Coupling Multiple Benzylic Activation of Simple Arenes by $CpFe^+$ with Multiple Alkene Metathesis using Grubb's Catalysts, An Efficient Carbon-Carbon Formation Strategy Leading to Polycycles, Cyclophanes, Capsules and Polymeric Compounds and their $CpFe^+$ Complexes.

Victor Martinez,[a] Jean-Claude Blais,[b] George Bravic,[c] Didier Astruc* [a]

SUPPLEMENTARY INFORMATION

Index

Experimental Section

Examples of ligand exchange reactions between ferrocene and arenes for the synthesis of the mono-and dinuclear complexes of the type [FeCp(η^6-arene)][PF_6] (compounds 3, 36, 39 and 44):

Compound **3**: ferrocene (14 g; 75 mmol), aluminium powder (2.0 g; 75 mmol) and aluminium trichloride (40 g; 300 mmol) were heated under N_2 in 150 mL of ethylbenzene at 100°C for 1h. 1.35 mL of H_2O was slowly added at RT, and the mixture was heated at 110°C for 24h, and hydrolyzed with 250 mL ice water. The aqueous solution was filtered over celite, decanted, washed with ether (3 x 200 mL) and, after addition of ammonia to *pH* 9, filtered off. A yellow precipitated was obtained from the solution upon metathesis using aqueous HPF_6. This precipitate was washed with ether and pentane, dissolved in 100 mL of acetonitrile and filtered over Al_2O_3. Addition of ethanol and removal of acetonitrile yielded [CpFe(η^6-C_6H_5Et)][PF_6] as a yellow solid (17 g; 63% yield). ^{1}H NMR (250 MHz, $CDCl_3$), δ_{ppm}: 6.30 and 6.22 (m, 5H, CH aromatic), 5.05 (s, 5H, cyclopentadienyl), 2.80 (c, J = 7.5 Hz, 2H, CH_2 aliphatic), 1.35 (t, J = 7.5Hz, 3H, CH_3 aliphatic).

Compound **36**: in a 250 mL three-necked round bottomed flask equipped with a nitrogen inlet and a reflux condenser topped with a gas outlet, a mixture of ferrocene (18.6 g; 100 mmol), aluminum trichloride (13.3 g; 100 mmol), aluminum powder (0.540 g; 20 mmol) and 3,3',5,5'-tetramethylbyphenyl (0.420 g; 2 mmol) was stirred for 5 min under Ar and heated in the melt at 120°C during 16h. The reaction mixture was slowly hydrolyzed using 100 mL of degassed ice water, addition of aqueous ammonia until *pH* 9 to precipitate $Al(OH)_3$. After filtration, a yellow solid was obtained by addition of an aqueous HPF_6 solution (10 mmol). The precipitate was filtered, dissolved in 50 mL of acetonitrile and dried over Na_2SO_4. The solution was filtered over Al_20_3. The addition of ethanol followed by slow evaporation of acetonitrile gave a yellow solid (0.393 g; 53% yield). ^{1}H NMR (200 MHz, CD_3CN), δ_{ppm}: 6.66 and 6.33 (s, 6H, CH aromatic), 4.85 (s, 10H, CH Cp) 2.56 (s, 12H, CH_3); ^{13}C NMR (50 MHz, CD_3CN), δ_{ppm}: 105.5, 91.46, 87.0 and 79.4 (aromatic), 80.5 (CH Cp) 21.9 (CH_3 aliphatic); MALDI-TOF calcd. for $C_{21}H_{23}Fe^+$: 331.25, found: 331.22.

Compound **39**: ferrocene (14 g; 75 mmol), aluminium powder (2.0 g; 75 mmol), aluminium trichloride (40 g; 300 mmol) and aniline (6.88 mL; 75 mmol) were heated under N_2 in 100 mL of decaline at 100°C for 1h. 1.35 mL of H_2O was slowly added at RT, and the mixture was heated at reflux for 24 h and hydrolyzed with 250 mL ice water. The aqueous solution was filtered over celite, decanted, washed with ether (3 x 200 mL) and, after addition of ammonia to *pH* 9, filtered off. A yellow product was extracted from the aqueous solution using dichloromethane upon metathesis with aqueous HPF_6. The solution was dried over Na_2SO_4 and evaporated. The solid residue was washed with ether and pentane, dissolved in 100 mL of acetonitrile and filtered over Al_2O_3. Addition of ethanol and removal of acetonitrile yields [CpFe(η^6-C_6H_5Et)][PF_6] as a yellow solid (1.7 g; 9% yield). ^{1}H NMR (250 MHz, acetone-d_6), δ_{ppm}: 6.17, 6.01 and 5.79 (t,t and d J = 6, 5.6 and 6.4 Hz, 5H, CH aromatic), 4.98 (s, 5H, cyclopentadienyl).

