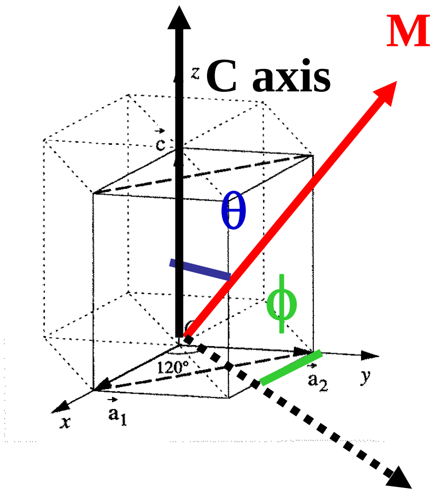
Magnetic anisotropy or better Magnetocrystalline anisotropy

- The magnetocrystalline anisotropy energy is expressed by the formula :

$$E_a(\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} K_n^m P_n^m(\cos\theta)\cos m\phi$$

- where P_n^m represents the Legendre polynoms,
- K_n^m anisotropy ~~constants~~,

□ θ and φ are the polar and azimutal angles (sphéric coordinates) of magnetization direction.



•K.H.J. Buschow and F.R. de Boer (2003) “Physics of Magnetism and materials” Kluver Academic/Plenum publisher

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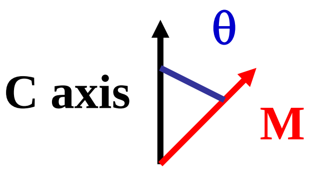
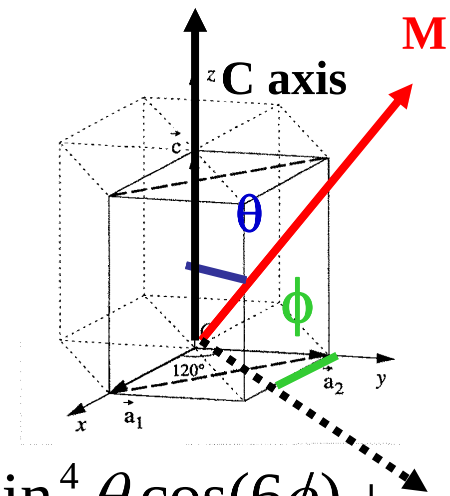
Magnetic anisotropy or better Magnetocrystalline anisotropy

uniaxial symmetry

$$E_a(\theta,\phi) = K_1 \sin^2\theta + K_2 \sin^4\theta + \cdots$$



Hexagonal symmetry



$$E_a(\theta,\phi) = K_1 \sin^2\theta + K_2 \sin^4\theta + K_3 \sin^6\theta + K_4 \sin^4\theta \cos(6\phi) + \ldots$$

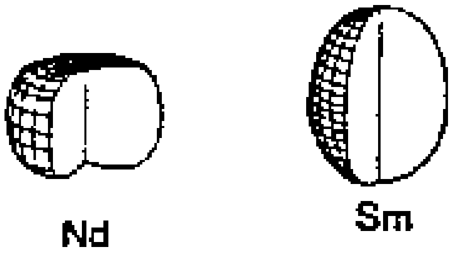
E_a is an important parameter for soft and hard magnetic materials

Crystal electric field

$$V(\vec{r}) = \sum_{l} \sum_{m=-l}^{+l} A_l^m r^l Y_l^m(\vec{r})$$

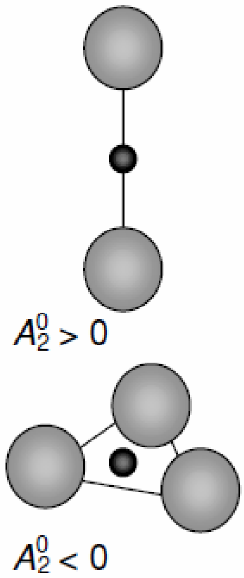
A_l^m Crystal electric field coefficients

