List of Electronic Supplementary Information (B614748H)

A photoswitchable molecular wire with the dithienylethene (DTE) linker, (dppe)(η^5-C_5Me_5)Fe-C≡C-DTE-C≡C-Fe(η^5-C_5Me_5)(dppe).

Yuya Tanaka, Akiko Inagaki and Munetaka Akita *

Chemical Resources Laboratory, Tokyo Institute of Technology, R1-27, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Experimental procedures for X-ray crystallography.

Single crystals of **2** were obtained by recrystallization from CH_2Cl_2-MeOH. Diffraction measurements were made on a Rigaku RAXIS IV imaging plate area detector with Mo Kα radiation (λ= 0.71069 Å) at –60°C. Indexing was performed from 3 oscillation images, which were exposed for 3 min. The crystal-to-detector distance was 110 mm ($2\theta_{max}$= 55°). In the reduction of data, Lorentz and polarization corrections and empirical absorption corrections were made.[1] The crystallographic data are summarized in Table S1.

The structural analysis was performed on an IRIS O2 computer using teXsan structure solving program system obtained from the Rigaku Corp., Tokyo, Japan.[2] Neutral scattering factors were obtained from the standard source.[3]

The structures were solved by a combination of the direct methods (SHELXS-86)[4] and Fourier synthesis (DIRDIF94).[5] Least-squares refinements were carried out using SHELXL-97 [4] (refined on F^2) linked to teXsan. All non-hydrogen atoms were refined anisotropically, methyl hydrogen atoms were refined using riding models, and other hydrogen atoms were fixed at the calculated positions.

(1) Higashi, T. *Program for absorption correction*, Rigaku Corp., Tokyo, Japan, 1995.

(2) *teXsan; Crystal Structure Analysis Package, ver. 1. 11*, Rigaku Corp., Tokyo, Japan, 2000.

(3) *International Tables for X-ray Crystallography*; Kynoch Press, Birmingham, 1975, Vol. 4.

(4) (a) Sheldrick, G. M. *SHELXS-86: Program for crystal structure determination*, University of Göttingen, Göttingen, Germany, 1986. (b) Sheldrick, G. M. *SHELXL-97: Program for crystal structure refinement*, University of Göttingen: Göttingen, Germany, 1997.

(5) Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Gould, R. O.; Smits, J. M. M.; Smykalla, C. *The DIRDIF program system, Technical Report of the Crystallography Laboratory*, University of Nijmegen, Nijmegen, The Netherland, 1992.

Table S1. Crystallographic data for **2**·CH_2Cl_2.

formula	$C_{92}H_{88}F_6P_4S_2Cl_2Fe_2$
formula weight	1678.31
crystal system	monoclinic
space group	$P2_1/n$
a / Å	42.28(2)
b / Å	16.460(8)
c / Å	12.019(5)
α / deg	90
β / deg	90.39(2)
γ / deg	90
V/ Å^3	8364(6)
Z	4
d_{calcd} / g·cm^{-3}	1.333
μ / mm^{-1}	0.595
no of diffractions collected	57814
no of variable	985
R1 for data	0.0817
with $I > 2\sigma(I)$	(for 13064 data)
wR2	0.1996
	(for all 18616 data)

