Supplementary Material

New Members of A Class of Iron-Thiolate-Nitrosyl Compounds: Trinuclear Iron-Thiolate-Nitrosyl Complexes Containing Fe_3S_6 Core

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Table S1. Crystallographic data of complexes **1** and **2**.

	1	**2**·2MeOH
chemical formula	$C_{18}H_{12}N_3O_3S_6Fe_3$	$C_{20}H_{20}O_5N_3S_6PF_6Fe_3$
Mw/gmol^{-1}	678.22	887.27
crystal system	monoclinic	orthorhombic
space group	$P2_1/c$	Pnma
λ/Å	0.7107	0.7107
a/Å	9.1440(3)	25.5399(6)
b/Å	17.5419(5)	10.2124(2)
c/Å	14.4173(4)	11.2987(3)
β/ °	94.435(2)	
V/Å ^{3}	2289.50(12)	2946.97(12)
Z	4	4
ρ_{calcd}/g cm^{-3}	1.968	2.000
μ/mm^{-1}	2.452	2.015
T/K	120(1)	150(1)
Uniq. Refln/obs.	5263/4592	3579/2332
R	0.0346[a]	0.0672[a]
R_{WF2}	0.0963[b]	0.1780[b]
GOF	1.167	1.117

[a] $R = \sum |(F_o - F_c)| / \sum F_o$. [b] $R_{WF}^2 = \{\sum w (F_o^2 - F_c^2)^2 / \sum[w (F_o^2)^2]\}^{1/2}$. for observed reflections.

Table S2. Selected SOMO coefficients of complex **1**.

MOs		170
occup:		1
Fe1	d_{z2}	0.5368
	d_{x2-y2}	-0.0195
	d_{xy}	0.0574
	d_{xz}	0.1844
	d_{yz}	0.1775
Fe2	d_{z2}	-0.0590
	d_{x2-y2}	0.0836
	d_{xy}	-0.0488
	d_{xz}	0.0729
	d_{yz}	-0.0626
Fe3	d_{z2}	0.0865
	d_{x2-y2}	0.3494
	d_{xy}	-0.0386
	d_{xz}	-0.0657
	d_{yz}	0.2008
O1	p_x	0.1195
	p_y	0.2448
	p_z	-0.0580
O2	p_x	-0.0136
	p_y	0.0320
	p_z	-0.1087
O3	p_x	-0.0627
	p_y	-0.0702
	p_z	-0.2066
N1	p_x	-0.1252
	p_y	-0.2425
	p_z	-0.0240
N2	p_x	0.0150
	p_y	-0.0566
	p_z	0.1233
N3	p_x	0.0654
	p_y	0.1359
	p_z	0.1935
S1	p_x	0.0323
	p_y	0.0695
	p_z	0.2675
S2	p_x	-0.0074
	p_y	-0.1269
	p_z	0.2810
S3	p_x	0.0339
	p_y	-0.1182
	p_z	0.3288
S4	p_x	-0.0137
	p_y	0.0003
	p_z	0.1722
S5	p_x	-0.0570
	p_y	-0.1562
	p_z	0.0147
S6	p_x	0.0416
	p_y	-0.0359
	p_z	-0.0033

Table S3. Composition[a] of the selected atomic orbitals in SOMO of complex **1**.

Orbital	%	Summation	%
Fe1(d_{z2})	23.41	Fe1	30.04
Fe3(d_{x2}-d_{y2})	10.07	Fe3	13.34
S2(p_z)	6.85	N1O1	11.79
S3(p_z)	4.88	N3O3	7.63
S4(p_z)	4.47	S1~S6	20.6
N1(p_z)	3.92		
O1(p_y)	3.84		
Fe3(d_{yz})	3.27		
N1(2s)	3.00		
Fe1(d_{xz})	2.78		
O3(p_z)	2.63		
Fe1(d_{yz})	2.59		
N3(p_z)	2.40		
S1(p_z)	1.77		
S5(p_y)	1.52		
N3(2s)	1.51		
Fe1(p_z)	1.26		
S3(p_y)	1.11		
N3(p_y)	1.09		
N1(p_x)	1.03		

[a] Only contributions of more than 1.0% are taken into account.