Supporting Information for

"New Fe(III)(cyclam) Complexes Bearing Axially Bound *geminal*-Diethynylethenes"

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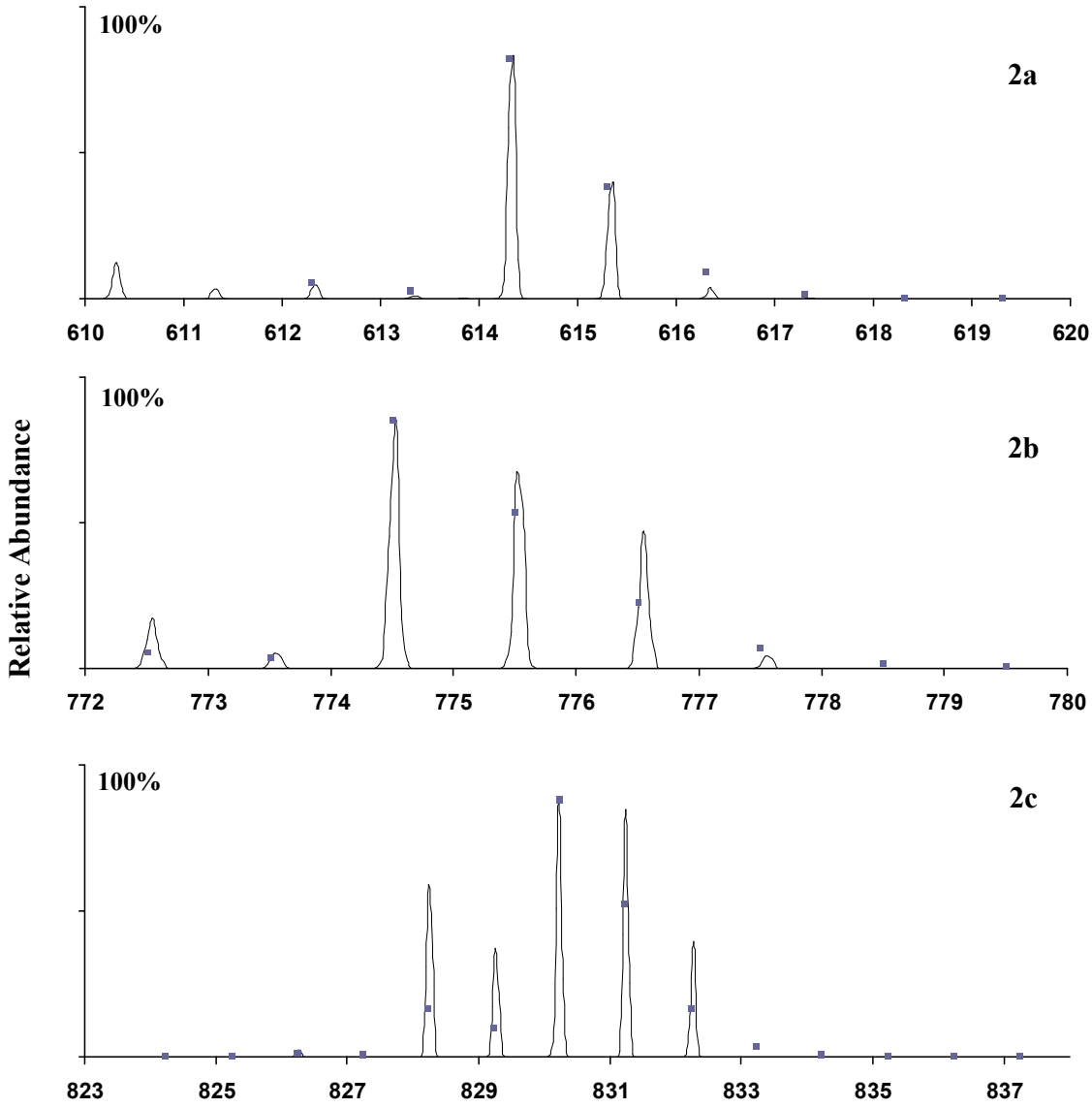

Fig. S1. HR-*n*ESI-MS spectra (solid line) of **2a**, **2b** and **2c** with isotopic distributions (blue dots) calculated by Analyst 1.4 software.

