Solving the time-independent Schrödinger equation for a hindered methyl rotor potential with *QRotor.py*

Pablo Gila-Herranz

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Time-independent Schrödinger equation for a hindered rotor

The time-independent Schrödinger equation is

$$H\Psi(\varphi) = E\Psi(\varphi)$$

The hamiltonian for a hindered methyl rotor can be expressed as a sum of the kinetic rotational energy and the potential energy,

$$H = -B\frac{d^2\Psi}{d\varphi^2} - V(\varphi)$$

with

$$B = \frac{1}{2I} = \frac{1}{2\sum_i m_i r_i^2}$$

The potential can be adjusted to the following form, where the coefficients are calculated via electronic calculation methods [1],

$$V(\varphi) = c_0 + c_1\sin(3\varphi) + c_2\cos(3\varphi) + c_3\sin(6\varphi) + c_4\cos(6\varphi)$$

Finite Difference Method

The time-independent Schrödinger equation is a second-order differential equation. It can be solved numerically using the finite difference method. The first derivative can be approximated as

$$\frac{d\Psi}{d\varphi} = \frac{\Psi(\varphi + \Delta\varphi) - \Psi(\varphi)}{\Delta\varphi}$$

References

[1] K. Titov, M. R. Ryder, A. Lamaire, Z. Zeng, A. K. Chaudhari, J. Taylor, E. M. Mahdi, S. M. J. Rogge, S. Mukhopadhyay, S. Rudić, V. Van Speybroeck, F. Fernandez-Alonso, and J.-C. Tan, "Quantum tunneling rotor as a sensitive atomistic probe of guests in a metal-organic framework," vol. 7, no. 7, p. 073402.