



<http://www.diva-portal.org>

Postprint

This is the accepted version of a paper published in *Journal of Chemical Physics*. This paper has been peer-reviewed but does not include the final publisher proof-corrections or journal pagination.

Citation for the original published paper (version of record):

Pinjari, R V., Delcey, M G., Guo, M., Odelius, M., Lundberg, M. (2014)

Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states.

Journal of Chemical Physics, 141(12): 124116

<http://dx.doi.org/10.1063/1.4896373>

Access to the published version may require subscription.

N.B. When citing this work, cite the original published paper.

Permanent link to this version:

<http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-236075>

Erratum: Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states [J. Chem. Phys. **141**, 124116 (2014)]

Rahul V. Pinjari,¹ Mickaël G. Delcey,¹ Meiyuan Guo,¹ Michael Odellius,² and Marcus Lundberg^{1, a)}

¹⁾*Department of Chemistry - Ångström laboratory, Uppsala University, SE-751 20 Uppsala, Sweden.*

²⁾*Department of Physics, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden.*

(Dated: 27 October 2016)

In the original paper, the core restricted active space (RAS) calculations of the ferric ion included the wrong number of sextet states in A_{1u} symmetry.¹ The correct number of states should be three instead of zero. The original description of the number of states should be changed from:

“For B_{1u} , B_{2u} , and B_{3u} this means 72 doublet, 37 quartet and 4 sextet states each, while the corresponding numbers for A_{1u} symmetry are 69, 39 and 0” to

“For B_{1u} , B_{2u} , and B_{3u} this means 72 doublet, 37 quartet and 4 sextet states each, while the corresponding num-

bers for A_{1u} symmetry are 69, 39 and 3”.

The original core RAS spectra of the high-spin systems included a minor peak at approx. 718 eV, not observed in spectra from the ligand-field multiplet model. The corrected core RAS spectra agrees well with the multiplet spectra, see Fig. 1.

The graphical analysis of the orbital contributions to the final spectra has also been updated, see Fig. 2.

The conclusions of the paper are not affected by the current corrections.

¹R. V. Pinjari, M. G. Delcey, M. Guo, M. Odellius, and M. Lundberg, J. Chem. Phys. **141**, 124116 (2014).

^{a)}Electronic mail: marcus.lundberg@kemi.uu.se

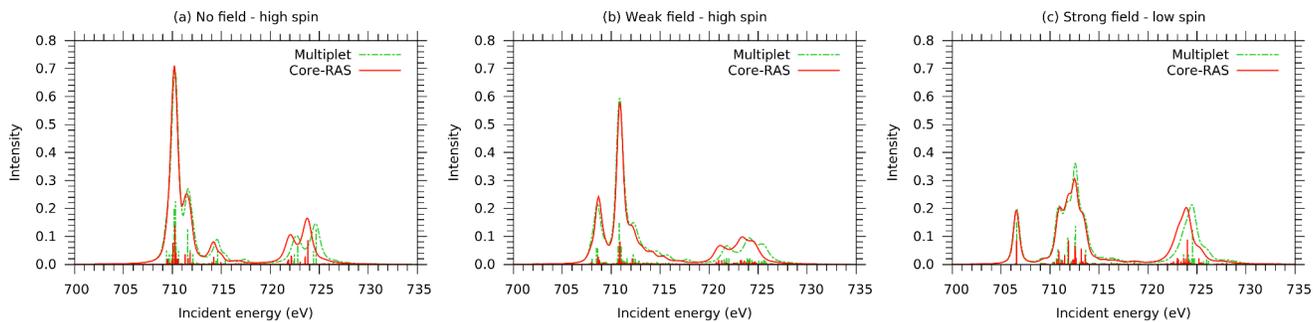


FIG. 1. L-edge XAS spectra of the Fe^{3+} ion, with different ligand-field splitting, calculated using RASPT2(11,1,0;3,5,0) (red solid line) and the ligand-field multiplet model (green dotted line).

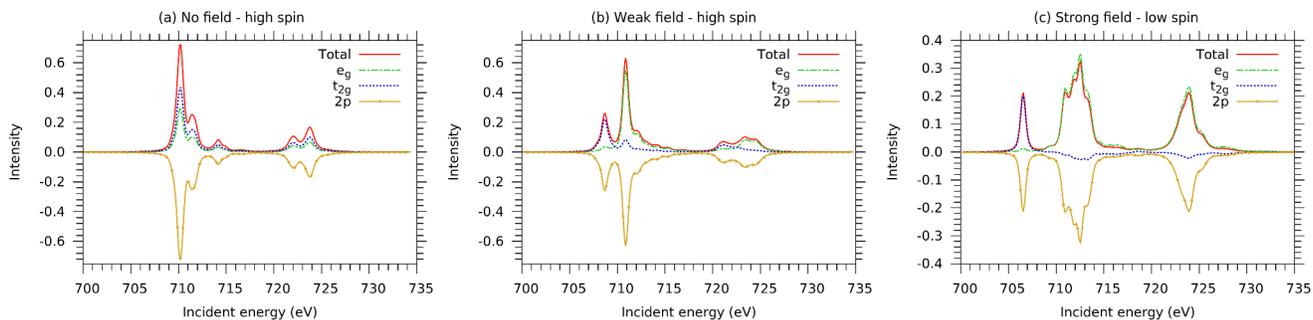


FIG. 2. Analysis of orbital contributions to the RASPT2(11,1,0;3,5,0) L-edge XAS spectra of the Fe^{3+} ion.