Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Prediction of High-Valent Iron K-edge Absorption Spectra by Time-Dependent Density Functional Theory

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Example ORCA input files

Geometry Optimization, Method 1

```
! UKS B3LYP TZVP TIGHTSCF SLOWCONV OPT
! Normalprint
! Cosmo
! grid4 nofinalgrid

%scf    MaxIter 500
        TolE 1e-7
        TolErr 1e-6
        End
*xyz a,b
xyz coordinates
*
```

Spectral Calculation, Method 1

```
! UKS BP86 TZVP TIGHTSCF SLOWCONV
! MORead
! Normalprint
! Cosmo
! grid4 nofinalgrid
%moinp "sces339.gbw"

%method SpecialGridAtoms 26
SpecialGridIntAcc 7
        end

%scf    MaxIter 500
        TolE 1e-7
        TolErr 1e-6
        end

%tddft orbwin[0] = 0,0,-1,-1
        orbwin[1] = 0,0,-1,-1
        doquad true
        maxdim 450
        maxcore 1500
        nroots 30
        triplets false
        end
```

Geometry Optimization, Method 2

```
! def2-TZVP(-f) def2-TZVP/J DeContractAux BP86 COSMO ZORA
! TightSCF Grid4 NoFinalGrid OPT
! Normalprint

%scf    MaxIter 500
        TolE 1e-7
        TolErr 1e-6
        end
```

Spectral Calcualtion, Method 2

```
! SP def2-TZVP(-f) def2-TZVP/J BP86 COSMO ZORA
! TightSCF Grid4 NoFinalGrid
! Normalprint

%scf    MaxIter 500
        TolE 1e-7
        TolErr 1e-6
        end

%tddft orbwin[0] = 0,0,-1,-1
        orbwin[1] = 0,0,-1,-1
        doquad true
        maxdim 450
        maxcore 1500
        nroots 30
        triplets false
        end
```