallic compounds(Miessler and Tarr, 1998)

Ligand	^{13}C chemical shift (range)*
M-CH_3	-28.9 to 23.5
M=C<	190 to 400
M ≡ C-	235 to 401
M-CO	177 to 275
Neutral binary CO	183 to 223
M-(η^5-C_5H_5)	-790 to 1430
Fe(η^5-C_5H_5)$_2$	69.2
M-(η^3-C_5H_5)	C_2(91 to 129), C_1 and C_3 (46 to 79)
M-C_6H_5	M-C (130 to 193), ortho (132 to 141) meta (127 to 130) and para (121 to 131)

*parts per million relative to $Si(CH_3)_4$

Finding the general formula

1. Calculate the composition of products using results from many techniques such as XRF, ICP-AES, TGA, and tritation as shown below.

Methods	Results
ICP-AES, WDXRF, EPMA/EDX	% of K, Na, Al, Cr
Tritration	% of $C_2O_4^{2-}$
TGA	% of water

2. Calculate the mole ratio of each component in products,

for example;

RedCubic 5% :

$$\frac{\%K}{Aw_K} : \frac{\%Na}{Aw_{Na}} : \frac{\%Al}{Aw_{Al}} : \frac{\%Cr}{Aw_{Cr}} : \frac{\%C_2O_4}{Mw_{ox}} : \frac{\%H_2O}{Mw_{H2O}}$$

$$\frac{7.277}{39.098} : \frac{9.531}{22.99} : \frac{6.358}{26.982} : \frac{0.895}{51.996} : \frac{57.62}{88} : \frac{16.10}{18}$$

$$0.186 : 0.415 : 0.236 : 0.017 : 0.655 : 0.894$$

$$1 : 2 : 0.95 : 0.05 : 3 : 4$$

General formula : $KNa_2[Al_{0.95}Cr_{0.05}(C_2O_4)_3]\cdot 4H_2O$