Useful relationships for rotational spectroscopy

CODATA 2014: $I_b(\text{uÅ}^2) = 505\,379.0089(86)/B(\text{MHz})$,
where $505\,379.01 = 10^{20}h/(8\pi^2 m_u 10^6)$
$k/hc = 0.695\,035\,6$ cm^{-1} K^{-1}

1 rad = 57.295 78° = 180/π
1 cal = 4.184 J
1 D = $3.335\,641 \times 10^{-30}$ C m
1 Pa = 7.500 617 mTorr

1 bohr = 1 $a_0 = 4\pi\varepsilon_0\hbar^2/(m_\text{e}e^2) = 0.529\,177\,2$ Å
1 hartree = 1 E_h = 27.211 395 eV = 2 625.500 7 kJ mol^{-1}
= 219 474.72 cm^{-1}

1 kJ mol^{-1} = 83.593 5 cm^{-1}
= 2 506.07 GHz

au of dipole= 2.541 746 D
au of quadrupole= 1.345 034 DÅ (DÅ = Buckingham = 10^{-20} esu)
au of octopole= $0.711\,761\,4 \times 10^{-34}$ esu
au of polarizability= 0.148 184 7 Å^3

$$\chi_{\alpha\alpha}\ (\text{MHz}) = -234.9647\ Q(\text{barn})\ \frac{\partial^2 V}{\partial \alpha^2}(\text{au})$$

Q(barn) = 0.002860(15) [D], 0.02044(3) [^{14}N]
−0.08165(80) [^{35}Cl]
0.313(3) [^{79}Br], −0.710(10) [^{127}I]

tetrahedral angle: $\alpha = \cos^{-1}(-1/3) = 109.471\,22°$
for an XCH$_3$-type molecule: $\sin\beta = \frac{2}{\sqrt{3}}\sin\frac{\alpha}{2}$, where: $\angle\text{XCH} = 180 - \beta$, $\angle\text{HCH} = \alpha$

Cartesian→Polar:

$R = (x^2 + y^2 + z^2)^{1/2}$
$\theta = \cos^{-1}(z/R)$
$\varphi = \tan^{-1}(y/x)$ [use ATAN2 for quadrant]

Polar→Cartesian:

$x = R\sin\theta\cos\varphi$
$y = R\sin\theta\sin\varphi$
$z = R\cos\theta$

Least-squares fit of a straight line $y = a + bx$:

$$C_{xx} = \sum x^2 - (\sum x)^2/N \qquad b = C_{xy}/C_{xx}$$

$$C_{yy} = \sum y^2 - (\sum y)^2/N \qquad (\delta b)^2 = \frac{1}{(N-2)C_{xx}}(C_{yy} - bC_{xy})$$

$$C_{xy} = \sum xy - \sum x \sum y/N \qquad a = \frac{1}{N}(\sum y - b\sum x)$$

$$(\delta a)^2 = \delta b^2 \sum x^2/N$$

Error propagation:

$x = aA \pm bB$:	$\delta x = (a^2\delta A^2 + b^2\delta B^2)^{1/2}$
$x = AB$:	$\delta x = (A^2\delta B^2 + B^2\delta A^2)^{1/2}$
$x = A/B$:	$\delta x = \left[(x/A)^2\delta A^2 + (x/B)^2\delta B^2\right]^{1/2} = (\delta A^2 + x^2\delta B^2)^{1/2}/B$
$x = 1/A$:	$\delta x = \delta A/A^2$
$x = A^2$:	$\delta x = 2A\,\delta A$
$x = \sqrt{A}$:	$\delta x = \delta A/(2\sqrt{A})$
$x = \ln A$:	$\delta x = \delta A/A$
$x = (A^2 + B^2)^{1/2}$:	$\delta x = (A^2\delta A^2 + B^2\delta B^2)^{1/2}/x$
$x = f(A, B, \ldots)$:	$\delta x^2 = \left(\frac{\partial f}{\partial A}\right)^2\delta A^2 + \left(\frac{\partial f}{\partial B}\right)^2\delta B^2 + \cdots$

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