Electronic Supplementary Material (ESI) for Dalton Transactions.


# Supporting Information

## OctaDist: A tool for calculating distortion parameters in spin crossover and coordination complexes

Rangsiman Ketkaew,[a] Yuthana Tantirungrotechai,[a] Phimphaka Harding,[b] Guillaume Chastanet,[c] Philippe Guionneau,[c] Mathieu Marchivie,[c*] and David J. Harding,[b*]

[a]Computational Chemistry Research Unit, Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathum Thani, 12120 Thailand.

[b]Functional Materials and Nanotechnology Center of Excellence, Walailak University, Thasala, Nakhon Si Thammarat, 80160, Thailand.

[c] CNRS, Univ. Bordeaux, Bordeaux INP, ICMCB, UMR 5026, 87 av. Dr A. Schweitzer, F-33600 Pessac, France.

*E-mail: mathieu.marchivie@icmcb.cnrs.fr; hdavid@mail.wu.ac.th

**Table S1**: Computed parameter of selected series of Fe complexes for high-spin state. Data were taken from Halcrow 2011 unless otherwise stated.[1]

| Structure | Temp (K) | OctaDist | Previous work |
|---|---|---|---|
| [Fe(saltrien)]$BF_4$ | 100 | 262 | 124 |
| | 250 | 263 | 127 |
| | 293 | 334 | 157 |
| [Fe(saltrien)]$BPh_4 \cdot ½(C_2H_4Cl_2)$ | 105 | 316 | 240 |
| [Fe(saltrien)]$BPh_4 \cdot ½(CH_3)_2CO$ | 120 | 316 | 239 |
| [Fe(saltrien)]$ClO_4$ | 140 | 450 | 254 |
| [Fe(saltrien)]$PF_6$ | 140 | 463 | 236 |
| | 240 | 408 | 323 |
| [Fe(saltrien)]$NO_3 \cdot C_2H_4Cl_2$ | 100 | 370 | 284 |
| [Fe(saltrien)][Ni(dmit)$_2$] | 293 | 295 | 295 |
| [Fe(1-bpp)$_2$][$BF_4$]$_2$ | 300 | 468 | 467 |
| [Fe(1-bpp)$_2$][$BF_4$]$_2 \cdot 3CH_3NO_2$ | 300 | 493 | 476 |
| [Fe(1-bpp)$_2$][$PF_6$]$_2$ | 300 | 643 | 599 |
| [Fe(1-bpp)$_2$][$ClO_4$]$_2$ | 300 | 653 | 547 |
| [Fe(1-bpp)$_2$][$SbF_6$]$_2$ | 300 | 640 | 560 |
| [Fe(1-bpp)$_2$][$I_3$]$_2$ | 300 | 490 | 488 |
| [Fe(1-bpp)$_2$]$I_{0.5}$[$I_3$]$_{1.5}$ | 300 | 629 | 522 |
| [Fe(1-bpp)$_2$][$Co(C_2B_9H_{11})_2$]$_2 \cdot CH_3NO_2$ | 300 | 488 | 482 |
| [Fe(qsal-I)$_2$]OTf.MeOH[2] | 293 | 210 | 189 |
| [Fe(qsal-I)$_2$]OTf.EtOH[2] | 213 | 247 | 200 |
| | 170 | 221 | 177 |
| [Fe(qsal-I)$_2$]OTf.n-PrOH[2] | 270 | 227 | 187 |
| [Fe(qsal-I)$_2$]OTf.i-PrOH[2] | 293 | 187 | 153 |
| [Fe(qsal-I)$_2$]OTf.Acetone[2] | 293 | 193 | 160 |

**Table S2**: Computed parameter of selected series of Fe complexes for low-spin state. Data were taken from Halcrow 2011 unless otherwise stated.[1]

