RELATIVISTIC COUPLED-CLUSTER CALCULATIONS OF CHLORINE L-EDGE SPECTRUM OF CH_2ICL

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We present a computational study of x-ray absorption spectra for CH_3Cl and CH_2ICl using relativistic equation-of-motion coupled-cluster methods with spin-orbit coupling. The 1:1 ratio of the peak intensities for the chlorine L_3 edge and L_2 edge in the experimental x-ray absorption spectrum of CH_2ICl [1] shows an interesting deviation from the ratio of 2:1 between $2p_{3/2}$ and $2p_{1/2}$ electrons. Here we study the origin of this phenomenon using high-accuracy *ab initio* calculations. Our computational results explain the relation between this anomaly in intensities and "multiplet effects" [2].

Reference:

[1] Z. Yang, K. Schnorr, A. Bhattacherjee, P.-L. Lefebvre, M. Epshtein, T. Xue, J.F. Stanton, and S.R. Leone, J. Am. Chem. Soc. **140**, 13360 (2018).

[2] F. de Groot, Coordination Chemistry Reviews **249**, 31 (2005).