Article

Three Novel Thiazole-Arm Containing 1,3,4-Oxadiazole-Based [HS-HS] Fe(II) Dinuclear Complexes

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Electronic Supplementary Information

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S1. **Infrared Spectra**

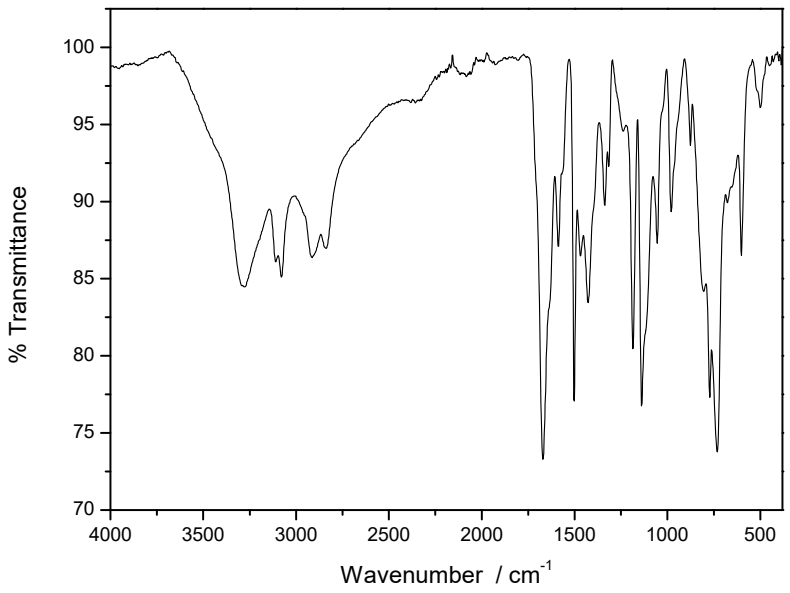

Figure S1: IR spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L^{Thiazole}**).

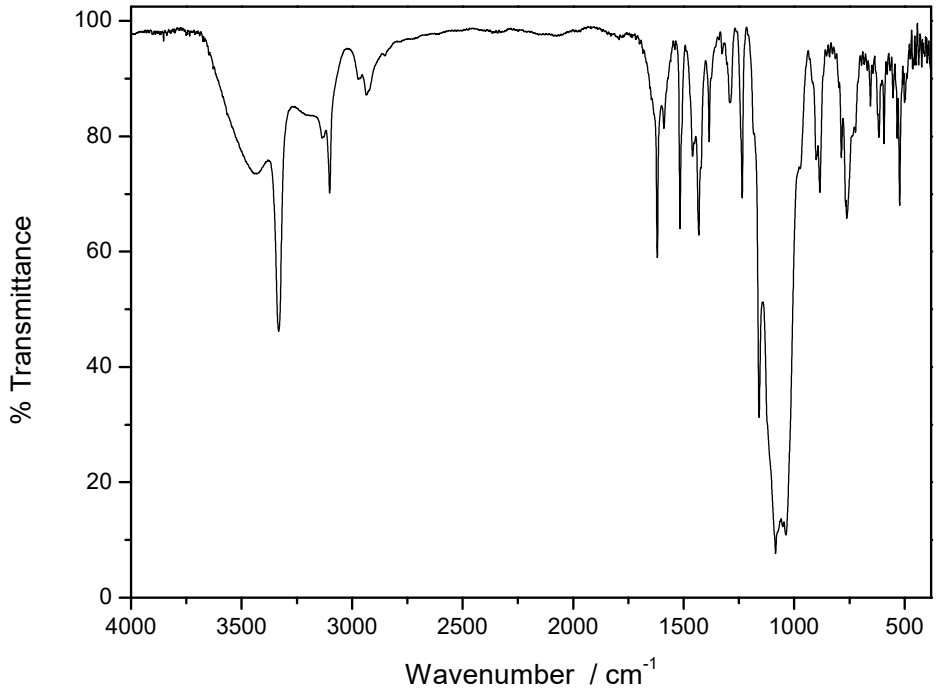

Figure S2: IR spectrum of $[Fe_2(\mu_2\text{-}L^{Thiazole})_2](BF_4)_4 \cdot 2MeCN$ (**1**).

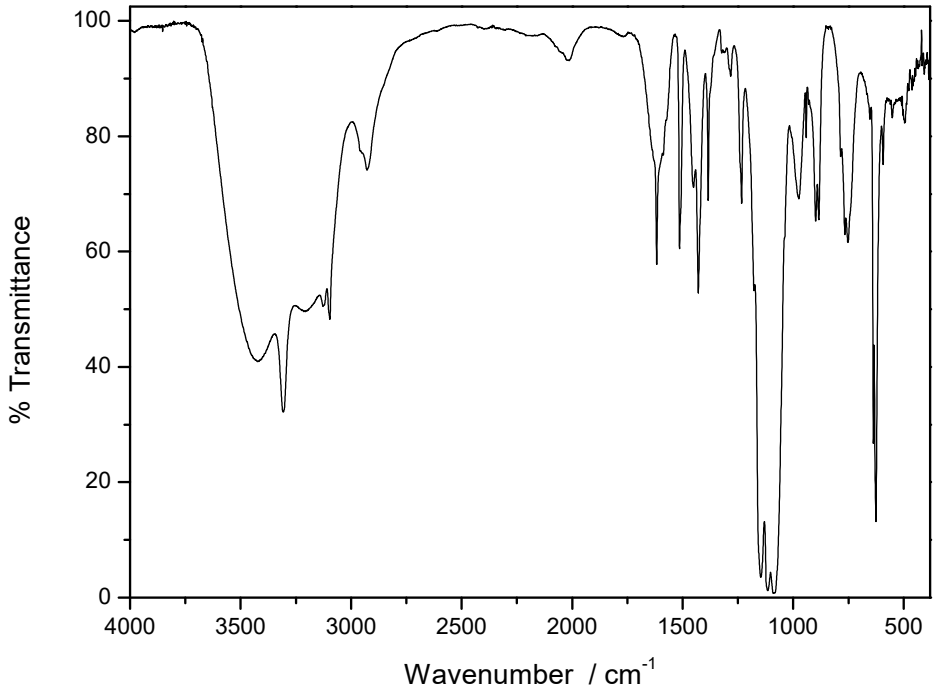

Figure S3: IR spectrum of $[Fe_2(\mu_2\text{-}L^{Thiazole})_2](ClO_4)_4$ (**2**)