Y_l^m Spherical harmonics



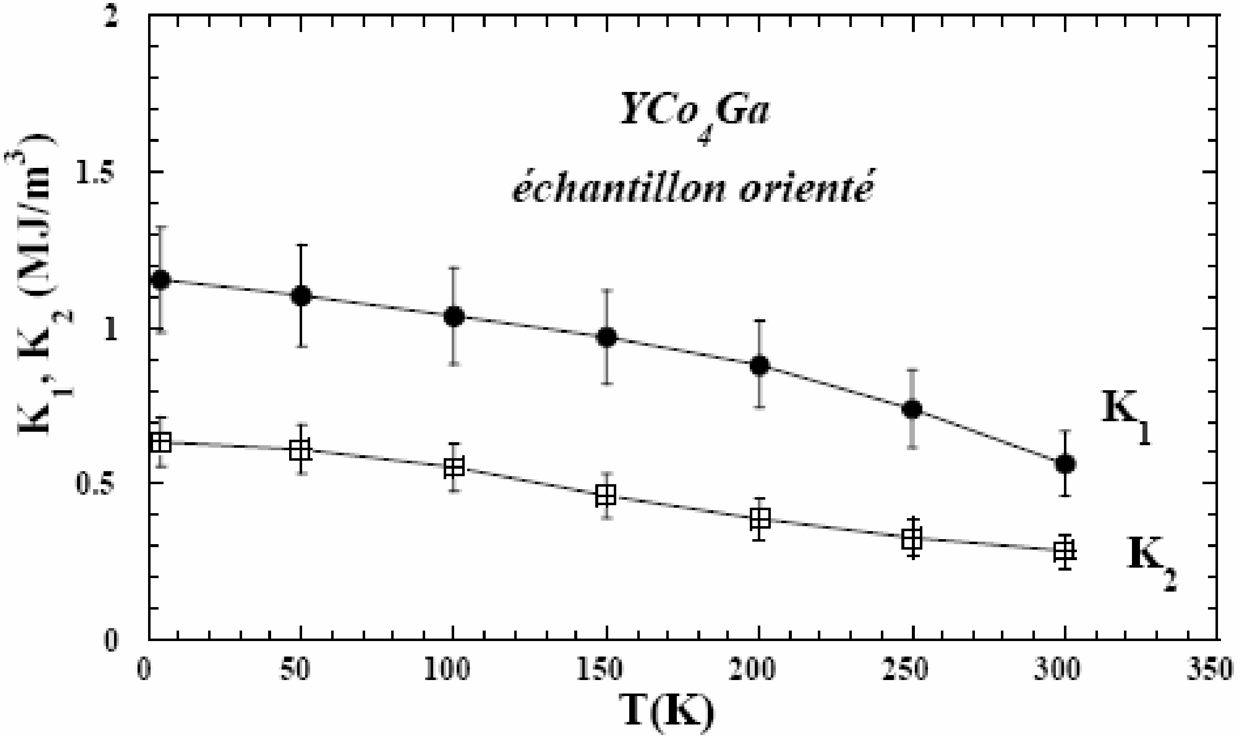
- Coupling with the 4f electronic shell
- Favors the orientation of the shell in the electric field gradient

- Hutchings, M. T. (1964) *Solid state phys.*, *16*, 227.
- Stevens coefficients



Examples of atomic configurations that produce positive and negative electric field gradients at the central site.

Anisotropy constant may vary with T !

