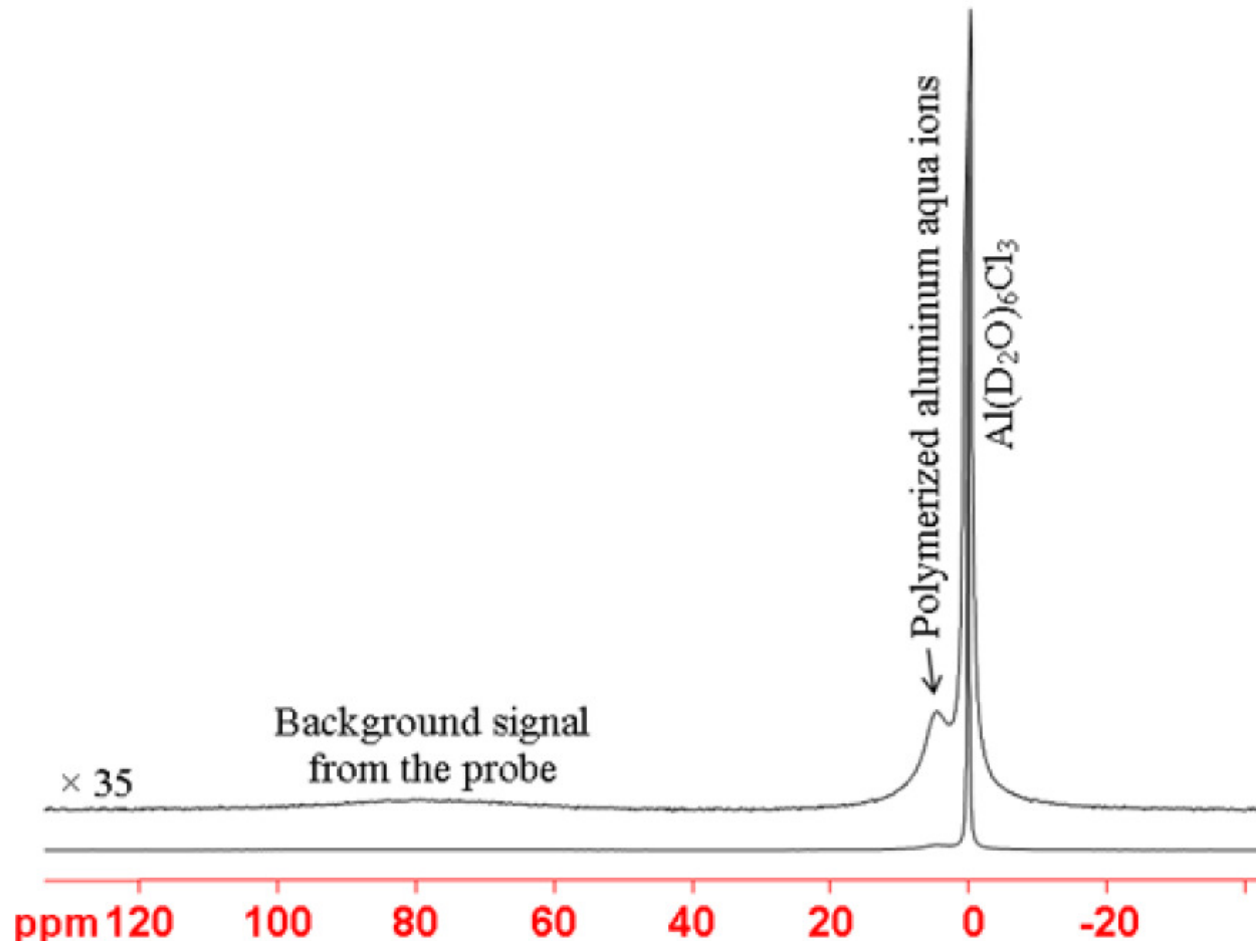


# Ressonância Magnética Nuclear de $^{27}\text{Al}$

# Dados Fundamentais de RMN de $^{27}\text{Al}$

- Spin Nuclear (I) =  $5/2$
- Abundância Natural do Isótopo 27 = 100%
- Faixa de Deslocamento Químico ( $\delta$ ) 400 ppm, de -200 até 200 ppm
- Razão de Frequência = 26.056859%
- Referência = 1,1 M  $\text{Al}(\text{NO}_3)_3$  em  $\text{D}_2\text{O}$  ( $\delta=0\text{ppm}$ ; FWHM= 11Hz;  $T_1=0,03\text{s}$  )
- Receptividade (em relação ao  $^1\text{H}$  = 0,20)