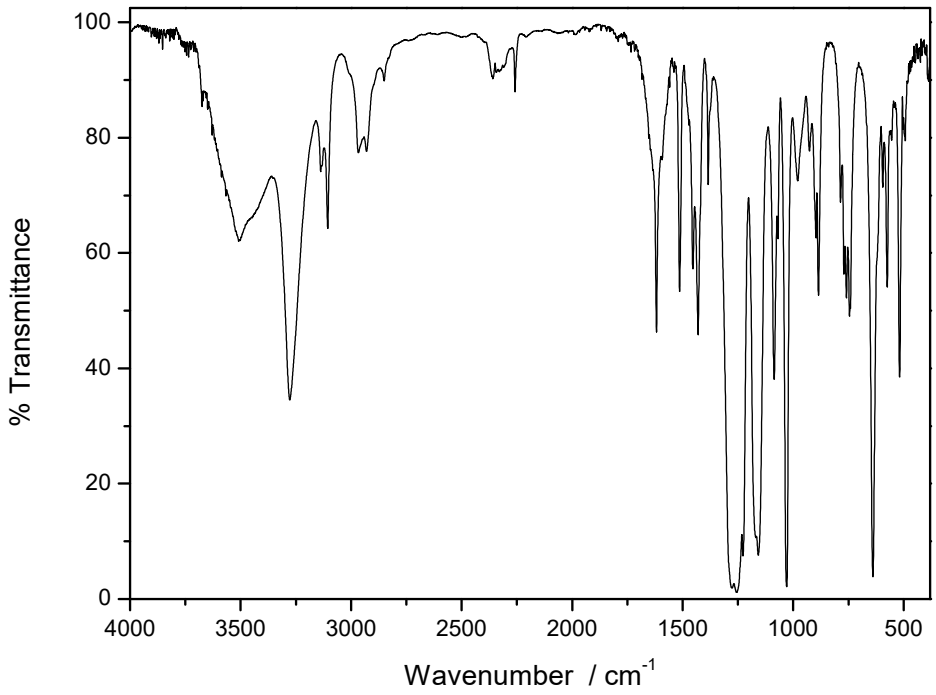

Figure S4: IR spectrum of $[Fe_2(\mu_2\text{-}\mathbf{L^{Thiazole}})_2](CF_3SO_3)_4{\cdot}2MeCN$ (**3**).

S2. NMR Spectroscopy

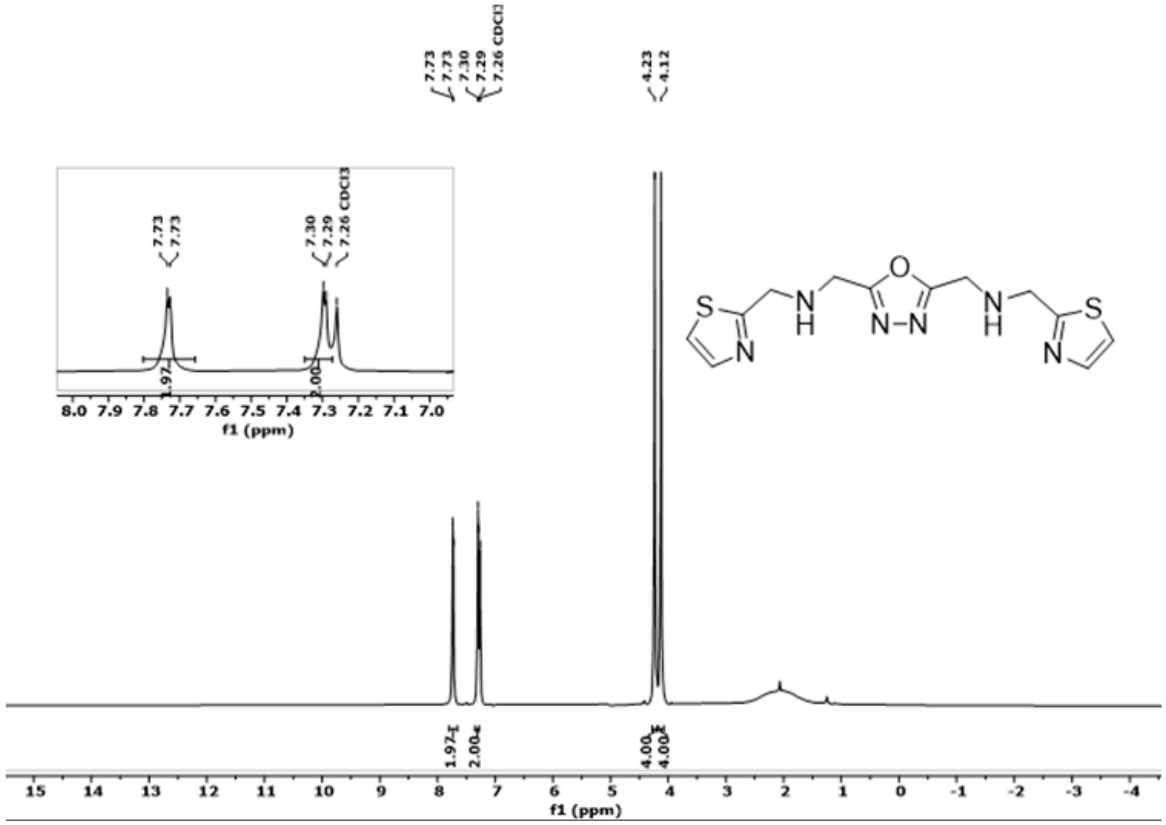

Figure S5: ^{1}H-NMR spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L^{Thiazole}**) in $CDCl_3$.

