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Fig. S1. Conformations of saltrien-type cation with classification of ethylene groups orientations. The arrows show the first carbon atom in each cycle. "w" is the statistical weight of conformer.

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Table S1. Comparison of $[Fe(Sal_2-trien)]^+$ cation conformations presented in the CCDC database with the magnetic state.

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Fig. S4. Total relative energies of conformers of $[Fe(Sal_2-trien)]^+$ cation in HS (a) and LS (b) states.

Table S3. Selected natural atomic charges (B3LYP/6-311++G(d,p)) for $[Fe(Sal_2-trien)]^+$ cation various conformations in LS state.

Fig. S5. Diagram of selected natural atomic charges (B3LYP/6-311++G(d,p)) for $[Fe(Sal_2-trien)]^+$ cation various conformations in LS state.

Table S4. Energy values for one singly-occupied (HOMO) molecular orbital of $[Fe(Sal_2-trien)]^+$ cation various conformations in the doublet state (LS).

Fig. S6. Energy diagram of one singly-occupied (HOMO) molecular orbital for $[Fe(Sal_2-trien)]^+$ cation various conformations in the doublet state (LS).

Table S5. Energy values for five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbitals of $[Fe(Sal_2-trien)]^+$ cation various conformations in the sextet state (**HS**).

Fig. S7. Energy diagram of five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbital for $[Fe(Sal_2-trien)]^+$ cation various conformations in the sextet state (**HS**).

Fig. S8. Five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbital for the HS state of $[Fe(Sal_2-trien)]^+$ cation various conformations.

Table S6. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(+ + +)) in the sextet state (HS). Units are in Å.

Table S7. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(+ + +)) in the doublet state (LS). Units are in Å.

Table S8. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(---)) in the sextet state (HS) at the B3LYP level. Units are in Å.

Table S9. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(---)) in the doublet state (LS). Units are in Å.

Table S10. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: II(- + -)) in the sextet state (HS). Units are in Å.

Table S11. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: II(- + -)) in the doublet state (LS). Units are in Å.

Table S12. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: II(+ - +)) in the sextet state (HS). Units are in Å.

Table S13. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: II(+ - +)) in the doublet state (LS). Units are in Å.

Table S14. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: III(+ + -)) in the sextet state (HS). Units are in Å.

Table S15. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: III(+ + -)) in the doublet state (LS). Units are in Å.

Table S16. Optimized parameters of $[Fe(Sal_2-trien]^+ (conformer: III(+ - -))$ in the sextet state (HS). Units are in Å.



Fig. S1. Conformations of saltrien-type cation with classification of ethylene groups orientations. The arrows show the first carbon atom in each cycle. "*w*" is the statistical weight of conformer.



Fig. S2. Optimized structures (B3LYP/6-311++G(d,p)) of [Fe(Sal₂-trien)]⁺ cation various conformations in HS (S=5/2) and LS (S=1/2) states.

№	Compound	Temp., K	Class	Confor- mation	α,°	<i>x</i> (HS), %	SCO	CCDC	Ref.
1	(1 [Ea(Sal_trian)][Ni(dmit)]	180	П	-+-	71.37	0 a	abmunt	246501	C 1
2		R.T.	Ι		107.43	100 b	abrupt	246500	51
3	$m_{-}L_{-}[Fe(Sa]_{-}trien)][Ni(dmit)]$	180	Т		117.55	100 ^{<i>a</i>} , <i>b</i>	no	729925	
4		R.T.	1		115.72	100 ^{<i>a</i>} , <i>b</i>	no	729927	S2
5	<i>t</i> -1"-[Fe(Sal ₂ - trien)][Ni(dmit) ₂] · acetone	R.T.	П	-+-	71.94	0 <i>a</i>	no	729931	
6	[Fe(Sal ₂ -trien)]ClO ₄	R.T.	III I II	++- +++ -+-	97.96 107.85 78.64	≈ 60 ^a	gradual	221922	S3, S4
7	$[Fe(Sal_2-trien)]BPh_4 \cdot \frac{1}{^2CH_2Cl_2}$	105	Ι		122.24	≈ 85 <i>ª</i>	no	676636	\$4
8	[Fe(Sal ₂ -trien)]BPh ₄ $\cdot \frac{1}{2}$ acetone	120	I		125.44	≈ 85 <i>ª</i>	gradual	676635	
9	[Fe(Sal ₂ -trien)]BPh ₄	R.T.	I		124.92	≈ 78 <i>ª</i>	gradual	-	
10		R.T.		+++	114.27 121.86	100 a		-	\$5
11	[Fe(Sal ₂ -trien)]PF ₆	240	Ι	+++	114.02 121.19	100 a	stepwise	676633	S4, S5
12		140		+++	114.67 120.83	≈ 73 <i>ª</i>		676634	
13	[Fe(Sal ₂ -trien)]BPh ₄ · acetone	R.T.	T/S (II⇔III)	0+-	94.18	$\approx 40^{a}$ (0^{b})	gradual	1187913	S6
14	[Fe(Sal ₂ -trien)]BF ₄	R.T.	I		104.86	100 <i>a</i>	no	746613	S7
15	[Fe(Sal ₂ -trien)]NO ₃ · H ₂ O	R.T.	П	-+-	63.61	≈ 18 ^a	not indicate	1254589	58
16	[Fe(Sal ₂ -trien)]Cl · 2H ₂ O	R.T.	П	-+-	64.52	$\approx 6^a$	not indicate	1178434	50
17	[Fe(Sal ₂ -trien)][Ni(dcbdt) ₂]	R.T.	III (disordered) II (disordered)	++- -+-	80.35	≈ 85 <i>ª</i>	no	626997	S9
18	$[Fe(Sal_{2}-trien)]_{2}[Mn_{2}(ox)_{3}]\cdot 4H_{2}O\cdot C_{3}H_{7}NO$	100	I (disordered) III (disordered) III	 ++- ++-	102.01 108.82	$\approx 48^{b}$ (80K) $\approx 74^{b}$ (160K)	gradual	707311	S10
19		180	П		71.60	≈ 6 ^b (165K)		749068	S11
20	[Fe(Sal-	92		-+-	71.38	0 b		813714	
21	trien)][Mn ^{II} Cr ^{III} (ox) ₃]·CH ₂ Cl ₂	120			70.57	0 b	gradual	807172	
22		250	II (disordered) I (disordered)	-+- 	78.22	≈ 50 b		813345	S12
23		R.T.	I II (disordered)	 -+-	81.51	≈ 80 b		807173	
24	[Fe(Sal ₂ - trien)][Mn ^{II} Cr ^{III} (ox) ₃]·CH ₃ OH	120	III I	++-	121.25 105.85	≈ 70 b	gradual	749069	S11
25	$[Fe(Sal_2-trien)][Mn^{II}Cr^{III}(Cl_2An)_3] \cdot \frac{1}{2} \frac{1}{CH_2Cl_2 \cdot CH_3OH \cdot \frac{1}{2}} \cdot \frac{1}{(H_2O) \cdot 5CH_3CN}$	120	I		116.9	> 50 ^a	gradual	998895	S13