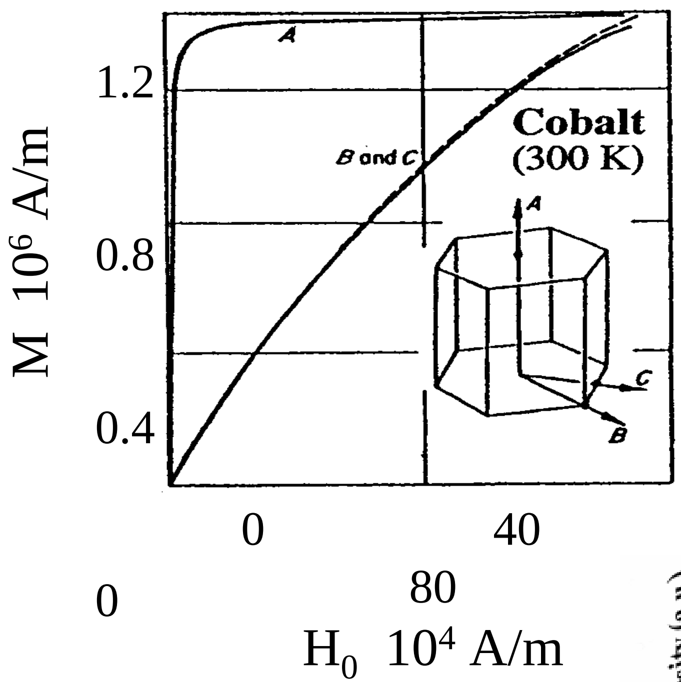


Not constants but PARAMETERS

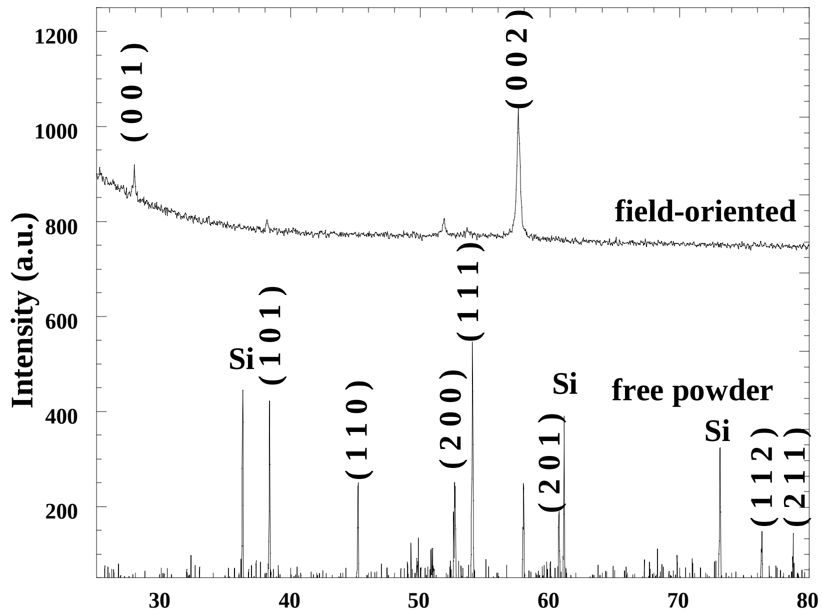
May even change of sign

How to identify the Easy Magnetization Direction

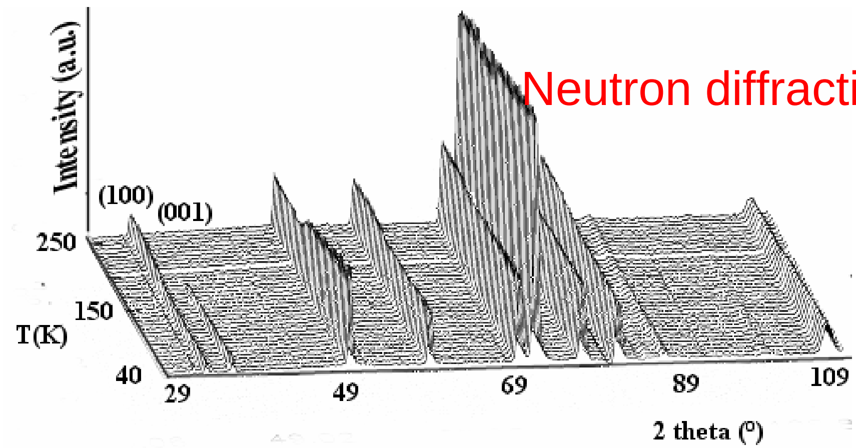
Magnetization curves



X-ray diffraction



Neutron diffraction experiments



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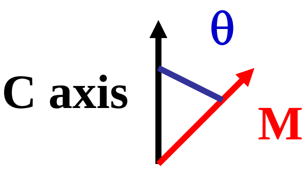
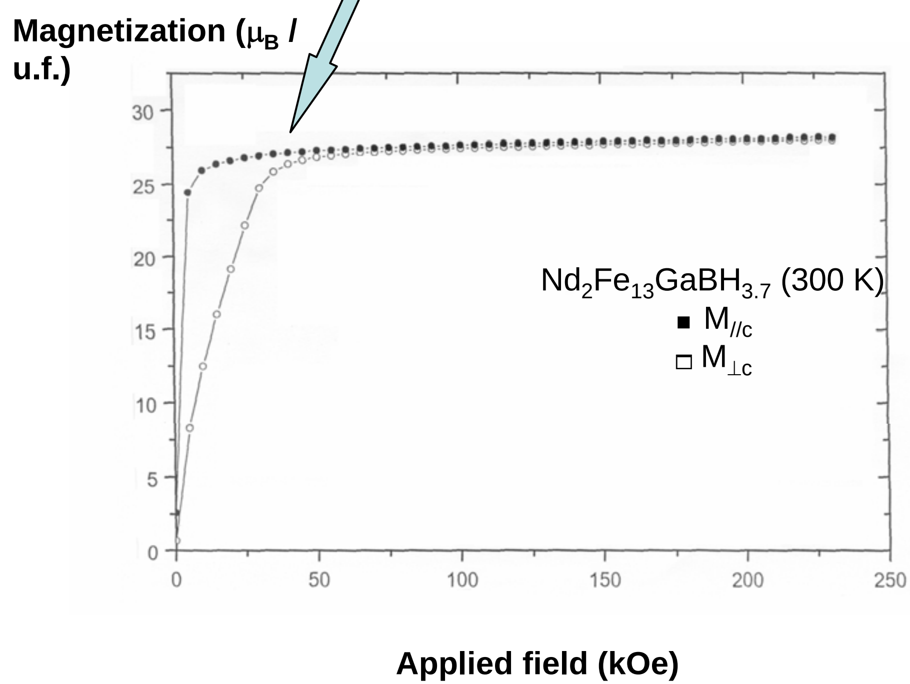
Anisotropy field

$H_a = 2\,K_1 / \ \mu_0\,M_s + \ldots$

$H_a = 2\,K_1 / \mu_0\,M_s$





$H_c < \ H_a$

Higher order :

$$\mu_0 H_a = (2K_1 + 4K_2)/\ M_S.$$

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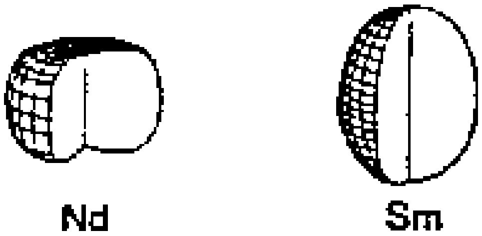
Rare earth contribution to magnetocrystalline anisotropy

$$K_1(T=0) = -\frac{3}{2}\alpha_J \langle r^2 \rangle^{4f} (3J_z - J(J+1))A_2^0$$

Purely Atomic parameter

α_J second order Stevens coefficient (α_J) for R^{3+}

