

The files C6CP08561J\_ESI\_001.zip to C6CP08561J\_ESI\_004.zip contain the dataset and utility scripts referred to as electronic supplementary information (ESI) for the paper:

On the calculation of second-order magnetic properties using subsystem approaches in the relativistic framework

by Malgorzata Olejniczak, Radovan Bast and Andre Severo Pereira Gomes

DOI: 10.1039/C6CP08561J

The md5 checksums for each file are:

MD5 (C6CP08561J\_ESI\_001.zip) = ac306cfa84bfd15dc394c9d40e645047

MD5 (C6CP08561J\_ESI\_002.zip) = 4fa186559eee50fff72a84a1e26cf749

MD5 (C6CP08561J\_ESI\_003.zip) = 8f047e7a7911b51e61e07829d25ce9c1

MD5 (C6CP08561J\_ESI\_004.zip) = 3f31b0b481f66e334ae28f3fd76a0ec7

The files contain, roughly:

C6CP08561J\_ESI\_001.zip: optimized structures, plots and scripts

C6CP08561J\_ESI\_002.zip: data for the h2se-h2o system

C6CP08561J\_ESI\_003.zip: data for the h2te-h2o system

C6CP08561J\_ESI\_004.zip: data for the h2po-h2o system

We note that, in addition to the hosting by RSC, the whole dataset is available at

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as a single gzipped tar file.

The authors, 8 march 2017