Electronic Supplementary Information for PCCP article

# Intra-molecular magnetic exchange interaction in tripyridinium bis[tetrachloroferrate(III)] chloride molecular magnet: A Broken Symmetry-DFT study

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**Structure of molecule**

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| | | | |
|---|---|---|---|
| Cl | 4.3505100000 | 0.1452260000 | -1.5019030000 |
| Fe | 5.9010630000 | -1.1226700000 | -0.6130520000 |
| Cl | 7.7378300000 | -0.8024470000 | -1.7160610000 |
| Cl | 4.9341690000 | -3.0724690000 | -0.3775880000 |
| Cl | 6.1878320000 | -0.3200860000 | 1.3899730000 |
| N | -1.0522280000 | -1.7520140000 | 0.1242440000 |
| -C | 0.0403820000 | -1.0350510000 | -0.2479850000 |
| C | 1.2104650000 | -1.7109330000 | -0.5740160000 |
| C | 1.2386690000 | -3.1110560000 | -0.5049400000 |
| C | 0.0862720000 | -3.8138390000 | -0.1233240000 |
| C | -1.0681070000 | -3.1088510000 | 0.1904130000 |

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| | | | |
|---|---|---|---|
| H | -1.9127450000 | -1.2402060000 | 0.3797060000 |
| H | -0.0575100000 | 0.0496350000 | -0.2708750000 |
| H | 2.0867310000 | -1.1501650000 | -0.8752530000 |
| H | 2.1568860000 | -3.6371220000 | -0.7397440000 |
| H | 0.0807180000 | -4.8946800000 | -0.0686250000 |
| H | -2.0101800000 | -3.5611290000 | 0.4767130000 |
| Cl | -0.1250660000 | 2.5054740000 | -0.3218310000 |
| N | 2.3024850000 | 3.1273180000 | 1.2802640000 |
| C | 3.5143600000 | 2.5457500000 | 1.1281410000 |
| C | 4.5481940000 | 2.8759210000 | 2.0012290000 |
| C | 4.3085220000 | 3.8096670000 | 3.0165750000 |
| C | 3.0395190000 | 4.3954400000 | 3.1441570000 |
| C | 2.0381240000 | 4.0303190000 | 2.2541170000 |
| H | 1.5219700000 | 2.8739130000 | 0.6528310000 |
| H | 3.6248320000 | 1.8343870000 | 0.3182990000 |
| H | 5.5072760000 | 2.3879320000 | 1.8873140000 |
| H | 5.1011580000 | 4.0758010000 | 3.7065710000 |
| H | 2.8305410000 | 5.1167500000 | 3.9236830000 |
| H | 1.0280410000 | 4.4169260000 | 2.2787190000 |
| N | -4.5024130000 | 1.9412870000 | -1.5378000000 |
| C | -3.3018180000 | 2.5376220000 | -1.3481030000 |
| C | -2.9680760000 | 3.6481940000 | -2.1179140000 |
| C | -3.8866820000 | 4.1261610000 | -3.0590370000 |
| C | -5.1247500000 | 3.4824850000 | -3.2217860000 |
| C | -5.4167380000 | 2.3715970000 | -2.4439980000 |
| H | -4.7373040000 | 1.1070570000 | -0.9844220000 |
| H | -2.6322610000 | 2.1198400000 | -0.6066500000 |
| H | -1.9941130000 | 4.0950490000 | -1.9668920000 |
| H | -3.6429420000 | 4.9899740000 | -3.6672230000 |

| | | | |
|---|---|---|---|
| H | -5.8488260000 | 3.8336280000 | -3.9453590000 |
| H | -6.3317670000 | 1.7982230000 | -2.5015680000 |
| Cl | -6.3523040000 | -0.6858050000 | -1.0534320000 |
| Fe | -5.5118810000 | -1.3983180000 | 0.8969840000 |
| Cl | -4.5641360000 | -3.3985530000 | 0.5126710000 |
| Cl | -3.6559840000 | -0.0843040000 | 0.9945020000 |
| Cl | -6.8802110000 | -0.6595190000 | 2.4579890000 |

**Simulation keywords**: To generate a BS state, keywords ‘stable’ and ‘guess=mix’ are used to stabilize the wave function and to find the BS state energy by generating symmetry broken initial guess in solution phase.