$$(3J_z - J(J+1))$$



$\alpha_J < 0$ $\alpha_J > 0$

$\langle r^2 \rangle^{4f}$ 4f shell

Atomic environment electric charges

A_2^0 **Crystal electric field gradient**

Remark : $\alpha_J \langle r^2 \rangle^{4f} (3J_z - J(J+1))$ **Quadrupolar moment**

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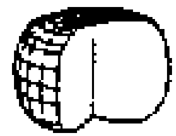
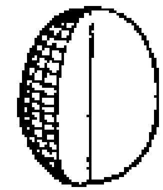
2^{nd} order Stevens coefficient

Ion	Ce^{3+}	Pr^{3+}	Nd^{3+}	Sm^{3+}	Tb^{3+}	Dy^{3+}	Ho^{3+}	Er^{3+}	Tm^{3+}	Yb^{3+}
α_J 10^2	-5,71	-2,10	-0,64	+4,13	-1,01	-0,63	-0,22	+0,25	+1,01	+3,17

Similar equation for K_2; K_3 and so on





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- K.H.J. Buschow, Magnetism and Processing of Permanent Magnet Materials, Handbook of Magnetic Materials Volume 10, édited by K.H.J. Buschow, Elsevier Science B.V., Amsterdam (1997), Ch. 4, p. 463. ISBN 0 444 853138.