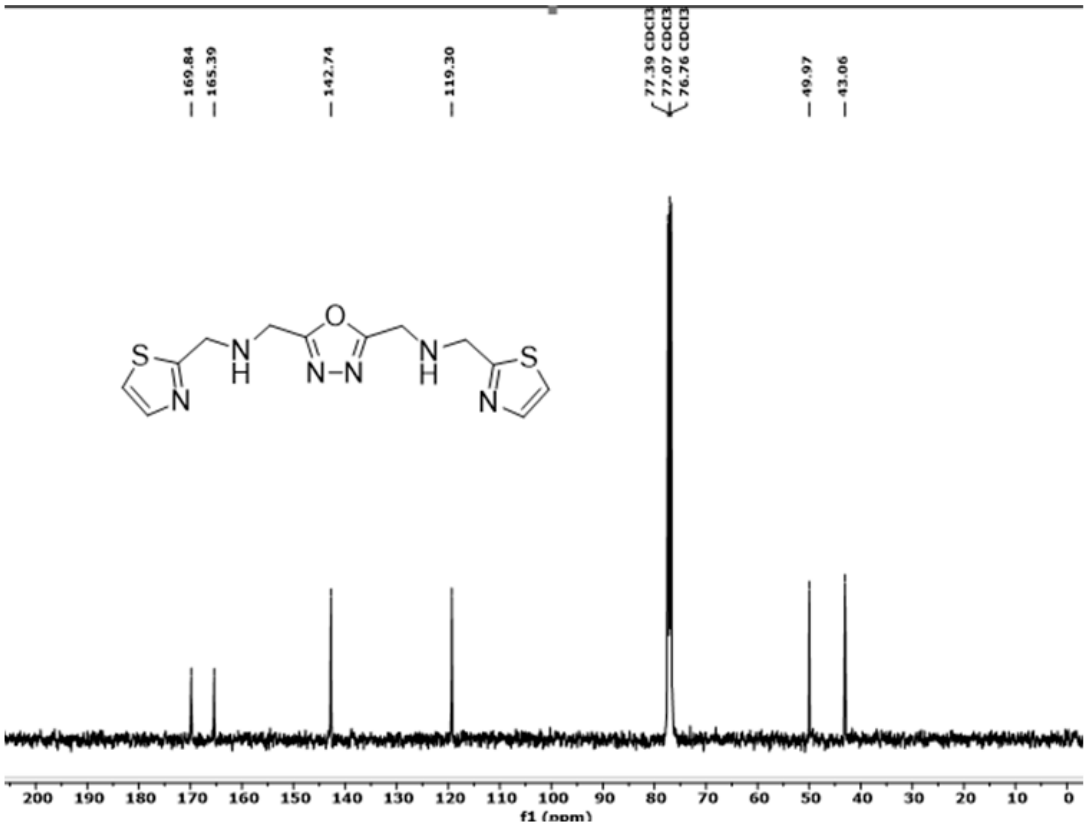

Figure S6: ^{13}C-NMR spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L**$^{\textbf{Thiazole}}$) in $CDCl_3$.