Table S1. Comparison of $[Fe(Sal_2-trien)]^+$ cation conformations presented in the CCDC database with the magnetic state.

^{*a*} According to SQUID magnetic measurement; ^{*b*} according to Mössbauer spectroscopy of ⁵⁷Fe.

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S13. A. Abherv^é, M. Clemente-Le^ón, E. Coronado, C.J.G^ómez-Garcⁱa and M.Verneret, *Inorg. Chem.*, 2014, **53**, 12014–12026.

Conformation		Fe – N _{im} , Å	Fe [–] N _{am} , Å	Fe-O, Å	α, °
	LS	1 96921	2 09390	1 87873	107 46
I (+ + +)	HS	2.13492	2.30902	1.92070	113.59
$\mathbf{I}()$	LS	1.98420	2.08226	1.87544	78.01
1()	HS	2.15887	2.27172	1.90976	93.84
$\mathbf{H}(-+-)$	LS	1.96462	2.06091	1.87318	66.41
п(т)	HS	2.14261	2.27214	1.90712	81.75
$\mathbf{H}(1 = 1)a$	LS	1.96750	2.02383	1.92304	50.79
II (+ +)"	HS	2.14409	2.28088	1.94075	97.60
	15	1.95779	2.06608	1.87926	86.12
III(++-)	LS	1.98621	2.08482	1.87113	00.12
m (+ + -)	н	2.13138	2.28237	1.90802	100.67
	115	2.15476	2.29288	1.91132	100.07
$\mathbf{H}(\mathbf{+}$	LS^b	-	-	-	-
)	HS	2.14000	2.25570	1.91280	106 49
)	110	2.17587	2.33126	1.92462	100.47

Table S2. Calculated (B3LYP/6-311++G(d,p)) Fe-Ligand bond lengths (Å) and dihedral angle α (°) for [Fe(Sal₂-trien)]⁺ cation various conformations.

Note: ^{*a*} conformation II (+ - +) is not observed experimentally. ^{*b*} conformation III (+ --) is not an energy minimum for LS state.



Fig. S3. Calculated (B3LYP/6-311++G(d,p) values of dihedral angle α between the least squares planes of the two phenoxy rings of [Fe(Sal₂-trien)]⁺ various cation conformations in HS (circle,
•) and LS (square, ■) states. Gray symbols correspond to the most thermodynamically stable conformers.



Fig. S4. Total relative energies of conformers of $[Fe(Sal_2-trien)]^+$ cation in HS (*a*) and LS (*b*) states.

Conformation	Fe (21), e	O(25), e	O(49), e
I(+ + +)	0.553	-0.626	-0.626
I()	0.537	-0.604	-0.617
II(-+-)	<u>0.507</u>	<u>-0.591</u>	<u>-0.591</u>
II(+ - +)	0.540	-0.648	-0.648
III(++ ⁻)	0.531	-0.618	-0.600

Table S3. Selected natural atomic charges (B3LYP/6-311++G(d,p)) for $[Fe(Sal_2-trien)]^+$ cation various conformations in LS state.



Fig. S5. Diagram of selected natural atomic charges (B3LYP/6-311++G(d,p)) for [Fe(Sal₂-trien)]⁺ cation various conformations in LS state.

Table S4. Energy values for one singly-occupied (HOMO) molecular orbital of $[Fe(Sal_2-trien)]^+$ cation various conformations in the doublet state (LS).

Conformation	HOMO (№ 107)
Conformation	Energy, eV
I(+++)	-8,5768
I()	-8,5330
II(-+-)	-8,5251
II(+ - +)	-8,7630
III(++ -)	-8,5510



Fig. S6. Energy diagram of one singly-occupied (HOMO) molecular orbital for $[Fe(Sal_2-trien)]^+$ cation various conformations in the doublet state (LS).

Table S5. Energy values for five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbitals of $[Fe(Sal_2-trien)]^+$ cation various conformations in the sextet state (**HS**).

	НОМО	HOMO-1	НОМО-2	HOMO-3	HOMO-4
Conformation	(№ 109)	(№ 108)	(№ 107)	(№ 106)	(№ 105)
	Energy, eV				
I(+++)	-8,7156	-8,7847	-9,6326	-9,6985	-9,7665
I()	-8,6990	-8,7406	-9,6903	-9,6996	-9,7570
II(-+-)	-8,6985	-8,7602	-9,7102	-9,7200	-9,7662
II(+ - +)	-8,6903	-8,8394	-9,6068	-9,6947	-9,7165
III(++-)	-8,7238	-8,7695	-9,6773	-9,7148	-9,7837
III(+)	-8,6898	-8,7747	-9,6569	-9,6743	-9,7581



Fig. S7. Energy diagram of five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbital for [Fe(Sal₂-trien)]⁺ cation various conformations in the sextet state (**HS**).



