Contribution ID: **130** Type: **Talk**

Can we reach the heaven of chemical accuracy by climbing Jacob's Ladder? A DFT validation study for Non-heme Iron complexes

Tuesday, 5 December 2017 14:00 (20 minutes)

HPC content

Gaussian 09 Code was used to optimize complexes. 20GB of RAM, 1 node of 24 processors and an average walltime of 50:00 was used for each optimization.

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