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135: 159517b **Electronic states of the manganese dimer ion probed by photodissociation spectroscopy.** Terasaki, Akira; Matsushita, Akira; Tono, Kensuke; Yadav, Ramkuber T.; Briere, Tina M.; Kondow, Tamotsu (Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo Laboratory, Genesis Research Institute, Inc., Ichikawa, Chiba, Japan 272–0001). *J. Chem. Phys.* 2001, 114(21), 9367–9370 (Eng), American Institute of Physics. The optical spectrum of the manganese dimer ion, Mn_2^+, was obtained by measurement of the photodissocn. action spectrum in the photon–energy range from 1.9 through 5.6 eV. The spectrum was analyzed by calcg. its electronic and geometric structures using d. functional theory including nonlocal corrections. The simulation was in reasonable agreement with the exptl. result, allowing the assignment of the electronic states involved in the optical transitions. The ground state was shown to be a $^{12}\Sigma_g^+$ state. The excited electronic states corresponding to the transitions around 2.9, 4.0, and 5.3 eV were assigned to $^{12}\Sigma_u^+$, $^{12}\Sigma_u^+$ together with $^{12}\Pi_u$, and $^{12}\Pi_u$, resp. The high–spin character indicates a ferromagnetic coupling of all the 3d electrons.

$^{12}\Sigma_u^+$

Refl. coef