Fig. S8. Five singly-occupied (HOMO, HOMO-1, HOMO-2, HOMO-3, and HOMO-4, respectively) molecular orbital for the HS state of [Fe(Sal₂-trien)]⁺ cation various conformations.

C 2.4971030	-1.149644000	-0.655944000
C 3.1827080	-1.870527000	-1.654778000
C 4.4027290	-2.466203000	-1.386118000
Н 4.9077560	-3.017462000	-2.171539000
C 4.9930720	-2.374015000	-0.114669000
Н 5.9458540	-2.848507000	0.082106000
C 4.3381640	-1.676120000	0.878775000
Н 4.7766590	-1.599802000	1.868628000
C 3.0923770	-1.052446000	0.638405000
C 2.4609340	-0.352415000	1.718841000
Н 2.9972490	-0.372771000	2.673099000
C 0.7960100	0.910656000	2.865217000
Н 1.5356840	0.958393000	3.671601000
Н -0.0517080	000 0.311249000	3.213965000
C 0.3250680	2.313558000	2.491224000
Н -0.1838310	2.796869000	3.331492000
Н 1.1915890	2.925865000	2.232922000
C -0.5867230	3.480854000	0.490570000
Н -1.5334470	3.505980000	-0.053482000
Н -0.5522770	4.377586000	1.119098000
Fe 0.000000	000 0.415783000	0.00000000
N 1.3338780	0.281352000	1.661500000
N -0.5590480	000 2.241425000	1.298480000
Н -1.4998520	2.005466000	1.602206000
O 1.3387500	-0.592334000	-0.938377000
C -2.4971010	-1.149647000	0.655940000
C -3.1827040	-1.870536000	1.654772000
С -4.4027260	-2.466211000	1.386111000
Н -4.9077510	-3.017474000	2.171530000
C -4.9930710	-2.374017000	0.114663000
Н -5.9458530	-2.848509000	-0.082112000
C -4.3381650	-1.676117000	-0.878778000
Н -4.7766610	-1.599795000	-1.868631000
C -3.0923780	-1.052444000	-0.638407000
C -2.4609350	-0.352408000	-1.718841000
Н -2.9972520	-0.372761000	-2.673099000
C -0.7960130	000 0.910667000	-2.865214000
Н -1.5356890	000 0.958408000	-3.671597000
Н 0.0517040	000 0.311261000	-3.213966000
C -0.3250710	2.313568000	-2.491217000
Н 0.1838270	000 2.796882000	-3.331483000
Н -1.1915910	000 2.925874000	-2.232912000
C 0.5867230	3.480855000	-0.490559000
Н 1.5334470	3.505979000	0.053494000
Н 0.5522770	4.377590000	-1.119083000
N -1.3338790	000 0.281359000	-1.661499000
N 0.5590470	2.241430000	-1.298473000
Н 1.4998510	2.005472000	-1.602202000
O -1.3387480	-0.592339000	0.938374000
Н 2.7231830	-1.951099000	-2.632336000
Н -2.7231780	-1.951112000	2.632329000

Table S6. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(+ + +)) in the sextet state (HS). Units are in Å.

С	-2.280551000	-1.168268000	0.571556000
С	-2.966980000	-1.968376000	1.512002000
С	-4.170641000	-2.568592000	1.192106000
Н	-4.668786000	-3.183605000	1.933411000
С	-4.752840000	-2.402727000	-0.076726000
Н	-5.693324000	-2.882348000	-0.315497000
С	-4.100705000	-1.629823000	-1.012518000
Н	-4.526794000	-1.498416000	-2.001997000
С	-2.869415000	-0.998005000	-0.715807000
C	-2.220819000	-0.245291000	-1.745458000
Н	-2.679316000	-0.286099000	-2.736471000
С	-0.447355000	0.942460000	-2.799269000
H	-1.141243000	1.108777000	-3.629358000
Н	0.276723000	0.180728000	-3.097962000
С	0.267919000	2.233133000	-2.432643000
Н	1.043969000	2.480385000	-3.160444000
Н	-0.444311000	3.059193000	-2.422213000
С	0.703497000	3.390221000	-0.292549000
Н	1.452885000	3.405042000	0.500504000
Н	0.872523000	4.267591000	-0.924178000
Fe	0.00000000	0.537327000	0.00000000
N	-1.136194000	0.444770000	-1.605706000
N	0.863349000	2,125319000	-1.057037000
Н	1.850173000	1.897395000	-1,143678000
0	-1.143296000	-0.615520000	0.945217000
Č	2.280555000	-1.168262000	-0.571560000
C	2,966987000	-1.968365000	-1.512009000
C	4,170646000	-2.568582000	-1.192112000
Н	4.668793000	-3.183592000	-1.933420000
С	4.752843000	-2.402723000	0.076721000
Н	5.693326000	-2.882345000	0.315492000
С	4.100705000	-1.629824000	1.012515000
Н	4.526792000	-1.498421000	2.001996000
С	2.869416000	-0.998005000	0.715805000
С	2.220818000	-0.245296000	1.745459000
Н	2.679313000	-0.286108000	2.736472000
С	0.447352000	0.942450000	2.799272000
Н	1.141239000	1.108766000	3.629362000
Н	-0.276725000	0.180716000	3.097962000
С	-0.267923000	2.233123000	2.432650000
Н	-1.043975000	2.480372000	3.160451000
Н	0.444305000	3.059185000	2.422222000
С	-0.703505000	3.390218000	0.292559000
Н	-1.452893000	3.405040000	-0.500493000
Н	-0.872534000	4.267585000	0.924192000
Ν	1.136192000	0.444766000	1.605707000
Ν	-0.863354000	2.125312000	1.057043000
Н	-1.850177000	1.897386000	1.143683000
0	1.143301000	-0.615512000	-0.945222000
Н	-2.513861000	-2.108726000	2.485798000
Н	2.513869000	-2.108710000	-2.485806000

Table S7. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(+ + +)) in the doublet state (LS). Units are in Å.