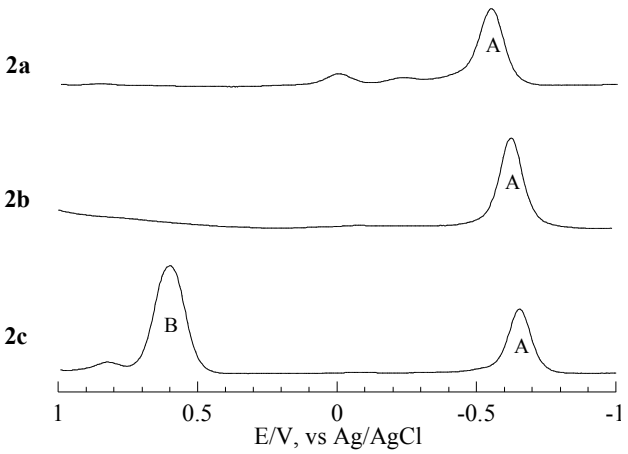

Fig. S2. Differential pulse voltammograms (DPV) recorded for compounds **2a – 2c** in 0.20 M THF solution of Bu_4NPF_6.

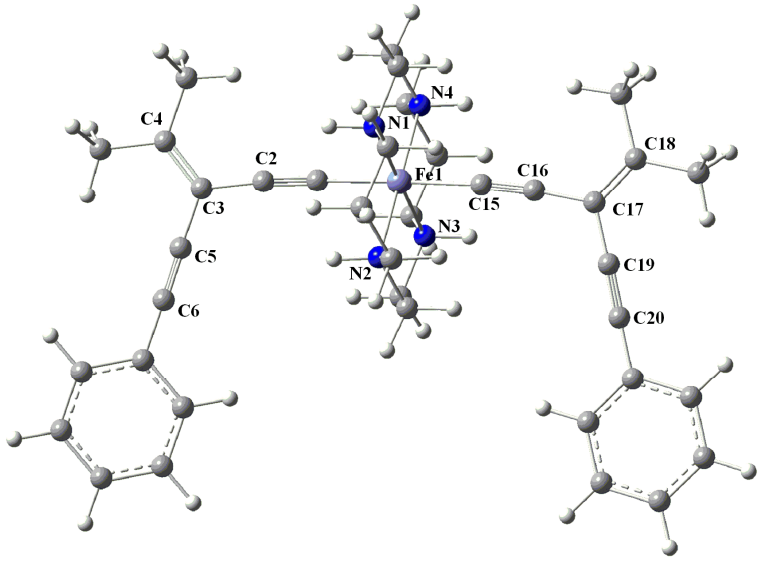

Fig. S3. Fully optimized structure of **2a'**$^+$ by using DFT method at LanL2DZ level.

Table S1. Relevant Bond Lengths (Å) and Angles (deg) Computed for **2a'**$^+$**.**

2a'$^+$			
Fe1 – C1	1.966	C1-Fe1-C15	178.6
Fe1 – C15	1.966	Fe1-C1-C2	173.1
Fe1 – N1	2.046	Fe1-C15-C16	174.2
Fe1 – N2	2.050	C1-Fe1-N1	88.2
Fe1 – N3	2.047	C1-Fe1-N2	87.3
Fe1 – N4	2.047	C1-Fe1-N3	91.9
C1 – C2	1.246	C1-Fe1-N4	92.8
C2 – C3	1.446	C1-C2-C3	174.5
C3 – C4	1.380	C2-C3-C4	122.8

C3 – C5	1.441	C2-C3-C5	115.2
C5 – C6	1.229	C3-C5-C6	178.4
C15 – C16	1.246	C15-C16-C17	174.9
C16 – C17	1.446	C16-C17-C18	122.8
C17 – C18	1.380	C16-C17-C19	115.0
C17 – C19	1.441	C17-C19-C20	178.4
C19 – C20	1.229		