# Espectro da Referência RMN de $^{27}\text{Al}$



# RMN de $^{27}\text{Al}$

## Octaédrico vs Tetraédrico

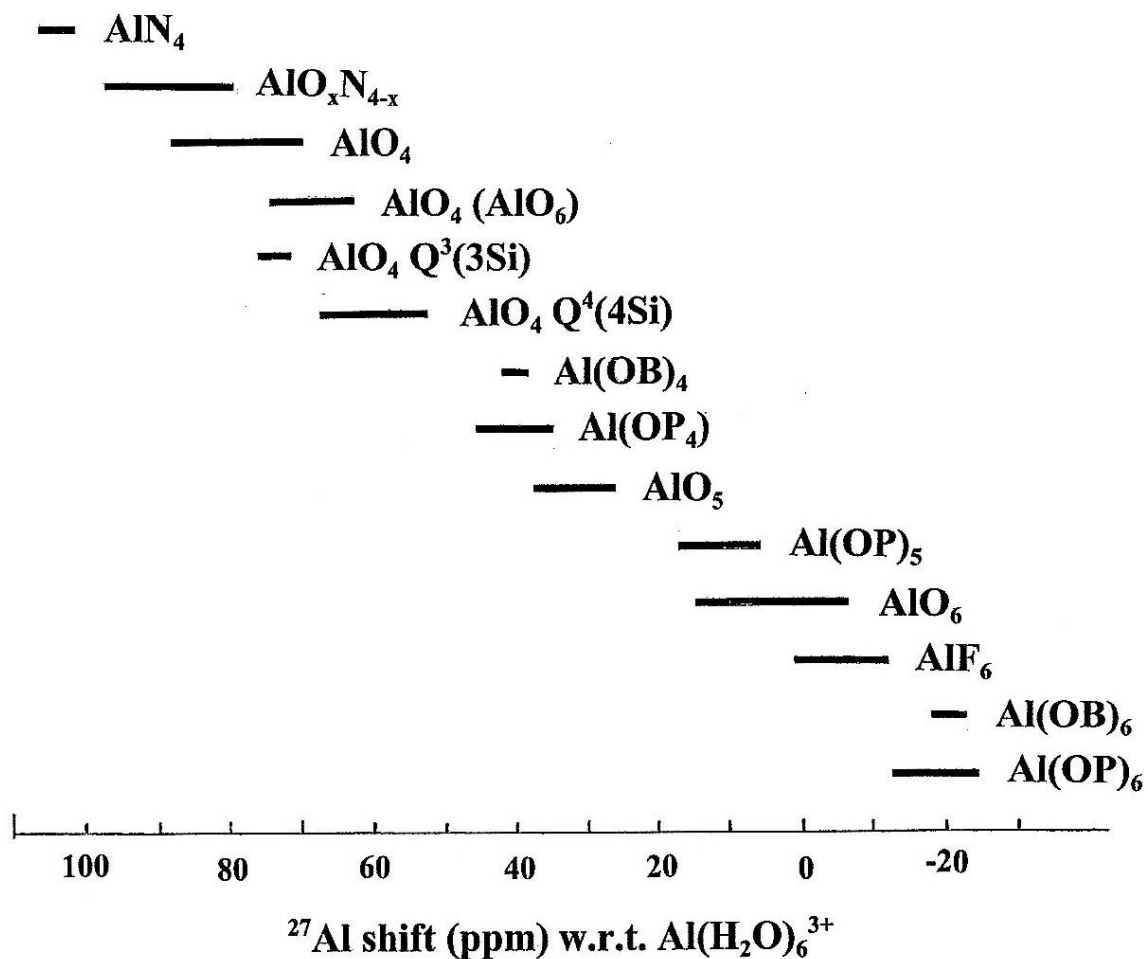


Figure 5.1. Range of  $^{27}\text{Al}$  chemical shifts in various Al compounds.