| Structure | Temp (K) | OctaDist | Previous work |
|---|---|---|---|
| [Fe(saltrien)]$ClO_4$ | 105 | 126 | 83 |
| [Fe(saltrien)][Ni(dmit)$_2$]$(CH_3)_2CO$ | 293 | 135 | 86 |
| [Fe(naphthtrien)]$PF_6(C_2H_5)_2O$ | 150 | 142 | 98 |
| [Fe(qsal-I)$_2$]OTf.MeOH[2] | 163 | 114 | 61 |
| [Fe(qsal-I)$_2$]OTf.EtOH[2] | 100 | 123 | 71 |
| [Fe(qsal-I)$_2$]OTf.n-PrOH[2] | 100 | 122 | 69 |
| [Fe(qsal-I)$_2$]OTf.i-PrOH[2] | 163 | 124 | 71 |
| [Fe(qsal-I)$_2$]OTf.Acetone[2] | 163 | 122 | 71 |
| [Fe(qsal-I)$_2$]OTf.MeCN[2] | 123 | 120 | 69 |
| [Fe(qsal)$_2$]NCS·$CH_2Cl_2$ | 113 | 125 | 76 |
| [Fe(qsal)$_2$]NCSe·MeOH | 230 | 137 | 81 |
| [Fe(qsal)$_2$][Ni(dmise)$_2$]·x$CH_3CN$ | 200 | 116 | 67 |
| [Fe(qnal)$_2$][Pd(dmit)$_2$]5·$(CH_3)_2CO$ | 105 | 114 | 69 |
| [Fe(qsal)$_2$]$I_3$ | 50 | 118 | 70 |
| [Fe(5-Cl-qsal)$_2$][Ni( -tpdt)$_2$]·$CH_3CN$ | 150 | 118 | 65 |
| [Fe(3-OMe-qsal)$_2$]$PF_6$ | 150 | 126 | 70 |
| [Fe(qsal)$_2$]$N_3$ | 200 | 130 | 76 |
| [Fe(pz*$_3$CH)(pz$_3$CH)][$BF_4$]$_2$, polymorph B | 173 | 60 | 30 |
| [Fe(pz*$_3$CH)(pz$^{4\text{-Me}}{}_3$CH)][$BF_4$]$_2$·2$CH_3CN$ | 25 | 86 | 44 |
| [Fe(pz*$_3$CH)(pz$_3$$CCH_2OH$)][$BF_4$]$_2$ | 25 | 66 | 33 |
| [Fe(pz$_3$CH)$_2$][$NO_3$]$_2$, α-polymorph | 293 | 68 | 34 |
| [Fe(pz$_3$CH)$_2$][$NO_3$]$_2$, β-polymorph | 293 | 69 | 35 |
| [Fe(pz$_3$CH)$_2$][$BF_4$]$_2$ | 173 | 73 | 38 |

```
$ octadist_cli

usage: octadist_cli [-h] [-v] [-a] [-c] [-g] [-i INPUT] [-o] [-s OUTPUT]
                    [--par PARAMETER [PARAMETER ...]] [--show MOL [MOL ...]]

Octahedral Distortion Calculator:
A tool for computing octahedral distortion parameters in coordination complex.
For more details, please visit https://github.com/OctaDist/OctaDist.

optional arguments:
  -h, --help            show this help message and exit
  -v, --version         show program's version number and exit
  -a, --about           show program info
  -c, --cite            show how to cite OctaDist
  -g, --gui             launch OctaDist GUI (this option is the same as
                        'octadist' command
  -i INPUT, --inp INPUT
                        input structure in .xyz format
  -o, --out             show formatted output summary
  -s OUTPUT, --save OUTPUT
                        save formatted output to text file, please specify
                        name of OUTPUT file without '.txt' extension
  --par PARAMETER [PARAMETER ...]
                        select which the parameter (zeta, delta, sigma, theta)
                        to show
  --show MOL [MOL ...]  show atomic symbol (atom) and atomic coordinate
                        (coord) of octahedral structure

Rangsiman Ketkaew       Updated on August 2019  E-mail: rangsiman1993@gmail.com
```

**Figure S1** Command-line in OctaDist.

```
$ octadist_cli --inp [Fe(1-bpp)2][BF4]2-LS-Full.xyz --out

Octahedral distortion parameters
--------------------------------
File: [Fe(1-bpp)2][BF4]2-LS-Full.xyz
Zeta   =   0.20319851
Delta  =   0.00034785
Sigma  =  86.08149397
Theta  = 281.23109091
```

**Figure S2** Command line interface in OctaDist for calculating the octahedral distortion parameters.

```
[1]: import octadist as oc

[2]: f = '[Fe(1-bpp)2][BF4]2-LS-Full.xyz'

[3]: atom, coord = oc.extract_coord(f)

[4]: atom, coord = oc.extract_octa(atom, coord)

[5]: atom

[5]: ['Fe', 'N', 'N', 'N', 'N', 'N', 'N']

[6]: coord

[6]: array([[ 4.0674,  7.204 , 13.6117],
            [ 4.3033,  7.375 , 11.7292],
            [ 3.8326,  6.9715, 15.4926],
            [ 5.8822,  6.4461, 13.4312],
            [ 3.3002,  5.3828, 13.6316],
            [ 4.8055,  8.9318, 14.2716],
            [ 2.3184,  8.0165, 13.1152]])
```

**Figure S3** OctaDist running on the interactive-python-based Jupyter Lab. This example shows how to parse an input file and extract atomic coordinates of an octahedral structure using the extract_coord and extract_octa functions.

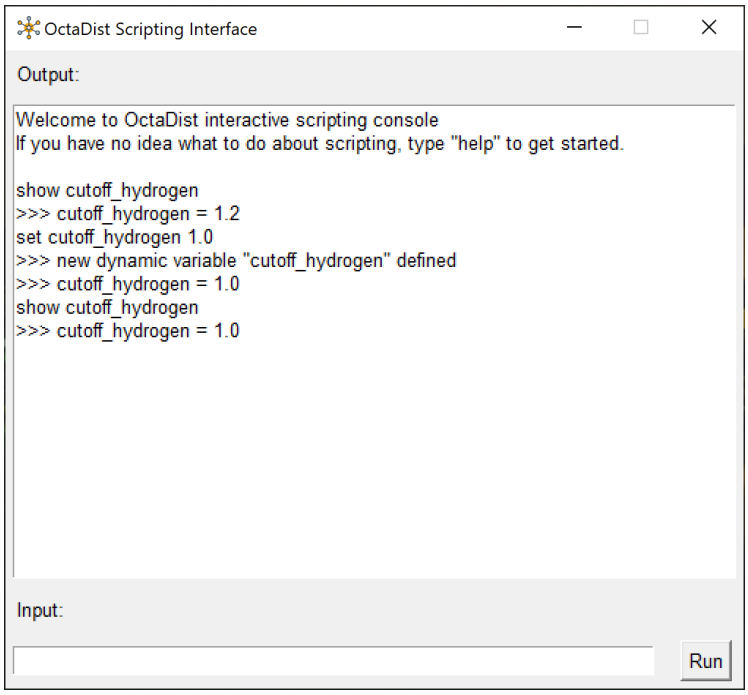


**Figure S4** Scripting console for interactive coding. A show command is used to set a new value to the cutoff_hydrogen variable.

## References


1 M. A. Halcrow, *Chem. Soc. Rev.*, 2011, **40**, 4119.

2 W. Phonsri, P. Harding, L. Liu, S. G. Telfer, K. S. Murray, B. Moubaraki, T. M. Ross, G. N. L. Jameson and D. J. Harding, *Chem. Sci.*, 2017, **8**, 3949–3959.