Compound **44**: ferrocene (14 g; 75 mmol), aluminium powder (2.0 g; 75 mmol) and aluminium trichloride (40 g; 300 mmol) were heated under N_2 in 150 mL of *p*-diisopropylbenzene at 100°C for 1 h, then the mixture was cooled to RT and 1.35 mL of H_2O was slowly added, then the mixture was heated at 110°C for 24 h, hydrolyzed with 250 mL ice water, the aqueous solution was filtered over celite, decanted, washed with ether (3 x 200 mL) and, after addition of ammonia to *pH* 9, filtered off. A yellow precipitate was obtained from the solution by metathesis with aqueous HPF_6. This precipitate was washed with ether and pentane, dissolved in 100 mL of acetonitrile and filtered over alumina. Addition of ethanol and removal of acetonitrile yielded a dark yellow oil, from which [FeCp(η^6-1,4-$i$$Pr_2C_6H_4$)][$PF_6$] was slowly crystallized giving yellow crystals. ^{1}H NMR (250 MHz, $CDCl_3$), δ_{ppm}: 6.18 (s, 4H, CH aromatic), 4.95 (s, 5H, CH Cp), 3.03 (m, 2H, CH_2 aliphatic), 1.36 (d, J = 6.9Hz, 12H, CH_2 aliphatic); ^{13}C NMR (63 MHz, $CDCl_3$), δ_{ppm}: 113.0 (C aromatic), 85.4 (CH aromatic), 76.8 (CH Cp), 33.0 and 23.3 (CH_2 and CH_3 aliphatic). Anal. calcd for $C_{17}H_{23}FePF_6$: H 5.41, C 47.69, found: H 5.52, C 47.72.

Synthesis and decaallylation of 39 (see also ref. 15)

Compound **39**: *n*-buthyllithium (48.8 mL; 1.6 M) was added to a THF (200 mL) solution of 1,2,3,4,5-pentamethylcyclopentadiene (15.2 g; 78 mmol) at -78°C, and a white solid (C_5Me_5Li) immediately precipitated from solution at RT. The mixture was cooled to -30°C, and $CoCl_2$ (10.1 g; 78 mmol) dissolved in 100 mL THF was slowly added. The reaction mixture was stirred at RT for 30 min and cooled to -10°C, and a THF solution of CpNa (18.1 g; 78 mmol) was added. After 6h, the temperature was raised to RT and the mixture was stirred with C_2Cl_6 for additional 3h. The solvent was then evaporated, the solid residue was dissolved in water, and the aqueous solution was washed with ether. After addition of an aqueous HPF_6 solution, a yellow solid precipitated and was filtered and dried. Recrystallitation from an acetonitrile-ethanol mixture gave **39** as yellow crystals (50% yield). ^1H NMR (250 MHz, acetone-d_6), δ_{ppm}: 5.1 (s, 5H, CH Cp), 2.1 (s, 15H, CH_3).

Compound **40**: allyl bromide (24 g; 200 mmol) was added to a mixture of **39** (2 g; 5 mmol) and KOH (11.1 g; 200 mmol), and the mixture was heated at 110°C for 24 h. The volatiles were evaporated and the residue was dissolved in dichloromethane and washed with water and with an aqueous HPF_6 solution. After drying over Na_2SO_4, the solvent are evaporated, and the residue was washed with pentane to afford **40** as a brown powder (15% yield). ^{13}C NMR (63 MHz, CD_3CN), δ_{ppm}: 134.9 et 136.4 (CH allylic), 117.4 et 116.1 (CH_2 allylic), 107.6 (C Cp), 85.7 (CH Cp), 35.3 (CH aliphatic) and 43.0 et 41.1 (CH_2 aliphatic); MALDI TOF calcd. for $C_{45}H_{60}Co^+$: 659.47, found: 659.28. Anal. calcd for $C_{45}H_{60}CoPF_6$: H 7.52, C 67.13, found: H 7.53, C 67.11.