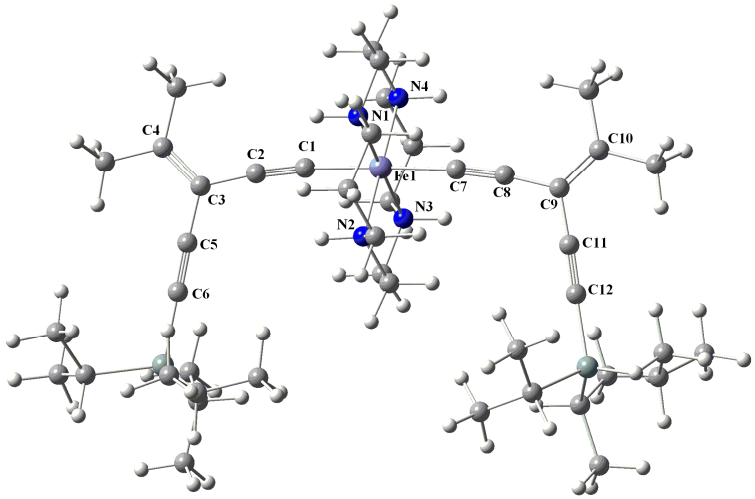

Fig. S4. Fully optimized structure of **2b'**$^{+}$ by using DFT method at LanL2DZ level.

Table S2. Relevant Bond Lengths (Å) and Angles (deg) Computed for **2b'**$^{+}$**.**

2b'$^{+}$			
Fe1 – C1	1.966	C1-Fe1-C7	178.2
Fe1 – C7	1.966	Fe1-C1-C2	171.9
Fe1 – N1	2.046	Fe1-C7-C8	174.1
Fe1 – N2	2.050	C1-Fe1-N1	88.4
Fe1 – N3	2.047	C1-Fe1-N2	87.1
Fe1 – N4	2.047	C1-Fe1-N3	91.6
C1 – C2	1.246	C1-Fe1-N4	92.9
C2 – C3	1.446	C1-C2-C3	173.7
C3 – C4	1.380	C2-C3-C4	123.1
C3 – C5	1.441	C2-C3-C5	114.6
C5 – C6	1.229	C3-C5-C6	177.8
C7 – C8	1.246	C7-C8-C9	173.6
C8 – C9	1.446	C8-C9-C10	123.1
C9 – C10	1.380	C8-C9-C11	114.7
C9 – C11	1.441	C9-C11-C12	178.1
C11 – C12	1.229		