С	-2.286096000	-1.238520000	0.733606000
С	-2.785366000	-2.142443000	1.692685000
С	-3.934103000	-2.873204000	1.444337000
Н	-4.294279000	-3.566325000	2.196470000
С	-4.637209000	-2.735444000	0.235726000
Н	-5.532887000	-3.315538000	0.054347000
С	-4.169024000	-1.852278000	-0.714395000
Н	-4.700679000	-1.732473000	-1.652943000
С	-2,998698000	-1.088329000	-0.494618000
C	-2.585597000	-0.176381000	-1.520319000
Н	-3.235785000	-0.149046000	-2.401034000
C	-1.346743000	1.495555000	-2.652326000
Н	-2.034715000	2 345418000	-2 575168000
Н	-1 572713000	0 989364000	-3 596013000
C	0 102783000	1 979954000	-2 674635000
Н	0.757109000	1 170015000	-2 998958000
Н	0.212509000	2 817740000	-3 372350000
C	-0.061947000	3 587264000	-0.760393000
Н	0 407943000	4 481672000	-1 183655000
Н	-1 116641000	3 613895000	-1 041705000
Fe	0.00000000	0 560364000	0.00000000
N	-1 549985000	0.603827000	-1 502121000
N	0 531423000	2 344403000	-1 302108000
Н	1 545718000	2.418457000	-1 286767000
0	-1 189264000	-0 559751000	0 989024000
C	2 286096000	-1 238521000	-0 733606000
C	2.2866,6000	-2 142443000	-1 692685000
C	3 934103000	-2 873205000	-1 444337000
Н	4 294279000	-3 566325000	-2 196470000
C	4 637209000	-2 735445000	-0.235726000
Н	5.532887000	-3.315538000	-0.054347000
С	4.169024000	-1.852278000	0.714395000
Н	4.700679000	-1.732473000	1.652943000
С	2.998697000	-1.088329000	0.494618000
С	2.585597000	-0.176381000	1.520319000
Н	3.235785000	-0.149046000	2.401034000
С	1.346743000	1.495554000	2.652326000
Н	2.034715000	2.345418000	2.575168000
Н	1.572713000	0.989364000	3.596013000
С	-0.102783000	1.979955000	2.674635000
Н	-0.757109000	1.170015000	2.998958000
Н	-0.212509000	2.817741000	3.372350000
С	0.061947000	3.587264000	0.760393000
Н	-0.407942000	4.481672000	1.183655000
Н	1.116641000	3.613895000	1.041705000
N	1.549985000	0.603827000	1.502121000
N	-0.531423000	2.344403000	1.302108000
Н	-1.545717000	2.418457000	1.286767000
0	1.189264000	-0.559752000	-0.989023000
Н	-2.238628000	-2.254550000	2.620934000
Н	2.238627000	-2.254550000	-2.620934000

Table S8. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(--)) in the sextet state (HS). Units are in Å.

С	1.902432000	-1.231899000	-0.758361000
С	2.286958000	-2.214038000	-1.697497000
С	3.299284000	-3.110892000	-1.412491000
Н	3.566144000	-3.860252000	-2.149504000
С	3.982891000	-3.071745000	-0.184108000
Н	4.771772000	-3.782241000	0.026817000
С	3.631898000	-2.116203000	0.743848000
Н	4.149865000	-2.066644000	1.696280000
С	2.599049000	-1.183218000	0.483795000
С	2.301278000	-0.204544000	1.481544000
Н	2.902965000	-0.256979000	2.392086000
С	1.197621000	1.592675000	2.572137000
Н	1.864110000	2.459536000	2,502200000
Н	1.446488000	1.074147000	3.501607000
С	-0.265655000	2.024186000	2.592734000
Н	-0.895008000	1.190097000	2.896494000
Н	-0.423224000	2.866478000	3.273835000
С	-0.069415000	3.673017000	0.755453000
Н	-0.673861000	4,519055000	1.095632000
Н	0.912792000	3.772723000	1.217177000
Fe	0.00000000	0.804245000	0.00000000
N	1.398125000	0.719964000	1.405418000
N	-0.655411000	2.376542000	1,197553000
Н	-1.670531000	2.423803000	1,142628000
0	0.940878000	-0.395634000	-1.091927000
C	-1.902433000	-1.231898000	0.758361000
C	-2.286960000	-2.214036000	1,697497000
C	-3.299286000	-3.110889000	1.412491000
Н	-3.566147000	-3.860249000	2.149505000
С	-3.982894000	-3.071742000	0.184108000
Н	-4.771775000	-3.782237000	-0.026817000
С	-3.631900000	-2.116200000	-0.743848000
Н	-4.149866000	-2.066641000	-1.696280000
С	-2.599050000	-1.183215000	-0.483795000
С	-2.301279000	-0.204542000	-1.481544000
Н	-2.902965000	-0.256976000	-2.392086000
С	-1.197620000	1.592676000	-2.572137000
Н	-1.864107000	2.459538000	-2.502200000
Н	-1.446487000	1.074148000	-3.501607000
С	0.265657000	2.024185000	-2.592735000
Н	0.895009000	1.190096000	-2.896494000
Н	0.423227000	2.866478000	-3.273835000
С	0.069418000	3.673017000	-0.755453000
Н	0.673866000	4.519054000	-1.095632000
Н	-0.912788000	3.772724000	-1.217177000
N	-1.398124000	0.719966000	-1.405418000
N	0.655414000	2.376541000	-1.197553000
Н	1.670533000	2.423801000	-1.142628000
0	-0.940878000	-0.395633000	1.091927000
Н	1.756376000	-2.249476000	-2.641110000
Н	-1.756378000	-2.249474000	2.641110000

Table S9. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: I(--))) in the doublet state (LS). Units are in Å.