MALDI-TOF mass spectra

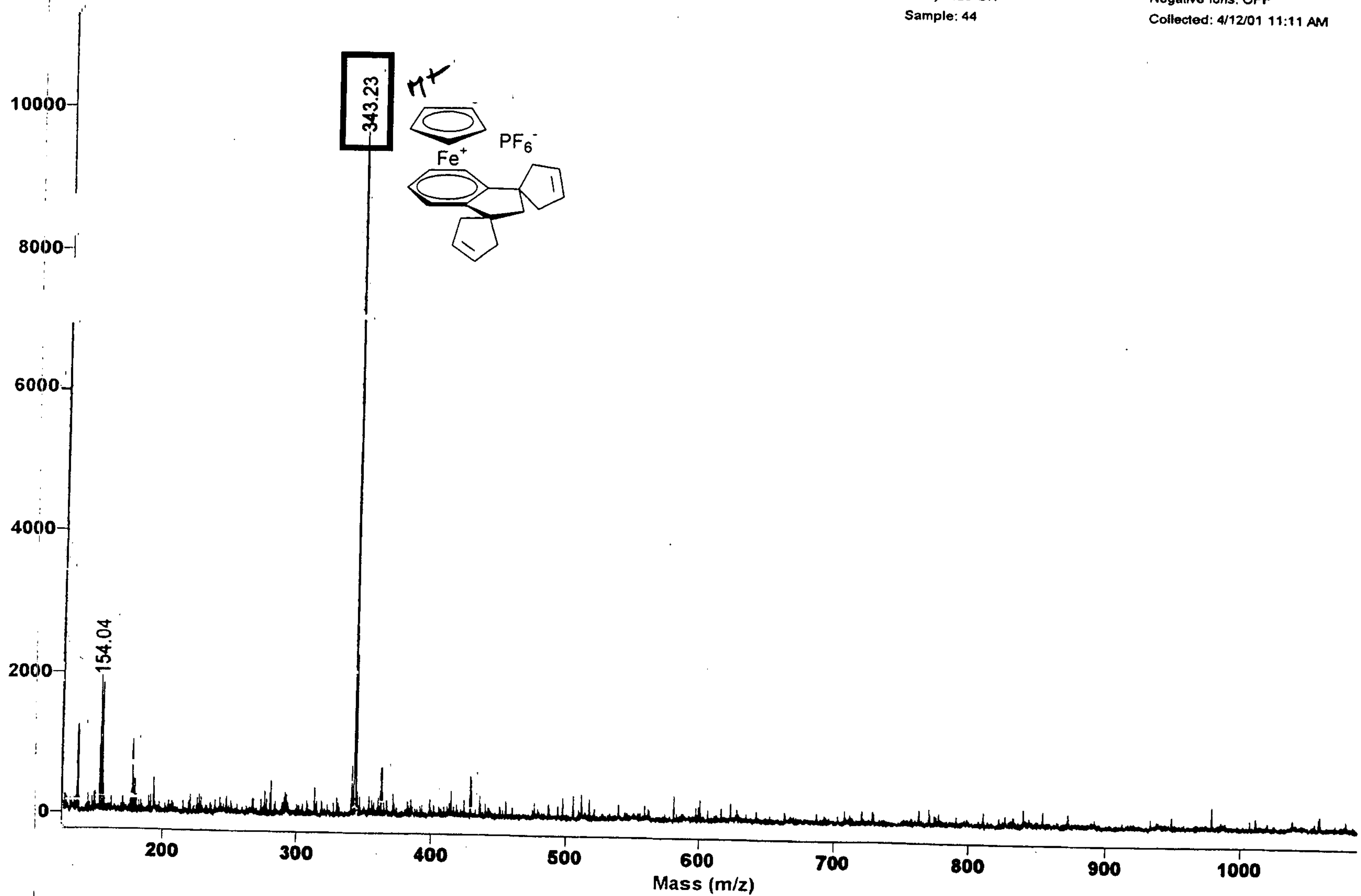
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast1004\12041015.ms
This File # 8 = C:\VOYAGER\DATA\JCB\AST1004\12041015.MS
Comment: 0404- DHB