Table S2. Interatomic distances (Å) and bond angles (deg) for **2**·CH_2Cl_2.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
Fe(1)	P(1)	2.187(1)	F(3)	C(4)	1.352(7)
Fe(1)	P(2)	2.195(1)	F(4)	C(4)	1.314(7)
Fe(1)	C(17)	1.896(4)	F(5)	C(5)	1.355(6)
Fe(1)	C(100)	2.102(4)	F(6)	C(5)	1.347(6)
Fe(1)	C(101)	2.126(4)	C(1)	C(2)	1.354(5)
Fe(1)	C(102)	2.128(4)	C(1)	C(5)	1.503(6)
Fe(1)	C(103)	2.133(5)	C(1)	C(12)	1.474(5)
Fe(1)	C(104)	2.133(4)	C(2)	C(3)	1.508(6)
Fe(2)	P(3)	2.188(1)	C(2)	C(22)	1.471(6)
Fe(2)	P(4)	2.207(1)	C(3)	C(4)	1.520(7)
Fe(2)	C(27)	1.877(4)	C(4)	C(5)	1.544(6)
Fe(2)	C(200)	2.139(5)	C(11)	C(12)	1.380(6)
Fe(2)	C(201)	2.119(5)	C(11)	C(15)	1.497(6)
Fe(2)	C(202)	2.099(5)	C(12)	C(13)	1.425(6)
Fe(2)	C(203)	2.130(5)	C(13)	C(14)	1.379(6)
Fe(2)	C(204)	2.153(5)	C(14)	C(16)	1.424(5)
Cl(1)	C(300)	1.81(1)	C(16)	C(17)	1.210(5)
Cl(2)	C(300)	1.68(1)	C(21)	C(22)	1.372(7)
S(1)	C(11)	1.726(4)	C(21)	C(25)	1.511(7)
S(1)	C(14)	1.742(4)	C(22)	C(23)	1.433(6)
S(2)	C(21)	1.739(5)	C(23)	C(24)	1.364(6)
S(2)	C(24)	1.747(5)	C(24)	C(26)	1.416(6)
P(1)	C(111)	1.849(4)	C(26)	C(27)	1.227(6)
P(1)	C(121)	1.841(4)	C(100)	C(101)	1.421(6)
P(1)	C(131)	1.846(4)	C(100)	C(104)	1.437(6)
P(2)	C(112)	1.864(4)	C(100)	C(105)	1.497(7)
P(2)	C(141)	1.854(4)	C(101)	C(102)	1.423(6)
P(2)	C(151)	1.852(4)	C(101)	C(106)	1.503(7)
P(3)	C(211)	1.839(5)	C(102)	C(103)	1.423(6)
P(3)	C(221)	1.834(5)	C(102)	C(107)	1.503(6)
P(3)	C(231)	1.852(5)	C(103)	C(104)	1.419(6)
P(4)	C(212)	1.848(5)	C(103)	C(108)	1.503(8)
P(4)	C(241)	1.842(5)	C(104)	C(109)	1.504(7)
P(4)	C(251)	1.846(5)	C(111)	C(112)	1.524(5)
F(1)	C(3)	1.346(6)	C(121)	C(122)	1.397(6)
F(2)	C(3)	1.348(7)	C(121)	C(126)	1.397(6)

Table S2. Interatomic distances (Å) for **2**·CH_2Cl_2. (cont'd.)

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
C(122)	C(123)	1.395(6)	C(223)	C(224)	1.373(9)
C(123)	C(124)	1.371(7)	C(224)	C(225)	1.367(9)
C(124)	C(125)	1.372(7)	C(225)	C(226)	1.385(9)
C(125)	C(126)	1.396(6)	C(231)	C(232)	1.399(8)
C(131)	C(132)	1.382(6)	C(231)	C(236)	1.399(8)
C(131)	C(136)	1.399(6)	C(232)	C(233)	1.363(9)
C(132)	C(133)	1.401(6)	C(233)	C(234)	1.37(1)
C(133)	C(134)	1.363(8)	C(234)	C(235)	1.36(1)
C(134)	C(135)	1.390(8)	C(235)	C(236)	1.42(1)
C(135)	C(136)	1.394(7)	C(241)	C(242)	1.393(8)
C(141)	C(142)	1.396(6)	C(241)	C(246)	1.380(8)
C(141)	C(146)	1.389(6)	C(242)	C(243)	1.40(1)
C(142)	C(143)	1.394(6)	C(243)	C(244)	1.36(1)
C(143)	C(144)	1.394(8)	C(244)	C(245)	1.39(1)
C(144)	C(145)	1.387(8)	C(245)	C(246)	1.39(1)
C(145)	C(146)	1.385(7)	C(251)	C(252)	1.402(8)
C(151)	C(152)	1.406(6)	C(251)	C(256)	1.381(8)
C(151)	C(156)	1.386(6)	C(252)	C(253)	1.395(9)
C(152)	C(153)	1.392(7)	C(253)	C(254)	1.37(1)
C(153)	C(154)	1.378(9)	C(254)	C(255)	1.38(1)
C(154)	C(155)	1.384(9)	C(255)	C(256)	1.387(9)
C(155)	C(156)	1.405(7)			
C(200)	C(201)	1.428(7)			
C(200)	C(204)	1.423(8)			
C(200)	C(205)	1.503(8)			
C(201)	C(202)	1.439(7)			
C(201)	C(206)	1.502(8)			
C(202)	C(203)	1.416(8)			
C(202)	C(207)	1.508(8)			
C(203)	C(204)	1.423(7)			
C(203)	C(208)	1.518(8)			
C(204)	C(209)	1.504(8)			
C(211)	C(212)	1.532(6)			
C(221)	C(222)	1.401(7)			
C(221)	C(226)	1.395(7)			
C(222)	C(223)	1.394(7)			