С	-2.187305000	-1.349290000	0.768744000
С	-2.580198000	-2.376969000	1.648917000
С	-3.721148000	-3.120597000	1.402853000
Н	-3.996981000	-3.911039000	2.092036000
С	-4.524974000	-2.870843000	0.277722000
Н	-5.414147000	-3.461408000	0.098233000
С	-4.166005000	-1.861851000	-0.590785000
Н	-4.778989000	-1.651568000	-1.461358000
С	-3.004045000	-1.083391000	-0.374224000
С	-2.719974000	-0.026731000	-1.300373000
Н	-3.467497000	0.111937000	-2.088245000
С	-1.637688000	1.858213000	-2.265608000
Н	-2.161544000	2.733664000	-1.864537000
Н	-2.141783000	1.587248000	-3.199348000
С	-0.176567000	2.200773000	-2.553291000
Н	0.269228000	1.398729000	-3.144614000
Н	-0.108658000	3.129210000	-3.131295000
С	0.553449000	3.553300000	-0.533570000
Н	1.525993000	3.685383000	-0.057319000
Н	0.408013000	4.411997000	-1.198988000
Fe	0.00000000	0.521885000	0.000000000
Ν	-1.697537000	0.772148000	-1.283164000
Ν	0.610257000	2.284314000	-1.297711000
Н	1.578675000	2.084958000	-1.524569000
0	-1.097326000	-0.657850000	1.020399000
С	2.187305000	-1.349289000	-0.768745000
С	2.580199000	-2.376967000	-1.648918000
С	3.721149000	-3.120595000	-1.402854000
Н	3.996983000	-3.911036000	-2.092037000
С	4.524975000	-2.870842000	-0.277722000
Н	5.414147000	-3.461407000	-0.098233000
С	4.166005000	-1.861851000	0.590785000
Н	4.778988000	-1.651569000	1.461359000
С	3.004045000	-1.083391000	0.374224000
С	2.719973000	-0.026732000	1.300374000
Н	3.467496000	0.111936000	2.088246000
С	1.637687000	1.858212000	2.265609000
Н	2.161544000	2.733663000	1.864539000
Н	2.141781000	1.587246000	3.199350000
С	0.176565000	2.200771000	2.553292000
Н	-0.269230000	1.398727000	3.144613000
Н	0.108656000	3.129208000	3.131296000
С	-0.553448000	3.553301000	0.533571000
Н	-1.525992000	3.685385000	0.057319000
Н	-0.408011000	4.411997000	1.198989000
N	1.697536000	0.772148000	1.283164000
N	-0.610258000	2.284314000	1.297711000
Н	-1.578676000	2.084959000	1.524568000
0	1.097326000	-0.657849000	-1.020400000
Н	-1.958058000	-2.571757000	2.513783000
H	1.958060000	-2.571755000	-2.513784000

Table S10. Optimized parameters of $[Fe(Sal_2-trien]^+ (conformer: II(- + -))$ in the sextet state (HS). Units are in Å.

C	1.297799000	1.722155000	-0.861823000
С	2.364989000	1.944199000	-1.759909000
С	3.318797000	2.910828000	-1.504733000
Н	4.133243000	3.049851000	-2.207093000
С	3.252967000	3.713767000	-0.351449000
Н	4.007621000	4.466958000	-0.164678000
С	2.211715000	3.529660000	0.530707000
Н	2.136861000	4.146779000	1.420364000
С	1.221957000	2.542137000	0.304774000
C	0.138455000	2.442195000	1.231448000
Н	0.119675000	3,181849000	2.035384000
C	-1.880294000	1.591657000	2,189907000
Н	-2.746826000	2,138337000	1.801345000
Н	-1 559916000	2 105371000	3 101115000
C	-2 246098000	0 143538000	2 499503000
Н	-1 437849000	-0 316415000	3 068110000
Н	-3 171627000	0.075414000	3 079000000
C	-3 660814000	-0 566740000	0 514478000
Н	-3 807373000	-1 527355000	0.019830000
Н	-4 488388000	-0.438553000	1 219014000
Fe	-0.819845000	0.00000000	0.00000000
N	-0.816309000	1 568907000	1 182470000
N	-2 352718000	-0 628827000	1 225649000
Н	-2 150745000	-1 600199000	1 444235000
0	0 409080000	0 798538000	-1 166563000
C	1 297799000	-1 722155000	0.861823000
C	2 364989000	-1 944199000	1 759909000
C	3 318797000	-2 910828000	1 504733000
Н	4 133243000	-3 049851000	2 207093000
C	3 252967000	-3 713767000	0 351449000
Н	4 007621000	-4 466958000	0 164678000
C	2 211715000	-3 529660000	-0 530707000
H	2,136862000	-4,146779000	-1.420365000
С	1.221958000	-2.542137000	-0.304774000
C	0.138455000	-2.442195000	-1.231448000
H	0.119675000	-3,181849000	-2.035385000
C	-1.880294000	-1.591657000	-2,189907000
H	-2.746826000	-2.138337000	-1.801345000
Н	-1.559916000	-2.105371000	-3.101115000
C	-2 246097000	-0 143538000	-2 499503000
H	-1,437849000	0.316415000	-3.068110000
Н	-3 171627000	-0.075414000	-3 079000000
C	-3 660814000	0 566739000	-0 514478000
Н	-3 807373000	1 527354000	-0.019830000
Н	-4 488388000	0 438553000	-1 219014000
N	-0.816309000	-1 568907000	-1 182470000
N	-2 352718000	0 628827000	-1 225649000
Н	-2 150745000	1 600199000	-1 444235000
0	0 409080000	-0 798539000	1 166563000
H	2 417019000	1 325094000	-2 647071000
H	2.417019000	-1.325094000	2.647071000

Table S11. Optimized parameters of $[Fe(Sal_2-trien]^+ (conformer: II(- + -))$ in the doublet state (LS). Units are in Å.

