



A computer-generated spectrum of a quadrupolar nucleus

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Field strength: 400 MHz

Why is this your favorite spectrum?

A program called SIMPSON was used, which allows us to simulate spectra of quadrupolar nuclei like vanadium. In this case we simulate a V51 spectrum of VOCl_3 , using literature values for anisotropic shift, eta, etc. The experimental conditions of this simulation could be fine-tuned to design novel pulse sequences to observe a nucleus like this one. I find this fascinating because lifelike spectra of complicated nuclei can be observed with a computer program.

