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Absorption spectrum of the Single Molecule Magnet [Ni(dbm)(MeOH)Cl] $_4^1$ DANIEL J. ARENAS, DIMITRIOS KOUKIS, SAITI DATTA, CHAO CAO, HAI-PING CHENG, DAVID B. TANNER, Department of Physics, University of Florida, STEPHEN HILL, Department of Physics, Florida State University, CHRISTOPHER BEEDLE, DAVID HENDRICKSON, Department of Chemistry and Biochemistry, University of California at San Diego — The room temperature optical absorption of the single-molecule magnet [Ni(dbm)(MeOH)(Cl)] $_4$ has been measured in the near-infrared-visible spectral region. The spectra show a strong absorption band around 3 eV and bands characteristic of d-d transitions in nickel. The results will be compared to various theoretical models in the literature; including DFT and DFT+U calculations [$Phys.\ Rev.\ Lett.\ 100$, 167206] that predict different energy gaps for the HOMO to LUMO optical transitions.

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