С	2.561519000	-0.874576000	-0.603953000
С	3.367762000	-1.392376000	-1.638045000
С	4.372967000	-2.303543000	-1.364001000
Н	4.973806000	-2.692028000	-2.178754000
С	4.627899000	-2.729905000	-0.050446000
Н	5.418185000	-3.442017000	0.149859000
С	3.863451000	-2.221774000	0.980301000
Н	4.055913000	-2.529970000	2.002953000
С	2.821612000	-1.301387000	0.732982000
С	2.102495000	-0.753030000	1.848270000
Н	2.497631000	-0.993926000	2.840594000
С	0.519016000	0.645239000	2.961146000
Н	1.115871000	0.427917000	3.853193000
Н	-0.497251000	0.275542000	3.117365000
C	0.497273000	2,152942000	2,692644000
Н	-0.003280000	2,692864000	3.502817000
H	1 523655000	2,520840000	2 627287000
C	0 254812000	3 665351000	0.718758000
Н	-0.107281000	4 553611000	1 248730000
Н	1 347803000	3 702685000	0 730204000
Fe	0,00000000	0.602371000	0.00000000
N	1 065623000	0.012536000	1 764560000
N	-0.155013000	2 410413000	1 381803000
Н	-1 165754000	2 403803000	1 513532000
0	1 618874000	0.003464000	-0.887179000
C	-2 561519000	-0.874576000	0.603953000
C	-3 367763000	-1 392376000	1 638045000
C	-4 372968000	-2 303542000	1 364001000
Н	-4 973806000	-2 692028000	2 178753000
C C	-4 627900000	-2 729904000	0.050446000
Н	-5 418186000	-3 442015000	-0 149860000
C C	-3 863451000	-2 221773000	-0.980301000
Н	-4 055914000	-2 529968000	-2 002953000
C	-2 821612000	-1 301386000	-0 732982000
C	-2 102495000	-0.753030000	-1 848270000
Н	-2 497632000	-0.993925000	-2 840594000
C C	-0.519016000	0.645239000	-2.961145000
Н	-1 115871000	0.043237000	-3 853193000
Н	0.497251000	0.775542000	-3 117365000
C	-0.497272000	2 152942000	-2 692644000
Н	0.003280000	2.152742000	-3 502817000
Н	-1 523655000	2.092804000	-2 627287000
C C	-0.254811000	3 665351000	-2.027287000
Н	0 107282000	4 553611000	-1.248730000
Н		3 702686000	-1.248750000
N	-1.047602000	0.012536000	
N	0 15501/000	2 /10/12000	-1.381803000
Н	1 165754000	2.410413000	-1.501005000
0	-1 619972000	0.002462000	0.887180000
Ч	2 177061000	1 060151000	2 6515/2000
Н	2 177061000	-1.000151000	-2.031343000
11	-3.1//901000	-1.000132000	2.031343000

Table S12. Optimized parameters of $[Fe(Sal_2-trien]^+ (conformer: II(+ - +))$ in the sextet state (HS). Units are in Å.

С	-2.572226000	-0.471675000	0.019504000
С	-3.755772000	-0.677543000	0.762375000
С	-4.481777000	-1.847027000	0.632093000
Н	-5.378026000	-1.983311000	1.227178000
С	-4.087320000	-2.854881000	-0.266378000
Н	-4.671705000	-3.761094000	-0.361427000
C	-2.964872000	-2.659174000	-1.041513000
Н	-2.666297000	-3,407907000	-1.767970000
C	-2,180020000	-1.491582000	-0.905055000
C	-1 144878000	-1 194540000	-1.847723000
Н	-1 207078000	-1 665859000	-2.831836000
C	0.414620000	0 360704000	-2 789433000
Н	0.093260000	-0.071303000	-3 740940000
H	1 500647000	0.278673000	-2 712328000
C	-0.014599000	1 839145000	-2 684880000
Н	0.489924000	2 457941000	-3 433744000
Н	-1 094088000	1 928795000	-2 821575000
C	-0.185846000	3 534937000	-0.746015000
Н	0.235338000	4 406569000	-1 256814000
Н	-1 271257000	3 556965000	-0.872092000
Fe	0.00000000	0 746602000	0.00000000
N	-0.217116000	-0.312401000	-1 643902000
N	0.324416000	2 260510000	-1 303358000
Н	1 343603000	2 257181000	-1 224393000
0	-1.915467000	0.665407000	0 149886000
C	2 572226000	-0.471675000	-0.019504000
C	3 755772000	-0 677543000	-0 762374000
C	4 481777000	-1 847027000	-0.632093000
Н	5 378026000	-1 983311000	-1 227178000
C	4 087320000	-2.854881000	0.266378000
Н	4 671705000	-3 761095000	0.361427000
C	2 964871000	-2 659174000	1 041513000
Н	2.666297000	-3 407908000	1 767970000
C	2 180020000	-1 491583000	0.905055000
C	1 144878000	-1 194540000	1 847723000
Н	1 207078000	-1 665859000	2 831836000
C	-0.414620000	0 360705000	2 789434000
Н	-0.093260000	-0.071303000	3 740940000
Н	-1 500647000	0.278673000	2 712328000
C	0.014599000	1 839145000	2 684880000
Н	-0.489924000	2 457941000	3 433744000
Н	1 094088000	1 928795000	2 821575000
C	0 185846000	3 534937000	0.746015000
H	-0 235338000	4 406569000	1 256814000
Н	1 271257000	3 556965000	0.872092000
N	0.217116000	-0.312401000	1 643902000
N	-0 324416000	2 260510000	1 303358000
Н	-1 343603000	2.257181000	1 224393000
0	1 915467000	0 665407000	-0 149886000
H	-4 081132000	0 107325000	1 435049000
H	4 081132000	0 107325000	-1 435048000

Table S13. Optimized parameters of $[Fe(Sal_2-trien]^+ (conformer: II(+ - +))$ in the doublet state (LS). Units are in Å.