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**·CH_2Cl_2.

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
P(1)	Fe(1)	P(2)	85.81(4)	P(4)	Fe(2)	C(200)	100.2(1)
P(1)	Fe(1)	C(17)	82.2(1)	P(4)	Fe(2)	C(201)	121.9(2)
P(1)	Fe(1)	C(100)	111.0(1)	P(4)	Fe(2)	C(202)	161.7(2)
P(1)	Fe(1)	C(101)	147.9(1)	P(4)	Fe(2)	C(203)	147.8(1)
P(1)	Fe(1)	C(102)	159.6(1)	P(4)	Fe(2)	C(204)	112.0(1)
P(1)	Fe(1)	C(103)	120.6(1)	C(27)	Fe(2)	C(200)	118.0(2)
P(1)	Fe(1)	C(104)	99.1(1)	C(27)	Fe(2)	C(201)	86.2(2)
P(2)	Fe(1)	C(17)	88.5(1)	C(27)	Fe(2)	C(202)	91.1(2)
P(2)	Fe(1)	C(100)	163.2(1)	C(27)	Fe(2)	C(203)	127.5(2)
P(2)	Fe(1)	C(101)	124.2(1)	C(27)	Fe(2)	C(204)	151.5(2)
P(2)	Fe(1)	C(102)	98.7(1)	C(200)	Fe(2)	C(201)	39.2(2)
P(2)	Fe(1)	C(103)	106.5(1)	C(200)	Fe(2)	C(202)	66.2(2)
P(2)	Fe(1)	C(104)	141.5(1)	C(200)	Fe(2)	C(203)	65.2(2)
C(17)	Fe(1)	C(100)	92.8(2)	C(200)	Fe(2)	C(204)	38.7(2)
C(17)	Fe(1)	C(101)	87.0(2)	C(201)	Fe(2)	C(202)	39.9(2)
C(17)	Fe(1)	C(102)	117.6(2)	C(201)	Fe(2)	C(203)	65.6(2)
C(17)	Fe(1)	C(103)	152.8(2)	C(201)	Fe(2)	C(204)	65.4(2)
C(17)	Fe(1)	C(104)	130.0(2)	C(202)	Fe(2)	C(203)	39.1(2)
C(100)	Fe(1)	C(101)	39.3(2)	C(202)	Fe(2)	C(204)	65.7(2)
C(100)	Fe(1)	C(102)	65.9(2)	C(203)	Fe(2)	C(204)	38.8(2)
C(100)	Fe(1)	C(103)	66.3(2)	C(11)	S(1)	C(14)	93.5(2)
C(100)	Fe(1)	C(104)	39.7(2)	C(21)	S(2)	C(24)	93.4(2)
C(101)	Fe(1)	C(102)	39.1(2)	Fe(1)	P(1)	C(111)	107.0(1)
C(101)	Fe(1)	C(103)	65.7(2)	Fe(1)	P(1)	C(121)	119.0(1)
C(101)	Fe(1)	C(104)	65.5(2)	Fe(1)	P(1)	C(131)	123.8(1)
C(102)	Fe(1)	C(103)	39.0(2)	C(111)	P(1)	C(121)	104.3(2)
C(102)	Fe(1)	C(104)	65.1(2)	C(111)	P(1)	C(131)	101.3(2)
C(103)	Fe(1)	C(104)	38.9(2)	C(121)	P(1)	C(131)	98.8(2)
P(3)	Fe(2)	P(4)	86.10(5)	Fe(1)	P(2)	C(112)	109.7(1)
P(3)	Fe(2)	C(27)	84.9(1)	Fe(1)	P(2)	C(141)	118.8(1)
P(3)	Fe(2)	C(200)	156.5(1)	Fe(1)	P(2)	C(151)	121.5(1)
P(3)	Fe(2)	C(201)	149.6(1)	C(112)	P(2)	C(141)	102.8(2)
P(3)	Fe(2)	C(202)	111.3(1)	C(112)	P(2)	C(151)	100.4(2)
P(3)	Fe(2)	C(203)	97.6(2)	C(141)	P(2)	C(151)	100.7(2)
P(3)	Fe(2)	C(204)	118.0(2)	Fe(2)	P(3)	C(211)	107.0(2)