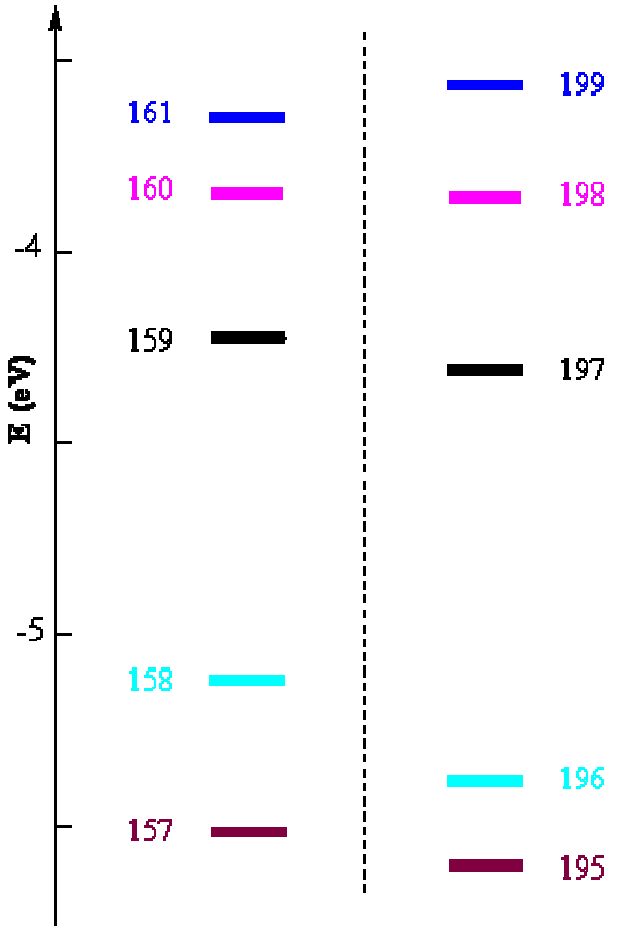

Fig. S5. MO energy level diagram for model compounds **2a**'$^{+}$ (left) and **2b**'$^{+}$ (right) based on β-spin.

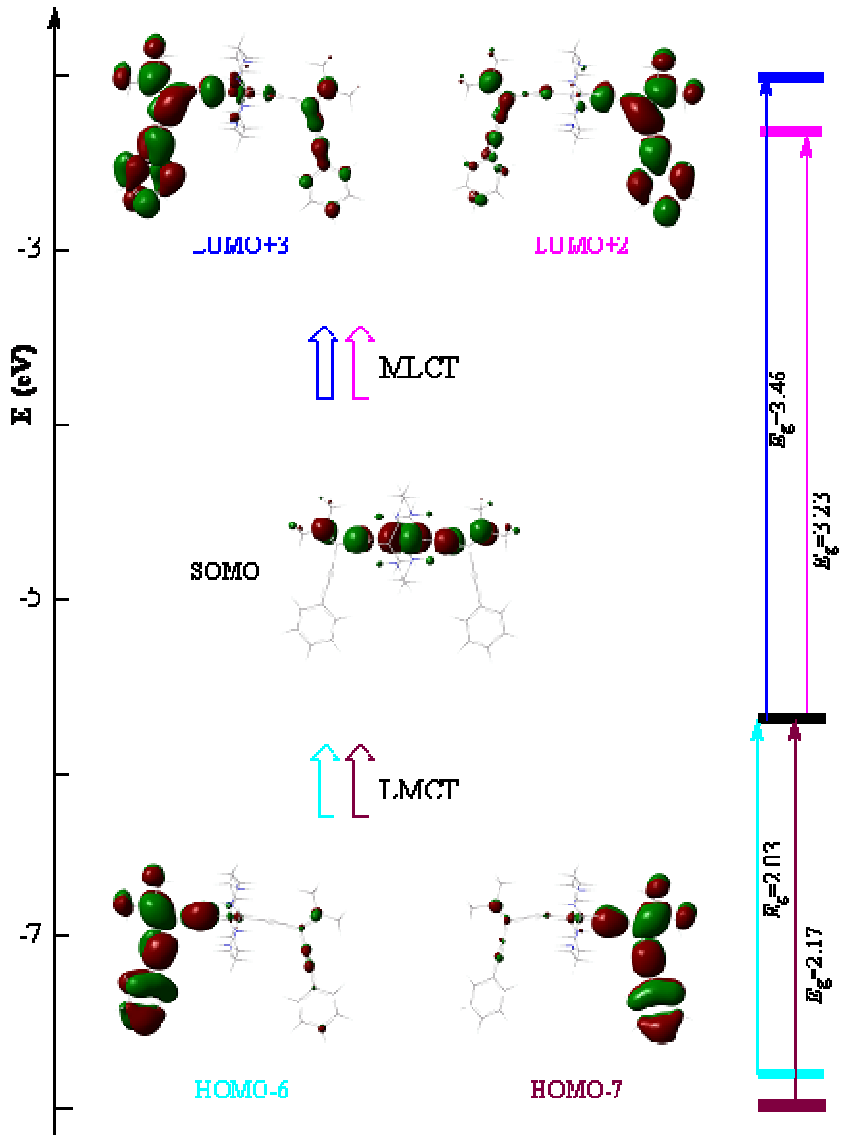

Fig. S6. MLCT and LMCT transition scheme for compound **2a**.