С	2.370566000	-1.231185000	-0.720395000
С	2.961587000	-2.014994000	-1.731595000
С	4.196761000	-2.608783000	-1.536650000
Н	4.627100000	-3.209362000	-2.330320000
С	4.896522000	-2.451796000	-0.329113000
Н	5.859700000	-2.925301000	-0.188699000
C	4.334852000	-1.692251000	0.676426000
Н	4.858474000	-1.567403000	1.618841000
С	3.077217000	-1.067455000	0.511180000
C	2.549510000	-0.308240000	1,609274000
Н	3,164263000	-0.301718000	2.515264000
С	0.999947000	1.027451000	2.839649000
Н	1.814642000	1,137379000	3,563447000
Н	0.212160000	0.425632000	3,307004000
C	0.445321000	2.395432000	2.447028000
Н	0.000200000	2 903137000	3 308762000
Н	1 260869000	3 021484000	2,080268000
C	-0.717029000	3 412378000	0 481993000
Н	-1 666493000	3 292902000	-0.041151000
Н	-0 780460000	4 339423000	1 064004000
Fe	-0.006632000	0.428160000	0.051989000
N	1 433744000	0.347236000	1 620928000
N	-0.541348000	2.227923000	1.349735000
Н	-1 438463000	1 963050000	1 748053000
0	1 194207000	-0.680461000	-0.932636000
Č	-2.396663000	-1.284561000	0.650945000
Ċ	-2.943207000	-2.242680000	1.528457000
Ċ	-4,133440000	-2.879963000	1.225270000
Н	-4.529628000	-3.617991000	1.913892000
С	-4.833608000	-2.591134000	0.041371000
Н	-5.762224000	-3.100000000	-0.183037000
С	-4.320717000	-1.651748000	-0.827863000
Н	-4.849813000	-1.414557000	-1.745293000
С	-3.106276000	-0.980178000	-0.550751000
С	-2.649284000	0.003412000	-1.486289000
Н	-3.307968000	0.163915000	-2.346062000
С	-1.327646000	1.719501000	-2.450265000
Н	-1.883695000	2.632659000	-2.206267000
Н	-1.687209000	1.379907000	-3.426980000
С	0.165978000	2.017374000	-2.531747000
Н	0.685372000	1.158389000	-2.959603000
Н	0.346427000	2.886862000	-3.173806000
С	0.440740000	3.519321000	-0.520135000
Н	1.347547000	3.839711000	-0.003397000
Н	0.212342000	4.294223000	-1.259451000
N	-1.565451000	0.713335000	-1.408058000
N	0.731426000	2.219318000	-1.174510000
Н	1.736828000	2.098001000	-1.237913000
0	-1.261708000	-0.695849000	0.954494000
Н	2.416496000	-2.145363000	-2.658463000
Н	-2.399417000	-2.470730000	2.436945000

Table S14. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: III(+ + -)) in the sextet state (HS). Units are in Å.

С	1.924158000	-1.320531000	-0.659112000
C	2.374535000	-2.264338000	-1.610337000
C	3 496387000	-3 034996000	-1 372798000
Н	3 810709000	-3 756569000	-2 118806000
C	4 231128000	-2.905261000	-0.180116000
Н	5 105955000	-3 518369000	-0.005851000
C	3 813760000	-1 992798000	0 762855000
Н	4 361571000	-1 882726000	1 693290000
C	2 669428000	-1 185236000	0 550918000
C	2 274842000	-0 279312000	1 583779000
Н	2.271012000	-0.323357000	2 512128000
n C	0.853096000	1 253903000	2 731397000
Н	1 674653000	1 398878000	3 439855000
Н	0.090274000	0.630981000	3 208315000
II C	0.050274000	2 587268000	2 316053000
Н	_0.311722000	3.048499000	3 129553000
Н	1 050/93000	3 277323000	2 034618000
II C	0.649799000	3.554709000	0.21/530000
Ч	1 536685000	3.770946000	0.214339000
Ч	0.727301000	1 403560000	0.773100000
Fe	0.009885000	0.711786000	0.773190000
N	1 292810000	0.561370000	1 516882000
N	0.621031000	2 379250000	1 118081000
Н	1 562677000	2.379230000	1 / 32680000
0	-1.302077000	2.130487000	0.054047000
C	2.094540000	-0.010314000	-0.334047000
C	2,591337000	2 004674000	1 668652000
C	-2.381337000	-2.094074000	1 222400000
U U	-3.004889000	-2.938133000	2.048008000
II C	4 108501000	-3.083913000	0.050312000
Ч	4,198501000	3 59//9/000	0.030312000
II C	3 749095000	1 0805/2000	0.861373000
Ч	4 200070000	1 022806000	1 8/6832000
C C	2 700286000	1.085963000	0 541725000
C	-2.700280000	-0.118360000	-1 520530000
Н	-2.507804000	-0.122100000	-2.451199000
C C	-1.070639000	1 657764000	-2.510244000
Н	-1.613275000	2 600195000	-2.375846000
Н	-1 397096000	1 234458000	-3 464215000
II C	0.433660000	1.254450000	-2 527229000
Н	0.42529000	0.99/388000	-2.327227000
Ч	0.942329000	2 727120000	3 189361000
II C	0.627494000	2.727129000	0.626461000
Н	1 /82600000	3.840025000	-0.020401000
Н	0 55/012000	A 252402000	-0.012545000
N	_1 358071000	<u></u>	_1 30/080000
N	0.806782000	2 15880/000	-1.394009000
Н	1 800563000	1 005220000	-1.132700000
0	_1 129810000	_0 332017000	1 138007000
Н	1 803350000	_2 37313/000	_2 52/237000
Н	_2 122007000	-2.373134000 -2 134164000	2 648745000
11	-2.122007000	-2.13-10-000	2.0707750000

Table S15. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: III(+ + -)) in the doublet state (LS). Units are in Å.