P(4)	Fe(2)	C(27)	84.6(1)	Fe(2)	P(3)	C(221)	119.3(2)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**·CH_2Cl_2. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
Fe(2)	P(3)	C(231)	123.7(2)	C(12)	C(11)	C(15)	129.9(4)
C(211)	P(3)	C(221)	103.9(2)	C(1)	C(12)	C(11)	123.4(4)
C(211)	P(3)	C(231)	99.6(2)	C(1)	C(12)	C(13)	123.0(4)
C(221)	P(3)	C(231)	100.3(2)	C(11)	C(12)	C(13)	113.4(4)
Fe(2)	P(4)	C(212)	108.9(2)	C(12)	C(13)	C(14)	113.6(4)
Fe(2)	P(4)	C(241)	116.6(2)	S(1)	C(14)	C(13)	109.5(3)
Fe(2)	P(4)	C(251)	124.8(2)	S(1)	C(14)	C(16)	121.0(3)
C(212)	P(4)	C(241)	104.1(2)	C(13)	C(14)	C(16)	129.4(4)
C(212)	P(4)	C(251)	99.3(2)	C(14)	C(16)	C(17)	175.5(4)
C(241)	P(4)	C(251)	100.4(2)	Fe(1)	C(17)	C(16)	175.8(4)
C(2)	C(1)	C(5)	111.2(3)	S(2)	C(21)	C(22)	109.4(3)
C(2)	C(1)	C(12)	128.8(4)	S(2)	C(21)	C(25)	120.1(4)
C(5)	C(1)	C(12)	119.8(3)	C(22)	C(21)	C(25)	130.4(4)
C(1)	C(2)	C(3)	110.8(3)	C(2)	C(22)	C(21)	122.9(4)
C(1)	C(2)	C(22)	128.9(4)	C(2)	C(22)	C(23)	123.2(4)
C(3)	C(2)	C(22)	120.3(3)	C(21)	C(22)	C(23)	113.9(4)
F(1)	C(3)	F(2)	105.9(4)	C(22)	C(23)	C(24)	113.7(4)
F(1)	C(3)	C(2)	113.6(4)	S(2)	C(24)	C(23)	109.5(3)
F(1)	C(3)	C(4)	111.4(4)	S(2)	C(24)	C(26)	119.7(3)
F(2)	C(3)	C(2)	111.1(4)	C(23)	C(24)	C(26)	130.7(4)
F(2)	C(3)	C(4)	109.3(4)	C(24)	C(26)	C(27)	176.4(5)
C(2)	C(3)	C(4)	105.6(3)	Fe(2)	C(27)	C(26)	176.0(4)
F(3)	C(4)	F(4)	105.1(4)	Fe(1)	C(100)	C(101)	71.3(2)
F(3)	C(4)	C(3)	108.9(4)	Fe(1)	C(100)	C(104)	71.3(2)
F(3)	C(4)	C(5)	108.9(4)	Fe(1)	C(100)	C(105)	126.6(3)
F(4)	C(4)	C(3)	115.1(5)	C(101)	C(100)	C(104)	107.5(4)
F(4)	C(4)	C(5)	113.3(4)	C(101)	C(100)	C(105)	125.9(4)
C(3)	C(4)	C(5)	105.4(3)	C(104)	C(100)	C(105)	126.3(4)
F(5)	C(5)	F(6)	104.2(4)	Fe(1)	C(101)	C(100)	69.5(2)
F(5)	C(5)	C(1)	113.0(4)	Fe(1)	C(101)	C(102)	70.5(2)
F(5)	C(5)	C(4)	109.7(4)	Fe(1)	C(101)	C(106)	130.2(3)
F(6)	C(5)	C(1)	113.0(4)	C(100)	C(101)	C(102)	107.9(4)
F(6)	C(5)	C(4)	111.8(4)	C(100)	C(101)	C(106)	125.1(4)
C(1)	C(5)	C(4)	105.4(3)	C(102)	C(101)	C(106)	126.7(4)
S(1)	C(11)	C(12)	110.0(3)	Fe(1)	C(102)	C(101)	70.4(2)
S(1)	C(11)	C(15)	120.0(3)	Fe(1)	C(102)	C(103)	70.7(2)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**·CH_2Cl_2. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