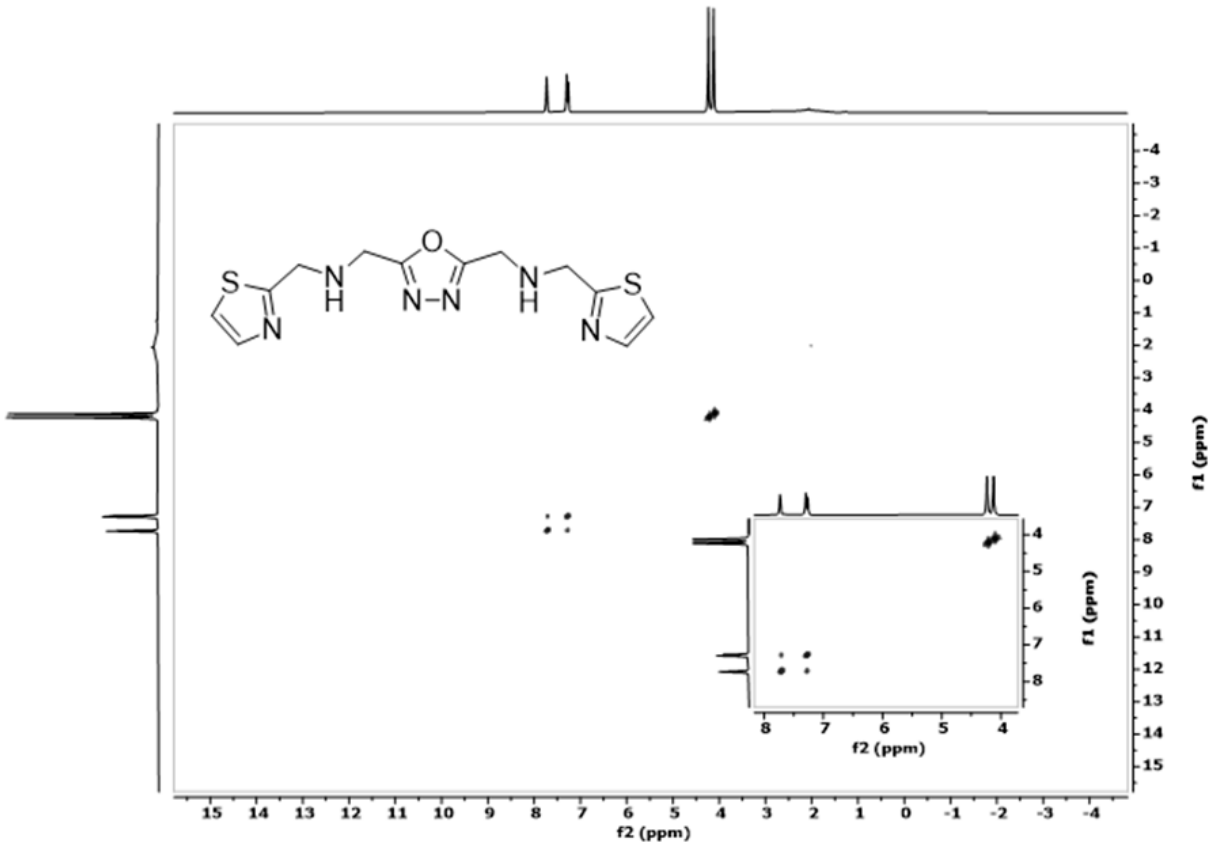

Figure S7: ^{1}H-^{1}H-COSY spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L**$^{\textbf{Thiazole}}$) in $CDCl_3$.

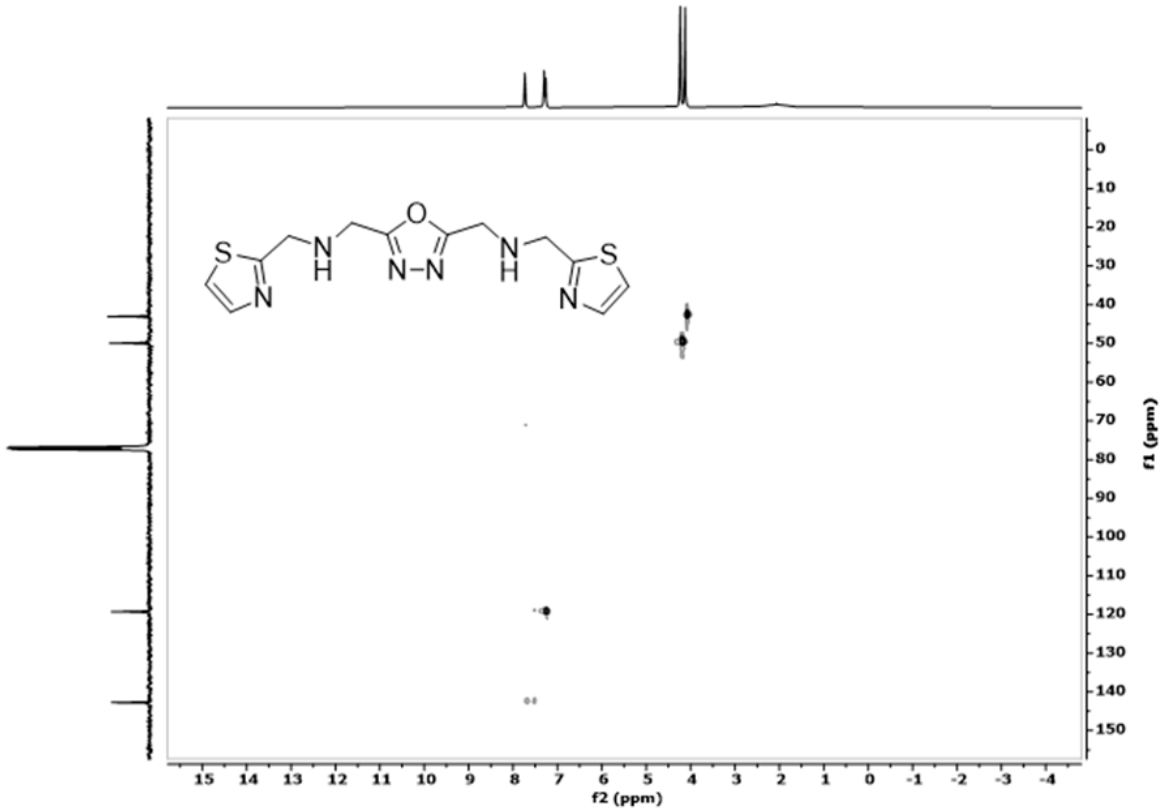

Figure S8: ^{1}H-^{13}C-HSQC spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole ($\mathbf{L^{5,TA}}$) in $CDCl_3$.