The quadrupole moment

$$Q_2 = \int \rho_{4f}(r)(3\cos^2\theta - 1)r^2 d^3r.$$

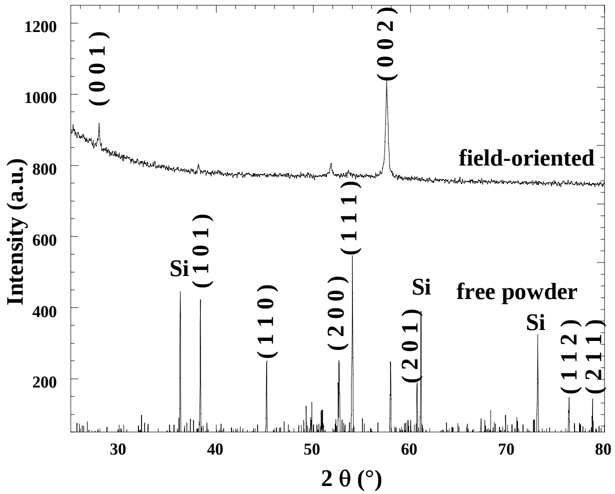
The hexadecapole moment

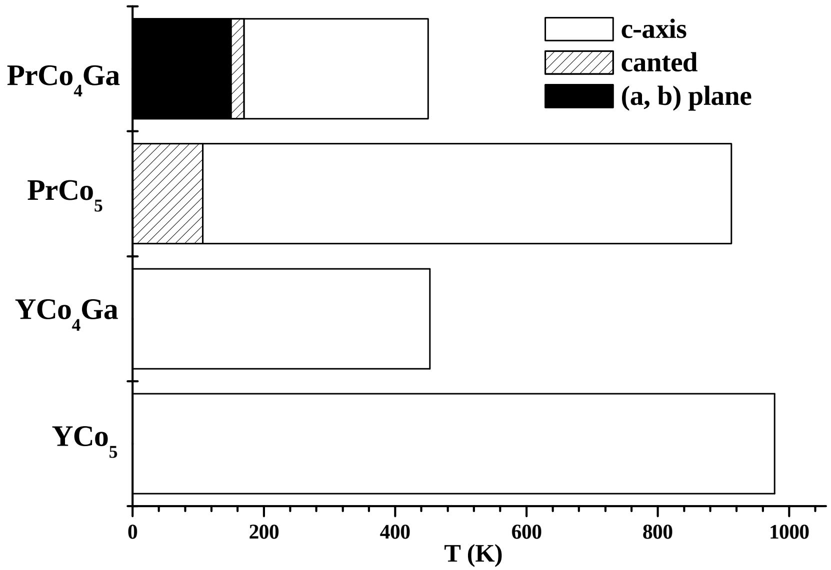
$$Q_4 = \int \rho_{4f}(r)(35\cos^4\theta - 30cos^2\theta + 3)r^4 d^3r,$$