# Acoplamento Quadropolar

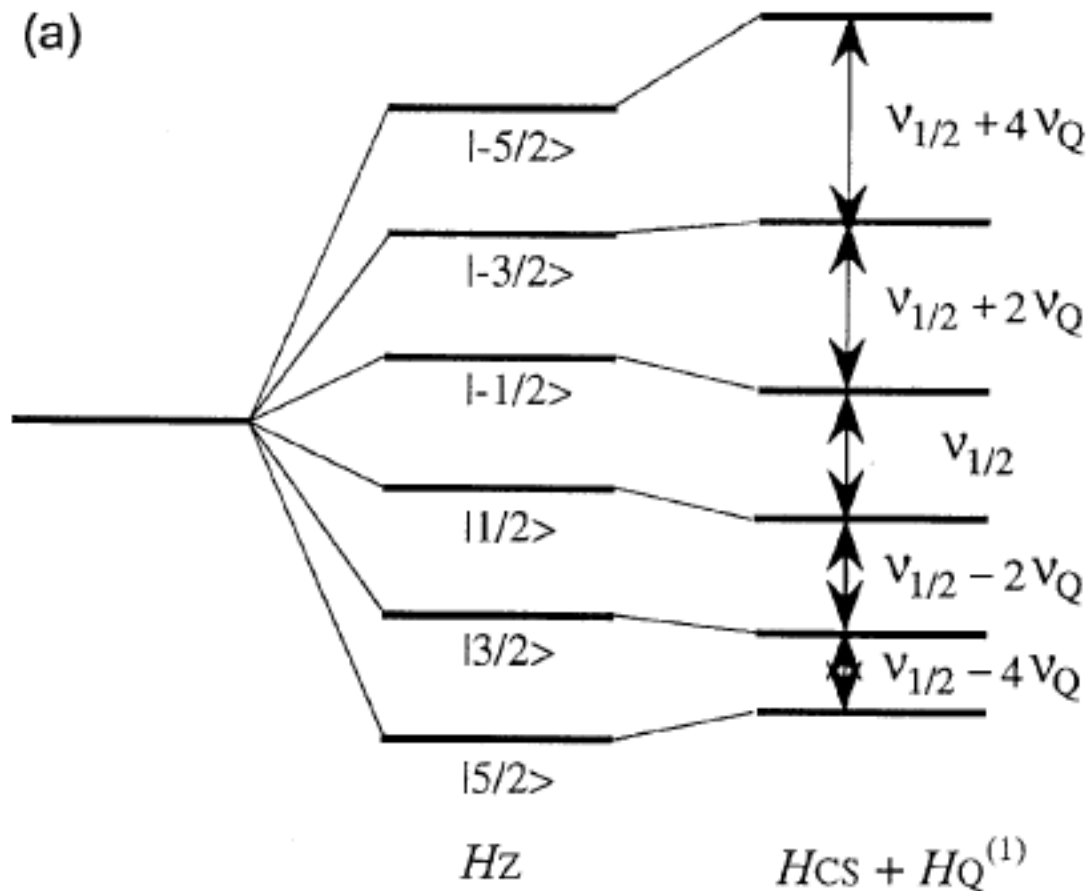
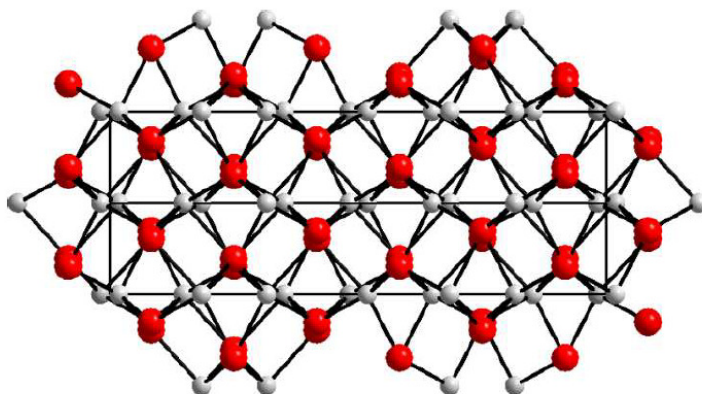


Diagrama de Níveis de Energia dos Estados de Spin Nuclear do  $^{27}\text{Al}$

# $^{27}\text{Al}$ MAS NMR Corundum e Safira

$\text{Al}_2\text{O}_3$ : SG =  $R\bar{3}c$  (No. 167)  $a = 4.759 \text{ \AA}$   $c = 12.992 \text{ \AA}$

Atom	$x$	$y$	$z$
Al	0	0	0.35217
O	0.30168	0	1/4



The corundum structure with the  $c$  axis going from left to right. Red spheres are O and grey are Al.

