

# Supplementary Materials: The Role of Coulombic Interactions for Spin Crossover Behaviors and Crystal Structural Transformation in Novel Anionic Fe(III) Complexes from a $\pi$ -Extended ONO Ligand

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Table S1. Cartesian coordinates of the HS  $[\text{Fe}(\text{aznp})_2]$  anion.

C	0.41109600	2.26279400	1.97710600
C	0.13475200	3.29434600	2.90799000
H	-0.87899500	3.37896000	3.29022500
C	1.13940400	4.16761600	3.31128200
H	0.90684100	4.95561700	4.02577600
C	2.44973100	4.05020800	2.80690100
H	3.22471400	4.74235200	3.12767600
C	2.74674300	3.04284200	1.89293500
H	3.74653600	2.93063900	1.48568000
C	1.74392100	2.15239600	1.47896500
C	2.34284800	-0.91201100	-1.41089600
C	2.77435900	-1.86859100	-2.40073500
H	1.99363800	-2.46463000	-2.86514800
C	4.08939000	-2.02328600	-2.73358800
H	4.37909300	-2.76000700	-3.48174200
C	5.11489100	-1.23686900	-2.11770400
C	6.47929600	-1.40257000	-2.45960500
H	6.74000900	-2.14928600	-3.20820400
C	7.46517500	-0.63896900	-1.86069000
H	8.50975300	-0.77595100	-2.13064800
C	7.09883800	0.32076200	-0.89119000
H	7.86715300	0.92462500	-0.41249900
C	5.77230000	0.50167600	-0.53859000
H	5.49919200	1.23656000	0.20973000
C	4.73977000	-0.26614700	-1.13814200
C	3.34174900	-0.09789900	-0.78326600
C	-0.41213100	-2.26626900	1.97388700
C	-0.13634300	-3.29920900	2.90333600
H	0.87702200	-3.38411200	3.28643400
C	-1.14096700	-4.17358000	3.30398800
H	-0.90878700	-4.96276300	4.01725700
C	-2.45084200	-4.05590600	2.79845400
H	-3.22580100	-4.74900200	3.11714200
C	-2.74739700	-3.04708000	1.88605700
H	-3.74680200	-2.93461300	1.47794300
C	-1.74451300	-2.15554200	1.47466500
C	-2.34199100	0.91350900	-1.41058000
C	-2.77310100	1.87182100	-2.39893100
H	-1.99207700	2.46815000	-2.86252600
C	-4.08819900	2.02804200	-2.73113300

Table S1. *Cont.*

H	−4.37761800	2.76627400	−3.47794600
C	−5.11403800	1.24132700	−2.11619200
C	−6.47846000	1.40863600	−2.45726400
H	−6.73893300	2.15685500	−3.20447100
C	−7.46464300	0.64468800	−1.85924300
H	−8.50924100	0.78290200	−2.12854200
C	−7.09864700	−0.31701400	−0.89152300
H	−7.86724700	−0.92112400	−0.41358100
C	−5.77210300	−0.49949200	−0.53969400
H	−5.49923100	−1.23581800	0.20730800
C	−4.73925100	0.26860500	−1.13836000
C	−3.34126600	0.09887100	−0.78415300
Fe	−0.00003500	−0.00063300	0.29043600
N	1.90314600	1.09593700	0.56646800
N	3.08707900	0.88903900	0.13140000
N	−1.90323200	−1.09758200	0.56394200
N	−3.08695600	−0.89005000	0.12854600
O	−0.50882600	1.42485800	1.56557700
O	1.08197600	−0.82830200	−1.16942500
O	0.50785200	−1.42745700	1.56451500
O	−1.08109800	0.82880100	−1.16919600

Table S2. Cartesian coordinates of the LS [Fe(aznp)<sub>2</sub>] anion.

C	−0.51548100	2.42610800	2.03973000
C	−0.41159000	3.40689000	3.05757300
H	0.53618500	3.92469100	3.17723500
C	−1.50351100	3.68952700	3.86986300
H	−1.40800300	4.44732100	4.64583900
C	−2.73135400	3.01474100	3.70665300
H	−3.57539900	3.25085500	4.35004500
C	−2.85725300	2.04514900	2.71607300
H	−3.78870600	1.50906200	2.56527100
C	−1.76187100	1.75222900	1.89134900
C	−1.72539000	−1.14027900	−1.24080600
C	−1.93861400	−2.15220800	−2.24377100
H	−1.10144300	−2.35081300	−2.90722800
C	−3.11972900	−2.82763500	−2.35962800
H	−3.23952600	−3.58753300	−3.13055600
C	−4.21867000	−2.55955300	−1.48474400
C	−5.44629900	−3.25709800	−1.60107700
H	−5.54131700	−4.01325100	−2.37906100
C	−6.50491300	−2.99055600	−0.75200900
H	−7.44247000	−3.53283000	−0.85130300
C	−6.35351400	−2.00389400	0.24798800
H	−7.18019700	−1.78677600	0.92153600
C	−5.16455900	−1.30818800	0.38301000
H	−5.05652100	−0.55357400	1.15330800
C	−4.06080700	−1.56037400	−0.47461000
C	−2.80508300	−0.84309900	−0.35001200
C	0.51554200	2.42623600	−2.03958900

Table S2. *Cont.*

C	0.41167200	3.40706100	−3.05739200
H	−0.53607600	3.92492300	−3.17700300
C	1.50358300	3.68967000	−3.86970800
H	1.40808900	4.44750100	−4.64565000
C	2.73139100	3.01480300	−3.70657000
H	3.57542600	3.25089000	−4.34998500
C	2.85726400	2.04515900	−2.71603900
H	3.78868800	1.50900300	−2.56529800
C	1.76189700	1.75227300	−1.89128500
C	1.72532300	−1.14045300	1.24066400
C	1.93849100	−2.15250200	2.24351800
H	1.10128100	−2.35119400	2.90689900
C	3.11961500	−2.82791400	2.35938800
H	3.23937500	−3.58789500	3.13024100
C	4.21861200	−2.55971100	1.48461100
C	5.44625600	−3.25722300	1.60097300
H	5.54123800	−4.01345100	2.37888800
C	6.50493500	−2.99054500	0.75202900
H	7.44250800	−3.53278700	0.85135100
C	6.35358500	−2.00378100	−0.24787400
H	7.18032100	−1.78654900	−0.92132000
C	5.16461200	−1.30811100	−0.38292800
H	5.05661500	−0.55341500	−1.15315200
C	4.06079300	−1.56043700	0.47456400
C	2.80505400	−0.84319200	0.34994300
Fe	−0.00000400	0.75494500	0.00000900
N	−1.73212700	0.79372200	0.86248100
N	−2.77943800	0.10440100	0.64725600
N	1.73213300	0.79371400	−0.86246500
N	2.77943200	0.10436900	−0.64726900
O	0.48066500	2.12885300	1.24209900
O	−0.55951600	−0.57352600	−1.24094000
O	−0.48059100	2.12901500	−1.24192600
O	0.55945800	−0.57368400	1.24081600



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