C 2.433398000 -1.092976000 -0.712721000 C 3.100173000 -1.759976000 -1.759757000 C 4.30001100 -2.412244000 -1.5528700 H 4.792052000 -2.918923000 -2.35545300 C 4.84811000 -2.433713000 -0.256574000 H 5.821121000 -2.951334000 -0.76974000 C 4.244705000 -1.799914000 0.78570400 C 3.022555000 -1.112782000 0.78577400 C 2.382055000 -0.4185449000 1.779971000 C 0.740323000 -0.717526000 2.93925700 C 0.740323000 0.717526000 2.798957000 H -0.1595100 0.139517000 3.169747000 C 0.38512000 2.768236000 2.758811000 H -0.29923000 2.6569200 2.6569200 C -0.174658000 3.64234000 0.77047600 H -0.35519000 3.34845000 0.78653000 H -0.85				
C 3 100173000 -1 759906000 -1 759757000 C 4 300011000 -2 412244000 -1 532687000 C 4 884811000 -2 412344000 -1 532687000 C 4 884811000 -2 433713000 -0 256274000 C 4 244705000 -1 792914000 -0.785074000 C 4 244705000 -1 789214000 -0.785074000 C 3 022255000 -1 112782000 0.587139000 C 2 398205000 -0.485449000 1.717492000 C 0.740332000 -0.620557000 3.773111000 C 0.74352000 2.186490000 2.71869000 C 0.38251200 2.18649000 2.71869000 C -0.174612000 2.85245000 3.57315000 H -0.174612000 2.85245000 3.673315000 C -0.171668000 3.64214300 0.7747600 H -0.35519000 3.96097300 0.96732800 Fe 0.003799000 0.53285600 0.02647000 N	С	2.433398000	-1.092976000	-0.712721000
C 4.300011000 -2.412244000 -1.532687000 H 4.792052000 -2.918923000 -2.355453000 C 4.84811000 -2.433713000 -0.256274000 H 5.821121000 -2.951334000 -0.091670000 C 4.244705000 -1.792914000 0.785074000 H 4.678159000 -1.80956000 1.779971000 C 2.398205000 -0.485449000 1.717492000 C 0.749323000 -0.717526000 2.939257000 C 0.749323000 0.717526000 2.939257000 H 1.438153000 0.620557000 3.778111000 C 0.382512000 2.186490000 2.71986900 H 0.1302952000 2.766236000 2.6529200 C -0.93814000 4.43324000 0.710476000 G -0.171658000 3.69273000 0.967328000 H -0.835190000 3.369973000 0.967328000 Fe 0.003709000 0.532856000 0.026447000 N	С	3,100173000	-1.759906000	-1.759757000
H 4.792052000 -2.918922000 -2.355453000 C 4.884811000 -2.433713000 -0.256274000 C 4.84811000 -2.4557134000 -0.256274000 C 4.244705000 -1.792914000 0.785074000 C 3.022255000 -1.112782000 0.785074000 C 3.022255000 -1.112782000 0.587139000 C 2.398205000 -0.485449000 1.717492000 C 0.740323000 -0.71526000 2.393257000 H 1.438153000 0.620557000 3.77811000 H -0.174612000 2.885245000 3.57315000 C 0.382512000 2.766336000 2.625692000 C -0.171668000 3.642342000 1.164462000 H 0.85194000 3.54097300 0.967328000 N 1.299292000 0.194729000 1.635159200 N 1.29929200 0.1947329000 1.635152000 N 1.29929200 0.1947329000 1.635152000 N 0.45	C	4,300011000	-2.412244000	-1.532687000
C 4.884811000 -2.433713000 -0.256274000 H 5.821121000 -2.951334000 -0.091670000 C 4.244705000 -1.792914000 0.785074000 H 4.678159000 -1.806956000 1.779971000 C 2.398205000 -0.485449000 1.71742200 C 2.398205000 -0.485449000 1.71742200 C 0.74032300 0.717526000 2.39257000 C 0.74032300 0.717526000 2.39257000 H 1.438153000 0.620557000 3.778111000 C 0.382512000 2.186490000 2.71986900 H -0.174612000 2.85245000 3.57331500 C -0.0171668000 3.642343000 0.70476000 H 0.85190000 3.9697300 0.96732800 N 1.299292000 0.194729000 1.69399000 N 1.299292000 0.194729000 1.65152000 O 1.29722000 -0.480744000 -0.958770000 C -2.42514	Н	4,792052000	-2.918923000	-2.355453000
H 5.821121000 -2.951334000 -0.091670000 C 4.244705000 -1.792914000 0.785074000 H 4.678157000 -1.800956000 1.779971000 C 3.022255000 -1.112782000 0.587139000 C 2.398255000 -0.485449000 1.717492000 H 2.911380000 -0.616033000 2.95257000 H 0.1438153000 0.620557000 3.778111000 H -0.139551000 0.139517000 3.169747000 C 0.382512000 2.186490000 2.719869000 H -0.17465000 3.642343000 7.70476000 C -0.717465000 3.642343000 0.770476000 H 0.855190000 3.96973000 0.96732800 Fe 0.003709000 0.532856000 0.02647000 N 1.29922000 0.194725000 1.6438515200 O 1.29272000 0.487413000 1.653152000 O 1.29272000 0.48741000 0.656382000 C -	C	4 884811000	-2 433713000	-0 256274000
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H 2.911380000 -0.616033000 2.675880000 C 0.740323000 0.717526000 2.939257000 H 1.438153000 0.620557000 3.778111000 H -0.159551000 0.139517000 3.169747000 C 0.382512000 2.186490000 2.719869000 H -0.174612000 2.858245000 3.573315000 H -0.171668000 3.642343000 0.70476000 H -0.85013400 4.43224000 1.164462000 H -0.85013400 4.43224000 1.164462000 H 0.85519000 3.960973000 0.967328000 Fe 0.003709000 0.532856000 0.26247000 N 1.29292000 0.194792000 1.693399000 N -0.37555000 2.340613000 1.448350000 C -2.425148000 -1.146035000 0.656382000 C -2.425148000 -1.146035000 0.656382000 C -3.033082000 -2.9735000 1.318015000 C -	C	2 398205000	-0.485449000	1 717492000
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II 2.04372/000 -1./33374000 -2./41722000 H 2.502420000 1.000506000 2.621420000	Н	2 643429000	_1 7535/31000	_2 741022000
	Н	-2 598480000	-1 990506000	2.741922000

Table S16. Optimized parameters of $[Fe(Sal_2-trien]^+$ (conformer: III(+ -)) in the sextet state (HS). Units are in Å.