THAT'S JUST, LIKE, YOUR OPINION, MAN - HOW DO WE KNOW WHEN WE HAVE A GOOD MATCH BETWEEN EXPERIMENTAL AND COMPUTED SPECTRA?

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The use of quantum chemistry to compute spectra, vibrational or electronic, for use in assigning gas phase spectra and structures, is common. However, there is no accepted standard for appropriate criteria for what constitutes an acceptable match, in particular for the purposes of structure determination. This is due to challenges associated with anharmonic effects, systematic deficiencies of electronic structure methods, and a host of other idiosyncratic effects. I will discuss examples of these challenges from my own lab and propose some best practices and figures of merit. I hope this will provide a judgement-free starting point for the development of more rigorous methods for comparing experimental and computed spectra.