Sample	Method	$\delta_{\text{iso}}$ (ppm)	QCC (MHz)
Corundum	SC NMR	7.4(4)	2.30(4)
Sapphire	SC NMR	18.8(3)	2.403(15)

Safira é corundo com impurezas de metais de transição.

# $^{27}\text{Al}$ MAS NMR Safirina



Foto de safirina  
(webmineral)

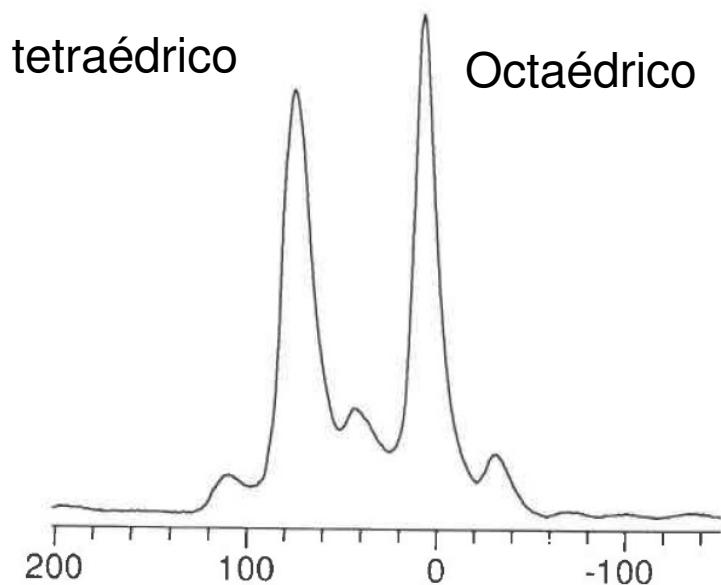
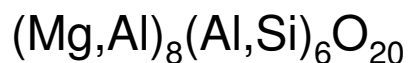
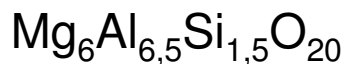
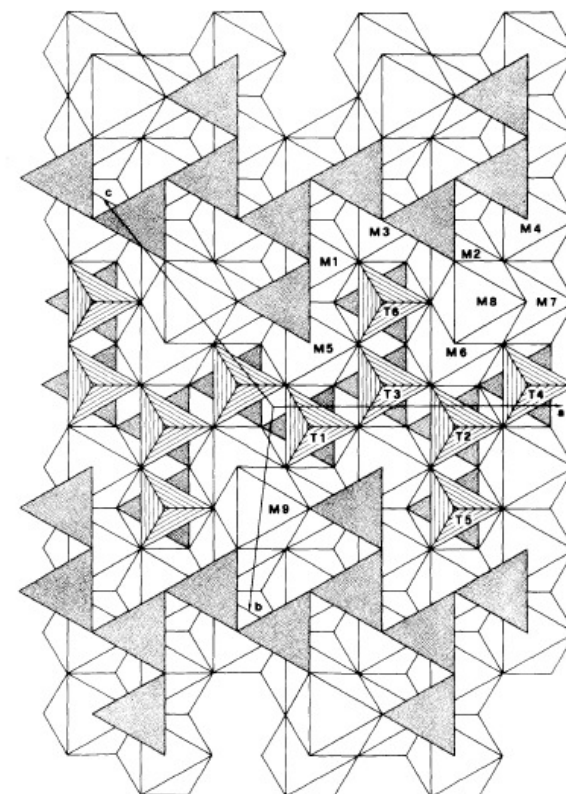


Fig. 2. The  $^{27}\text{Al}$  NMR spectrum for synthetic sapphire. The two largest peaks are real maxima; the smaller ones are spinning side bands.



Estrutura idealizada da safirina.

Zeitschrift für Kristallographie 151, 91 – 100 (1980)