Fe(1)	C(102)	C(107)	132.1(3)	C(142)	C(141)	C(146)	118.4(4)
C(101)	C(102)	C(103)	108.6(4)	C(141)	C(142)	C(143)	120.7(4)
C(101)	C(102)	C(107)	126.1(5)	C(142)	C(143)	C(144)	119.8(5)
C(103)	C(102)	C(107)	124.6(5)	C(143)	C(144)	C(145)	119.7(5)
Fe(1)	C(103)	C(102)	70.3(2)	C(144)	C(145)	C(146)	119.9(5)
Fe(1)	C(103)	C(104)	70.6(2)	C(141)	C(146)	C(145)	121.4(4)
Fe(1)	C(103)	C(108)	133.4(3)	P(2)	C(151)	C(152)	119.0(3)
C(102)	C(103)	C(104)	107.6(4)	P(2)	C(151)	C(156)	122.2(3)
C(102)	C(103)	C(108)	124.4(4)	C(152)	C(151)	C(156)	118.8(4)
C(104)	C(103)	C(108)	127.0(4)	C(151)	C(152)	C(153)	120.5(4)
Fe(1)	C(104)	C(100)	69.0(2)	C(152)	C(153)	C(154)	119.8(5)
Fe(1)	C(104)	C(103)	70.6(2)	C(153)	C(154)	C(155)	120.7(5)
Fe(1)	C(104)	C(109)	134.4(3)	C(154)	C(155)	C(156)	119.6(5)
C(100)	C(104)	C(103)	108.3(4)	C(151)	C(156)	C(155)	120.5(4)
C(100)	C(104)	C(109)	124.1(4)	Fe(2)	C(200)	C(201)	69.6(3)
C(103)	C(104)	C(109)	126.8(4)	Fe(2)	C(200)	C(204)	71.1(3)
P(1)	C(111)	C(112)	106.7(3)	Fe(2)	C(200)	C(205)	132.8(4)
P(2)	C(112)	C(111)	110.2(3)	C(201)	C(200)	C(204)	108.1(4)
P(1)	C(121)	C(122)	121.3(3)	C(201)	C(200)	C(205)	127.1(5)
P(1)	C(121)	C(126)	120.0(3)	C(204)	C(200)	C(205)	124.0(4)
C(122)	C(121)	C(126)	118.6(3)	Fe(2)	C(201)	C(200)	71.2(3)
C(121)	C(122)	C(123)	120.4(4)	Fe(2)	C(201)	C(202)	69.3(3)
C(122)	C(123)	C(124)	120.1(4)	Fe(2)	C(201)	C(206)	128.2(4)
C(123)	C(124)	C(125)	120.4(4)	C(200)	C(201)	C(202)	107.7(4)
C(124)	C(125)	C(126)	120.4(4)	C(200)	C(201)	C(206)	126.8(5)
C(121)	C(126)	C(125)	120.0(4)	C(202)	C(201)	C(206)	125.4(5)
P(1)	C(131)	C(132)	120.8(3)	Fe(2)	C(202)	C(201)	70.8(3)
P(1)	C(131)	C(136)	121.3(3)	Fe(2)	C(202)	C(203)	71.6(3)
C(132)	C(131)	C(136)	118.0(4)	Fe(2)	C(202)	C(207)	126.7(4)
C(131)	C(132)	C(133)	121.2(4)	C(201)	C(202)	C(203)	107.5(4)
C(132)	C(133)	C(134)	120.4(5)	C(201)	C(202)	C(207)	126.0(5)
C(133)	C(134)	C(135)	119.4(4)	C(203)	C(202)	C(207)	126.3(5)
C(134)	C(135)	C(136)	120.4(5)	Fe(2)	C(203)	C(202)	69.3(3)
C(131)	C(136)	C(135)	120.5(4)	Fe(2)	C(203)	C(204)	71.4(3)
P(2)	C(141)	C(142)	120.3(3)	Fe(2)	C(203)	C(208)	133.1(4)
P(2)	C(141)	C(146)	121.2(3)	C(202)	C(203)	C(204)	108.8(5)