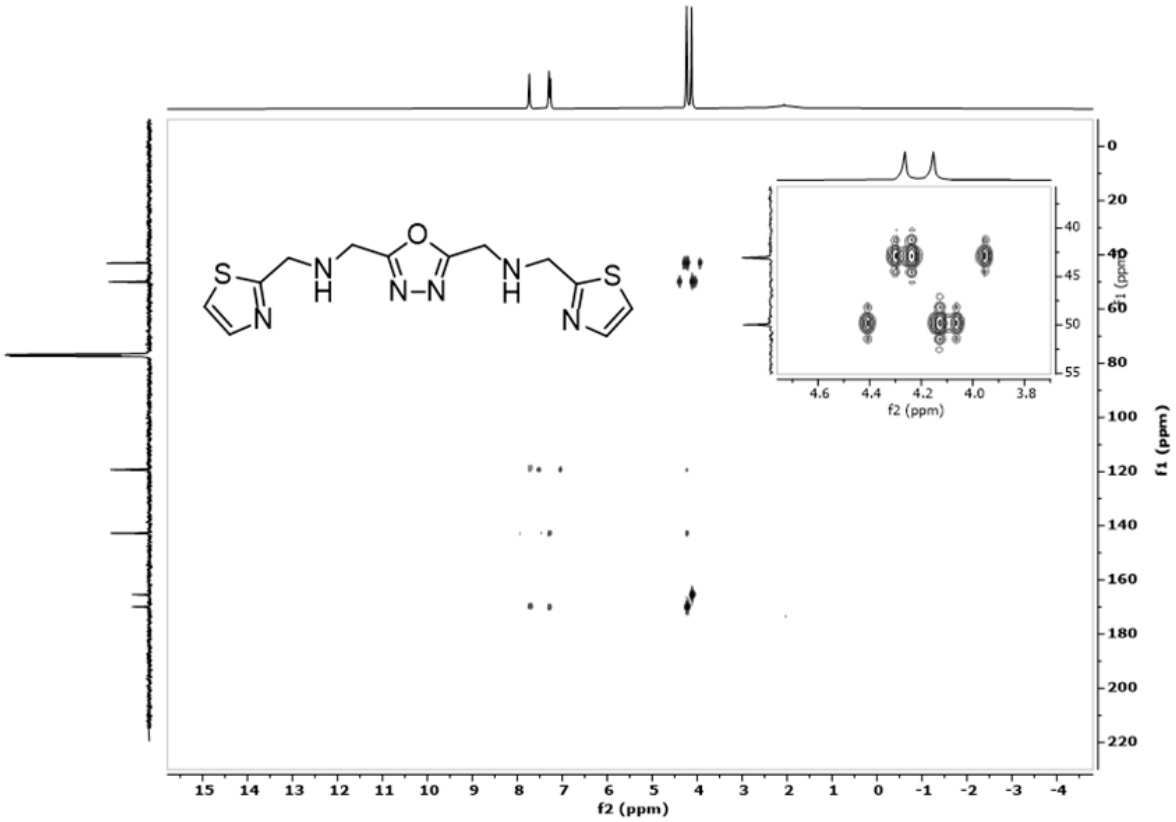

Figure S9: ^{1}H-^{13}C-HMBC spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L^{5,TA}**) in $CDCl_3$.

S3. FD Mass spectroscopy

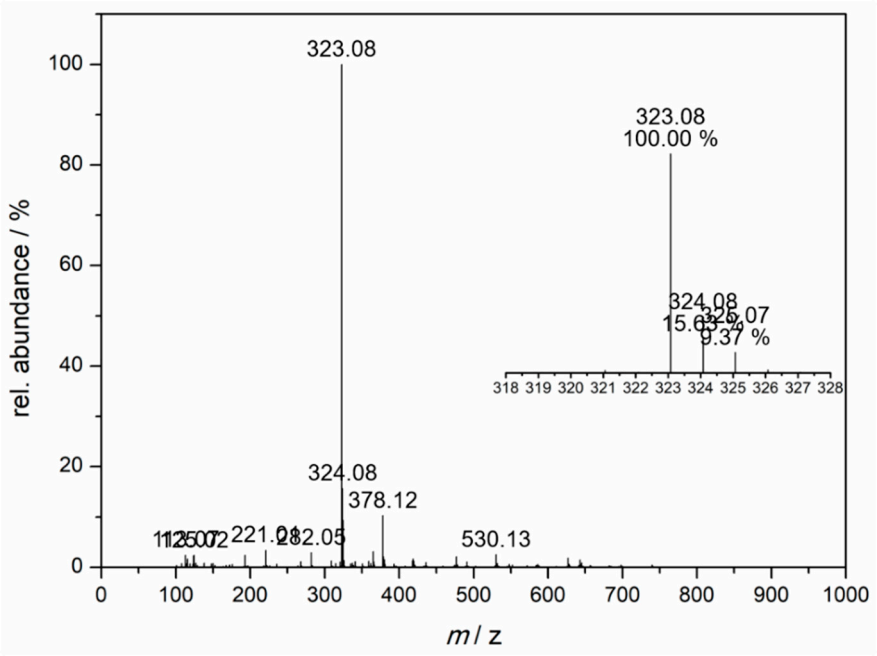

Figure S10: FD mass spectrum of 2,5-Bis[(1,3-thiazol-2-ylmethyl)amino]methyl-1,3,4-oxadiazole (**L^{Thiazole}**).