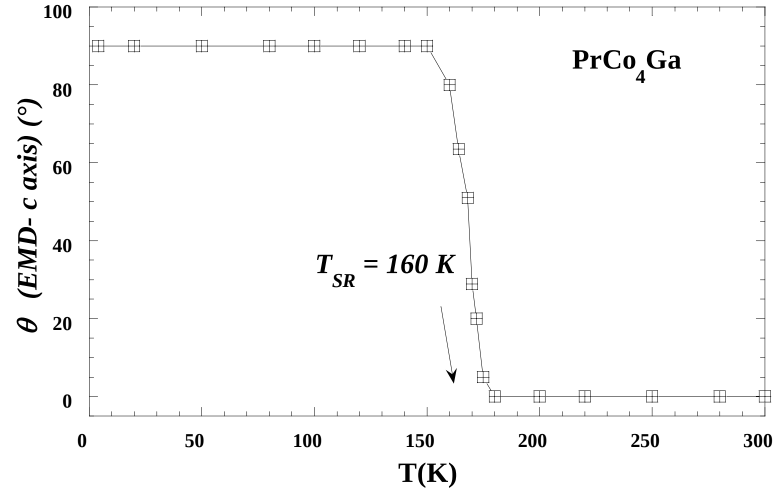
The 64-pole moment

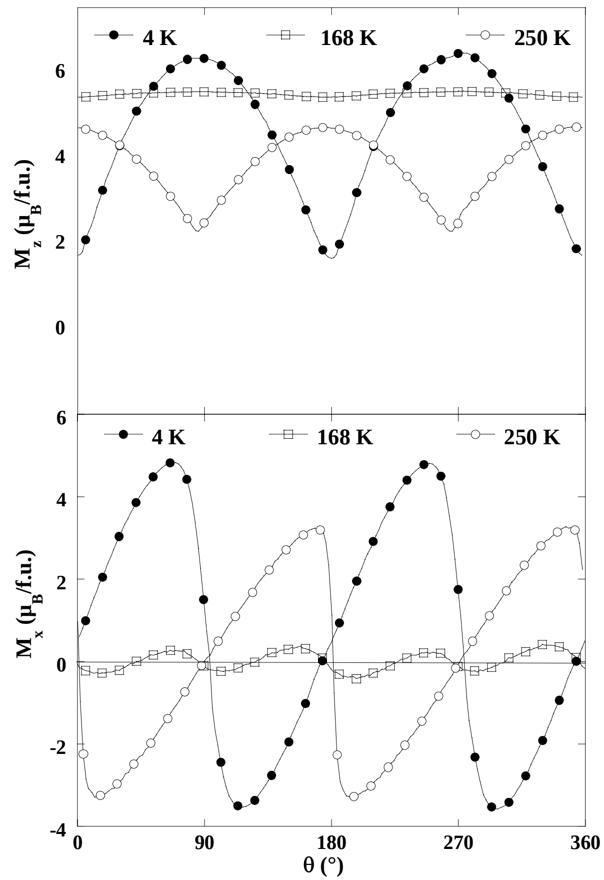
$$Q_6 = \int \rho_{4f}(r)(231\cos^6\theta - 315\cos^4\theta + 105\cos^2\theta - 5)r^6 d^3r.$$

More complex behaviour :









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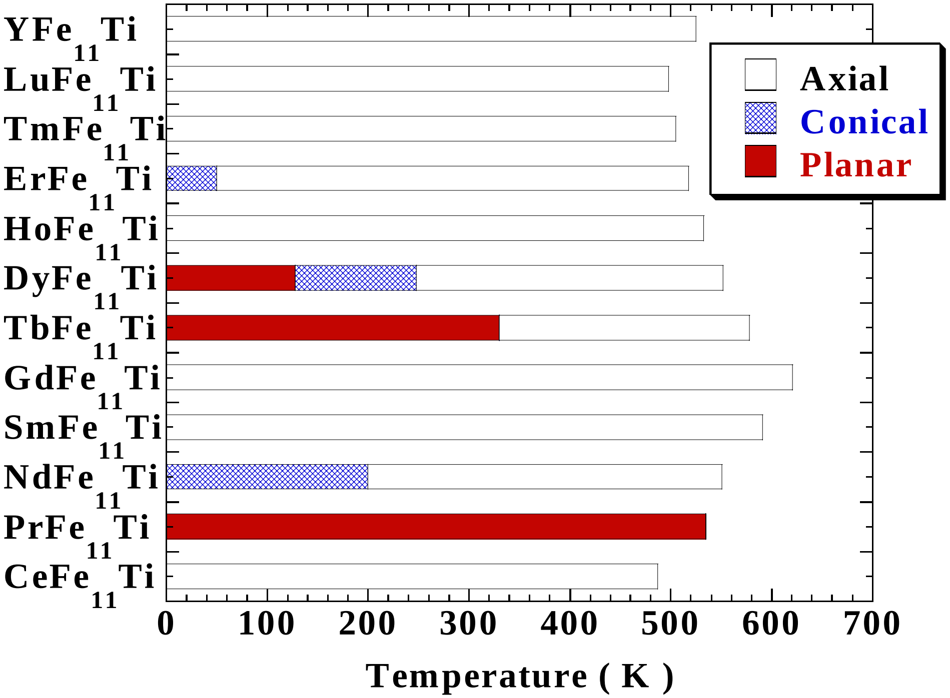
Complex behaviour



Magnetic phase diagram

K_1	$K_1 > 0$	$K_1 > 0$	$K_1 < 0$	$K_1 < 0$
K_2	$\infty > K_2 > -K_1$	$-K_1 > K_2 > -\infty$	$-K_1/2 > K_2 > -\infty$	$\infty > K_2 > -K_1/2$
EMD	$\theta = 0$; axe c	$\theta = 90$; plan de base		$\theta = \arcsin(-K_1/2K_2)^{1/2}$; cône

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Magnetic phase diagram for K1 and K2 values of an uniaxial magnet

Note that in the metastable region there are 2 energy minima a Theta=0 and Theta =π/2