8

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 44

Laser : 2180
Scans Averaged: 159
Pressure: 5.21e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 4/12/01 11:11 AM



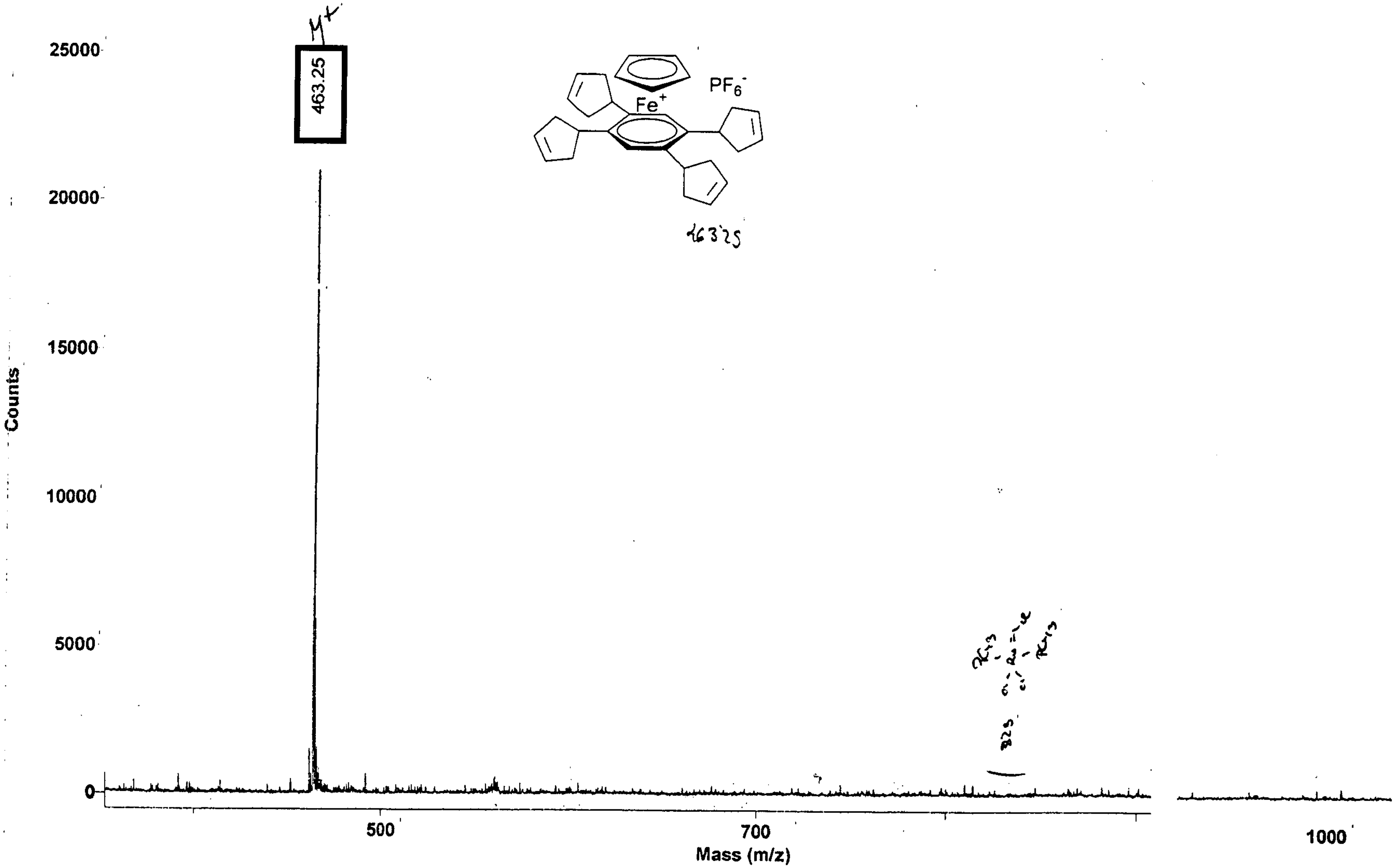
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast1403\27031009.ms
This File #11 = C:\MESDOC~1\JCB4DATA\AST1403\27031009.MS
Comment: V0503 - DHB

11

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 62

Laser : 2020
Scans Averaged: 118
Pressure: 7.41e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 27/03/01 11:15