S4. Crystallography

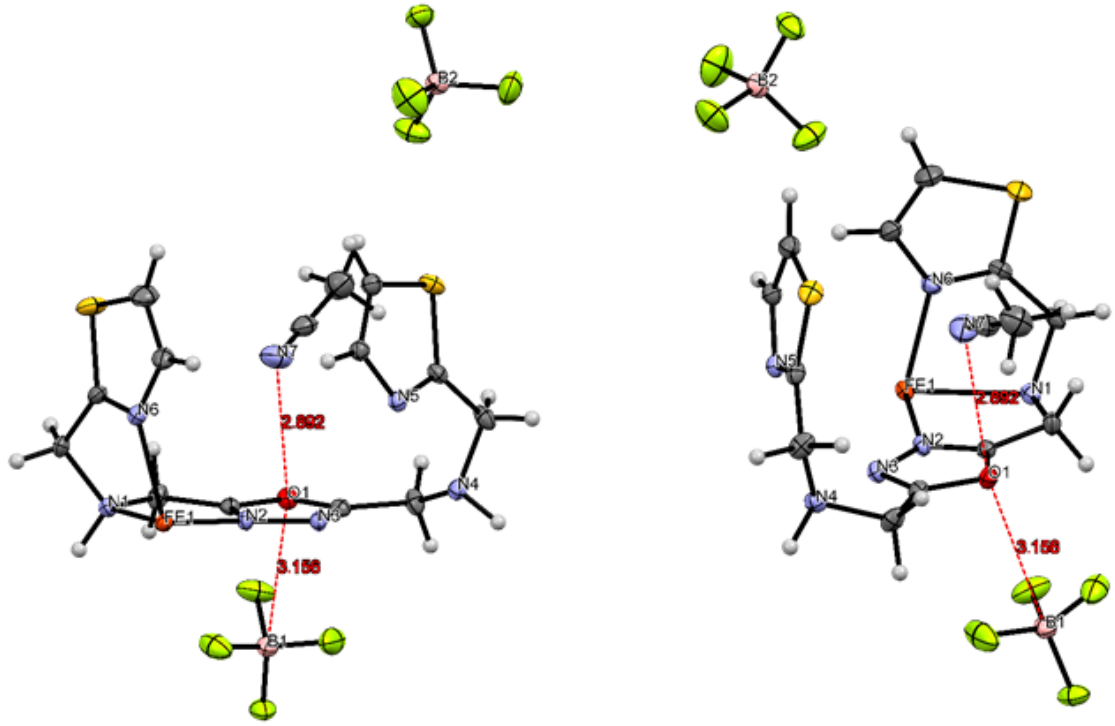

Figure S11: Asymmetric Unit of **1** with front view (left) and side view (right). Measured distances are displayed as red dashed lines. ORTEP representation with atomic displacement parameters set to 50 % probability.

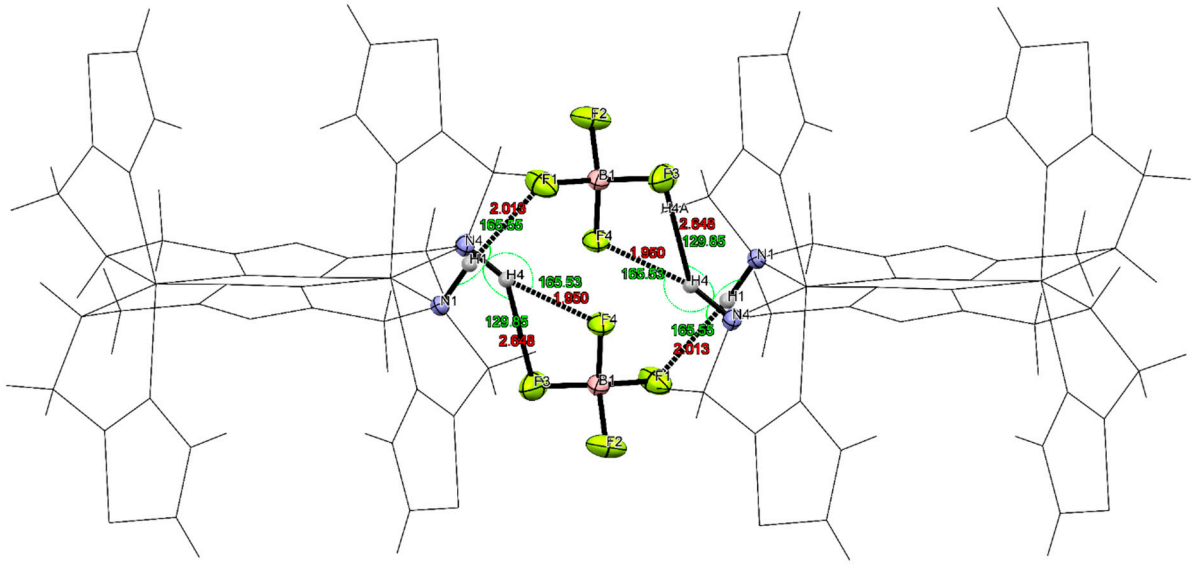

Figure S12: Unique hydrogen bonds (dashed black lines) in **1** between complex cations and tetrafluoroborate anions. Acetonitrile molecules and irrelevant tetrafluoroborate anions are omitted for clarity. N-H···F distances are displayed in red. N-H-F angles are shown in green. ORTEP representation with atomic displacement parameters set to 50 % probability.

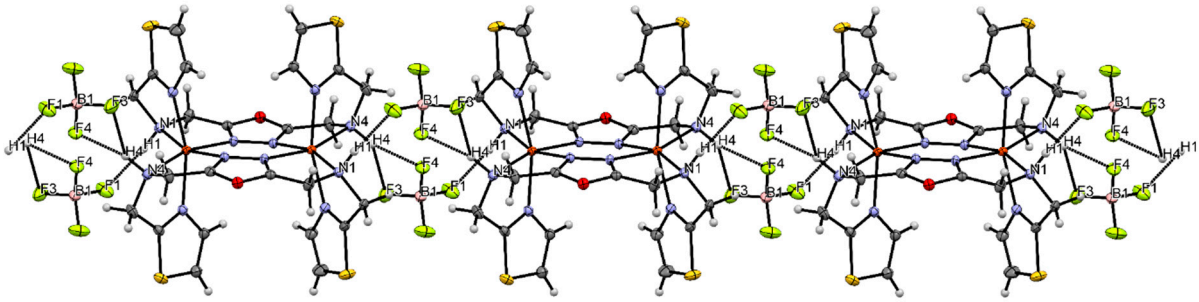

Figure S13: One-dimensional network of complex cations via hydrogen bonds (dashed black lines) in **1**. Acetonitrile molecules and irrelevant tetrafluoroborate anions are omitted for clarity. ORTEP representation with atomic displacement parameters set to 50 % probability.