Table S3. Interatomic distances (Å) and bond angles (deg) for **2**·CH_2Cl_2. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
C(202)	C(203)	C(208)	124.8(5)	C(252)	C(251)	C(256)	118.7(5)
C(204)	C(203)	C(208)	125.7(5)	C(251)	C(252)	C(253)	120.2(5)
Fe(2)	C(204)	C(200)	70.1(3)	C(252)	C(253)	C(254)	120.2(6)
Fe(2)	C(204)	C(203)	69.7(3)	C(253)	C(254)	C(255)	119.7(6)
Fe(2)	C(204)	C(209)	136.8(4)	C(254)	C(255)	C(256)	120.7(7)
C(200)	C(204)	C(203)	107.9(4)	C(251)	C(256)	C(255)	120.4(6)
C(200)	C(204)	C(209)	124.3(5)	Cl(1)	C(300)	Cl(2)	107.5(6)
C(203)	C(204)	C(209)	126.2(5)				
P(3)	C(211)	C(212)	105.7(3)				
P(4)	C(212)	C(211)	109.5(3)				
P(3)	C(221)	C(222)	121.0(4)				
P(3)	C(221)	C(226)	121.2(4)				
C(222)	C(221)	C(226)	117.7(4)				
C(221)	C(222)	C(223)	120.3(5)				
C(222)	C(223)	C(224)	120.6(5)				
C(223)	C(224)	C(225)	119.9(5)				
C(224)	C(225)	C(226)	120.4(6)				
C(221)	C(226)	C(225)	121.2(5)				
P(3)	C(231)	C(232)	121.0(4)				
P(3)	C(231)	C(236)	120.3(4)				
C(232)	C(231)	C(236)	118.6(5)				
C(231)	C(232)	C(233)	121.6(6)				
C(232)	C(233)	C(234)	119.6(6)				
C(233)	C(234)	C(235)	121.4(7)				
C(234)	C(235)	C(236)	119.7(6)				
C(231)	C(236)	C(235)	119.1(6)				
P(4)	C(241)	C(242)	124.0(5)				
P(4)	C(241)	C(246)	118.3(4)				
C(242)	C(241)	C(246)	117.6(5)				
C(241)	C(242)	C(243)	121.3(7)				
C(242)	C(243)	C(244)	119.9(7)				
C(243)	C(244)	C(245)	120.0(7)				
C(244)	C(245)	C(246)	119.5(7)				
C(241)	C(246)	C(245)	121.6(6)				
P(4)	C(251)	C(252)	117.1(4)				
P(4)	C(251)	C(256)	124.1(4)				