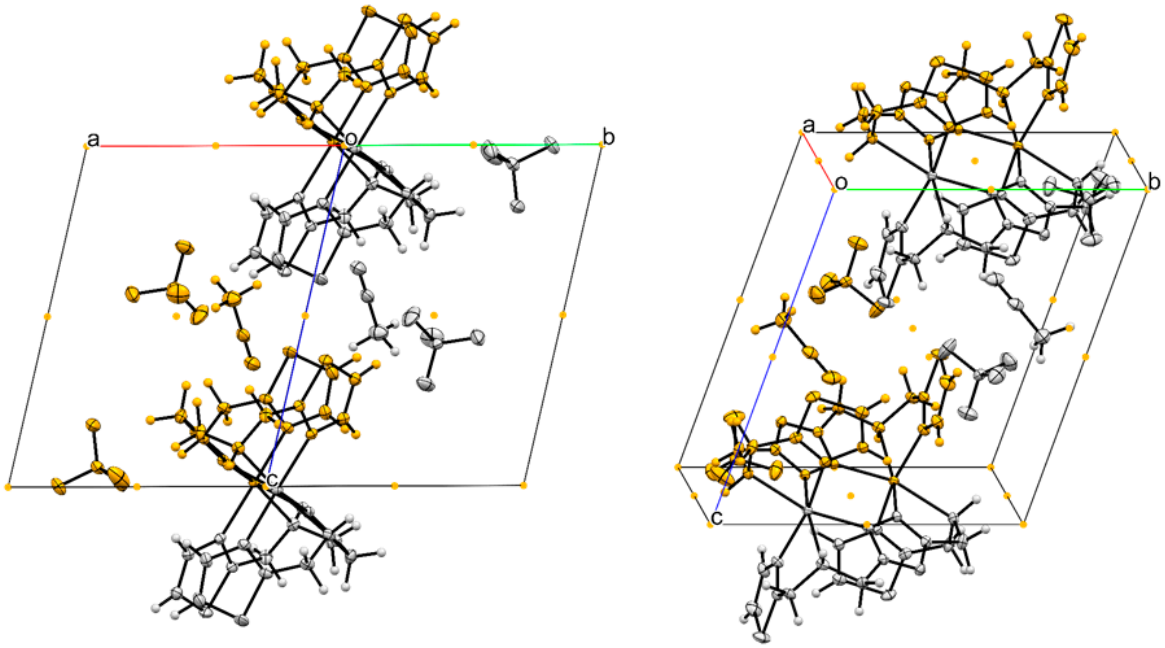

Figure S14: Unit cell of **1** with view along the bisector of γ (left) and perspective (right). The colour scheme is set according to symmetry equivalent moieties. Yellow dots represent a center of inversion. ORTEP representation with atomic displacement parameters set to 50 % probability.

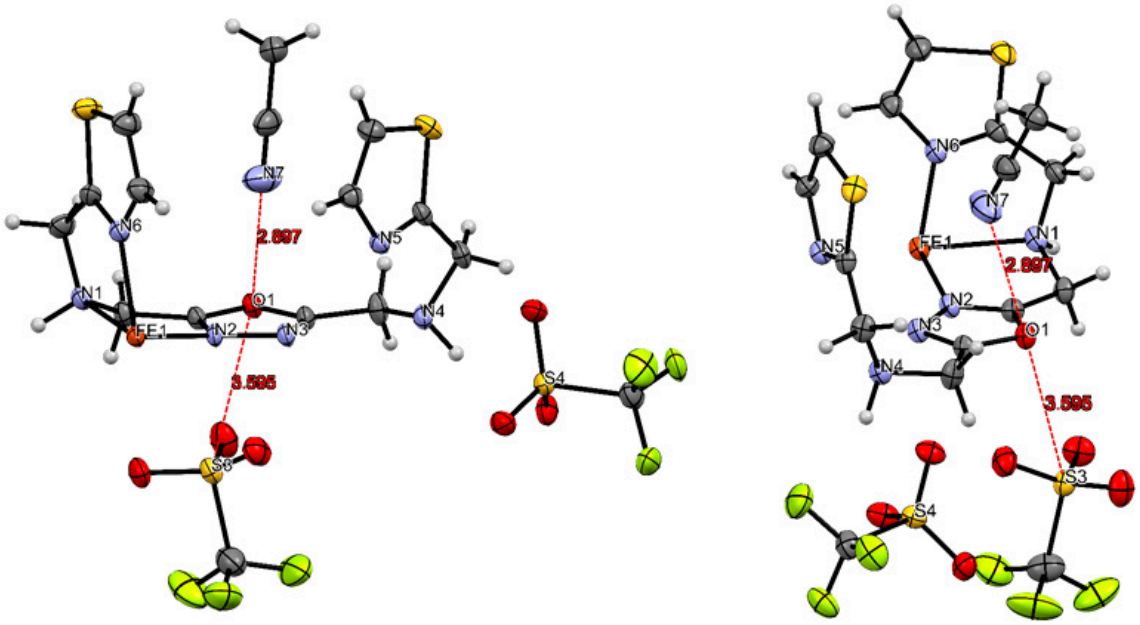

Figure S15: Asymmetric Unit of **3** with front view (left) and side view (right). Measured distances are displayed as red dashed lines. ORTEP representation with atomic displacement parameters set to 50 % probability.

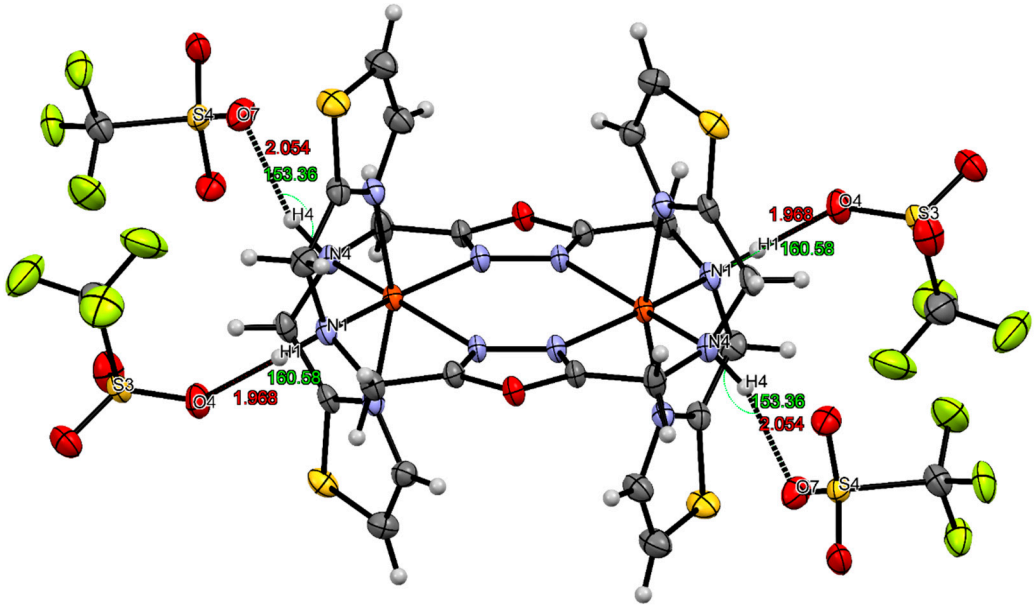

Figure S16: Unique hydrogen bonds (dashed black lines) in **3** between complex cations and tetrafluoroborate anions. Acetonitrile molecules and irrelevant tetrafluoroborate anions are omitted for clarity. N-H···O distances are displayed in red. N-H-O angles are shown in green. ORTEP representation with atomic displacement parameters set to 50 % probability.

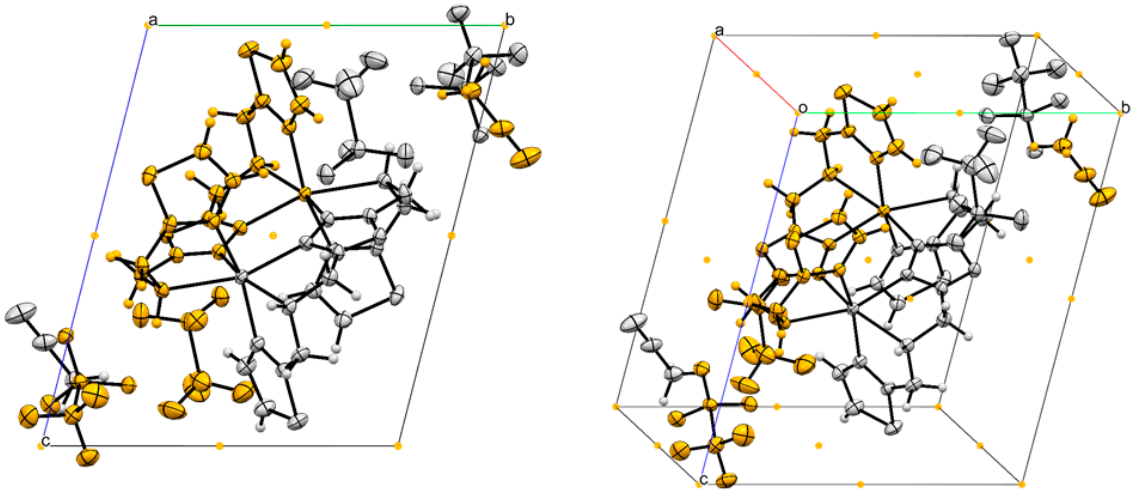

Figure S17: Unit cell of **3** with view along the a-axis (left) and perspective (right). The colour scheme is set according to symmetry equivalent moieties. Yellow dots represent a center of inversion. ORTEP representation with atomic displacement parameters set to 50 % probability.

Table S1: Selected angles of complex 1 and 3. Labeling of the atoms follows the scheme in Figure 3 (left).

	1 120 K	**3** 120 K
cis-Angles / °		
N1-Fe-N2	74.57(4)	74.69(10)
N2-Fe-N3	90.63(4)	90.67(10)
N3-Fe-N4	75.64(4)	74.47(10)
N4-Fe-N1	120.95(4)	122.24(10)
N1-Fe-N5	97.88(4)	96.63(10)
N2-Fe-N5	94.31(4)	92.48(11)
N3-Fe-N5	94.61(4)	95.11(11)
N4-Fe-N5	76.26(4)	76.07(10)
N1-Fe-N6	75.80(4)	75.84(11)
N2-Fe-N6	98.43(4)	101.61(11)
N3-Fe-N6	95.53(4)	96.75(11)
N4-Fe-N6	93.83(4)	93.41(11)
trans-Angles / °		
N1-Fe-N3	161.24(4)	161.56(10)
N2-Fe-N4	162.43(4)	160.07(11)
N5-Fe-N6	163.60(4)	161.42(11)
Torsions / °		
Fe-N2-N3-Fe1'	9.03(18)	10