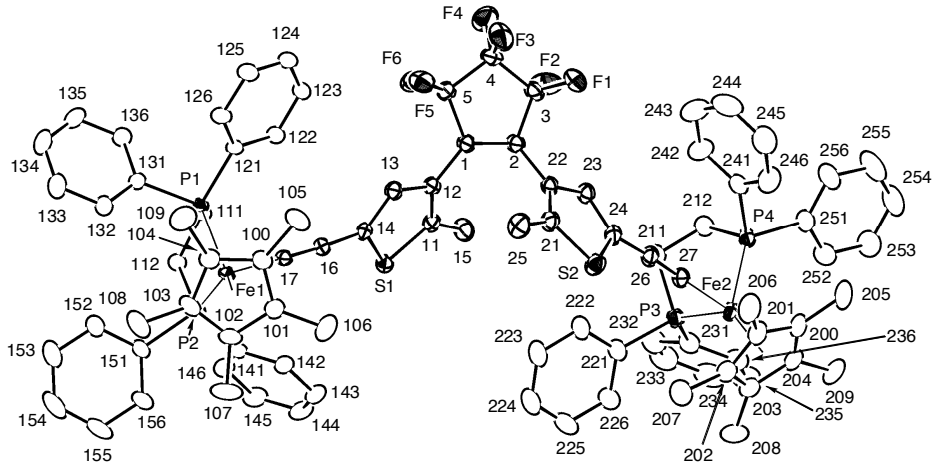

Figure S1. Atomic numbering scheme for **2**·CH_2Cl_2. Labels without atom names are for carbon atoms.

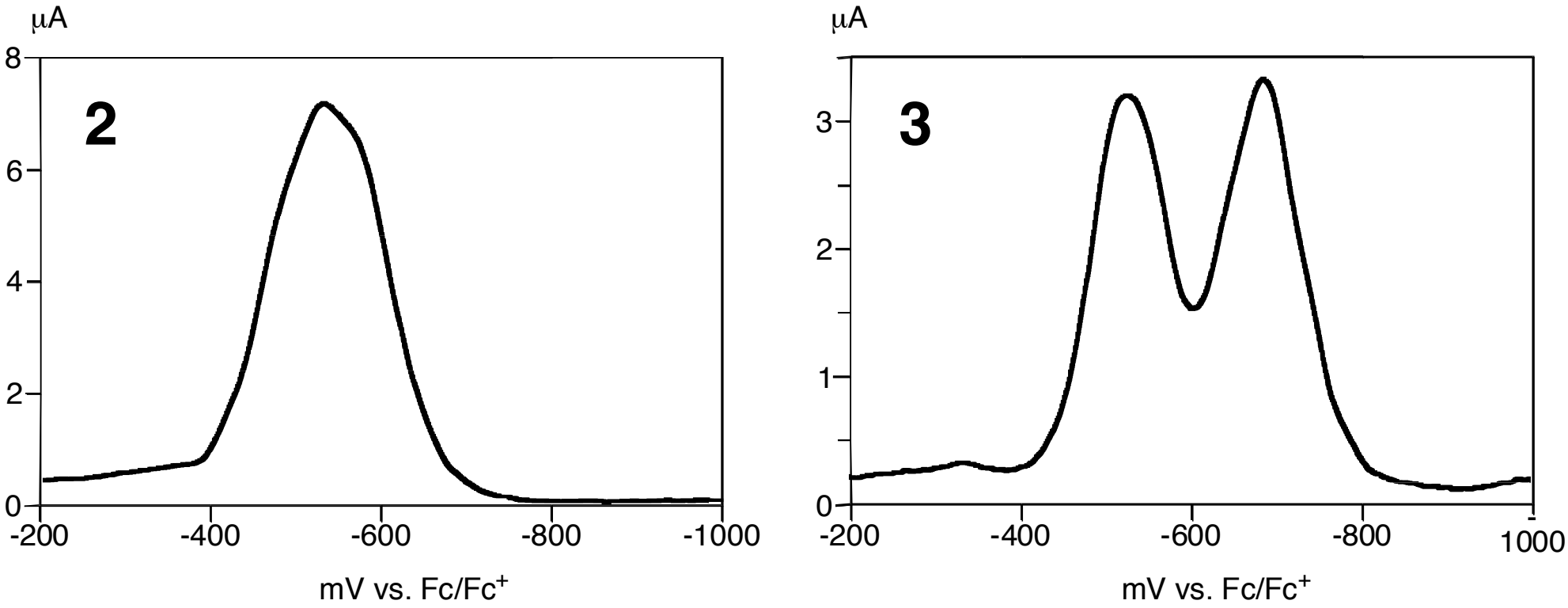

Figure S2. DPV traces for **2** and **3**. (the reduction processes)

[**2**]= 1.3 x 10^{-3} M, [**3**]= 6.4 x 10^{-4} M in CH_2Cl_2; for other measurement conditions see footnote ⊥.