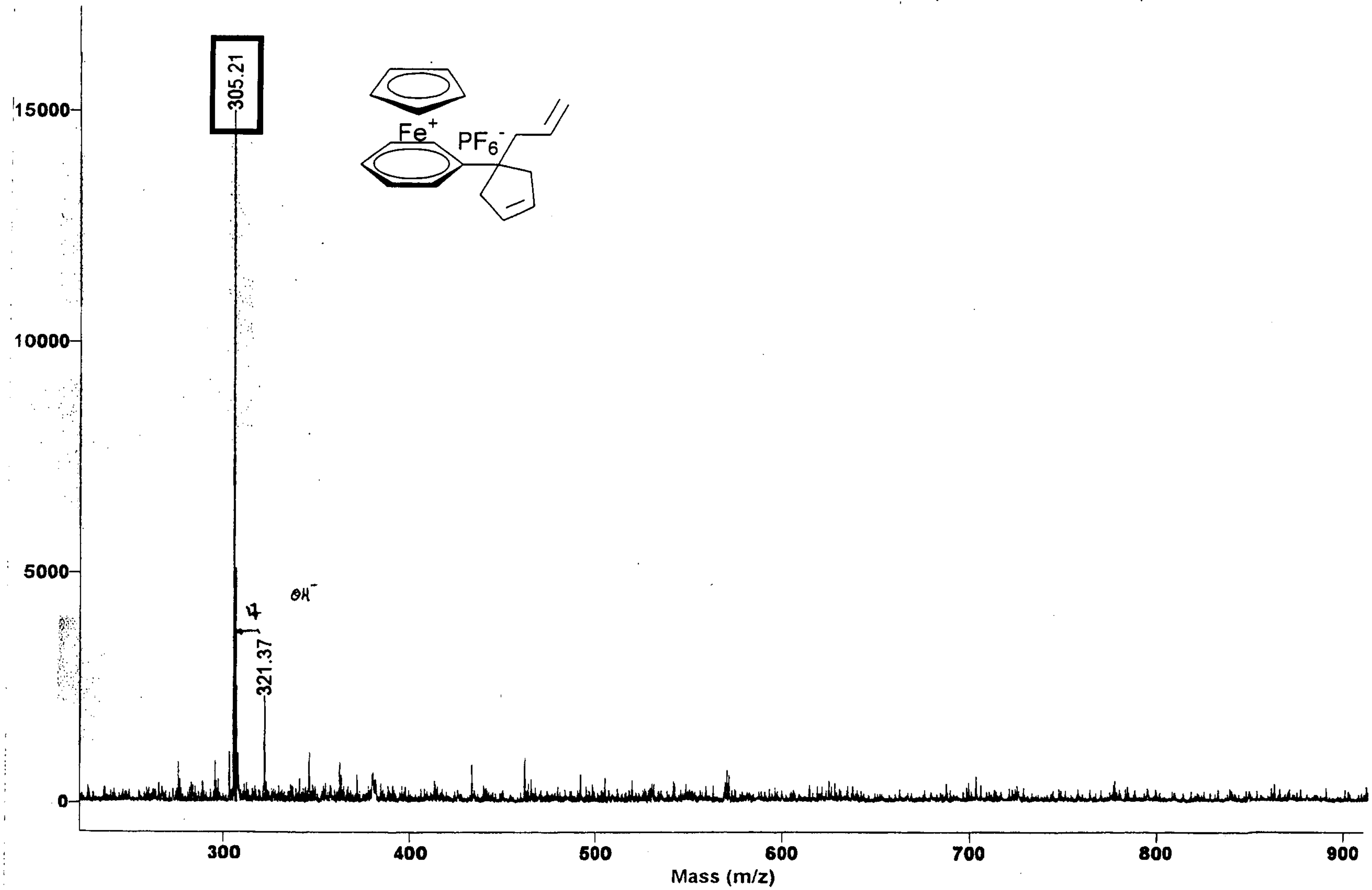
UPMC - LCSOB

Original Filename: c:\voyager\data\jcb\ast2606\28061019.ms
This File # 1 = C:\VOYAGER\DATA\JCB\AST2606\28061019.MS
Comment: MAR 1106 - DHB

16

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 86

Laser : 2320
Scans Averaged: 128
Pressure: 1.32e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 6/28/01 12:24 PM



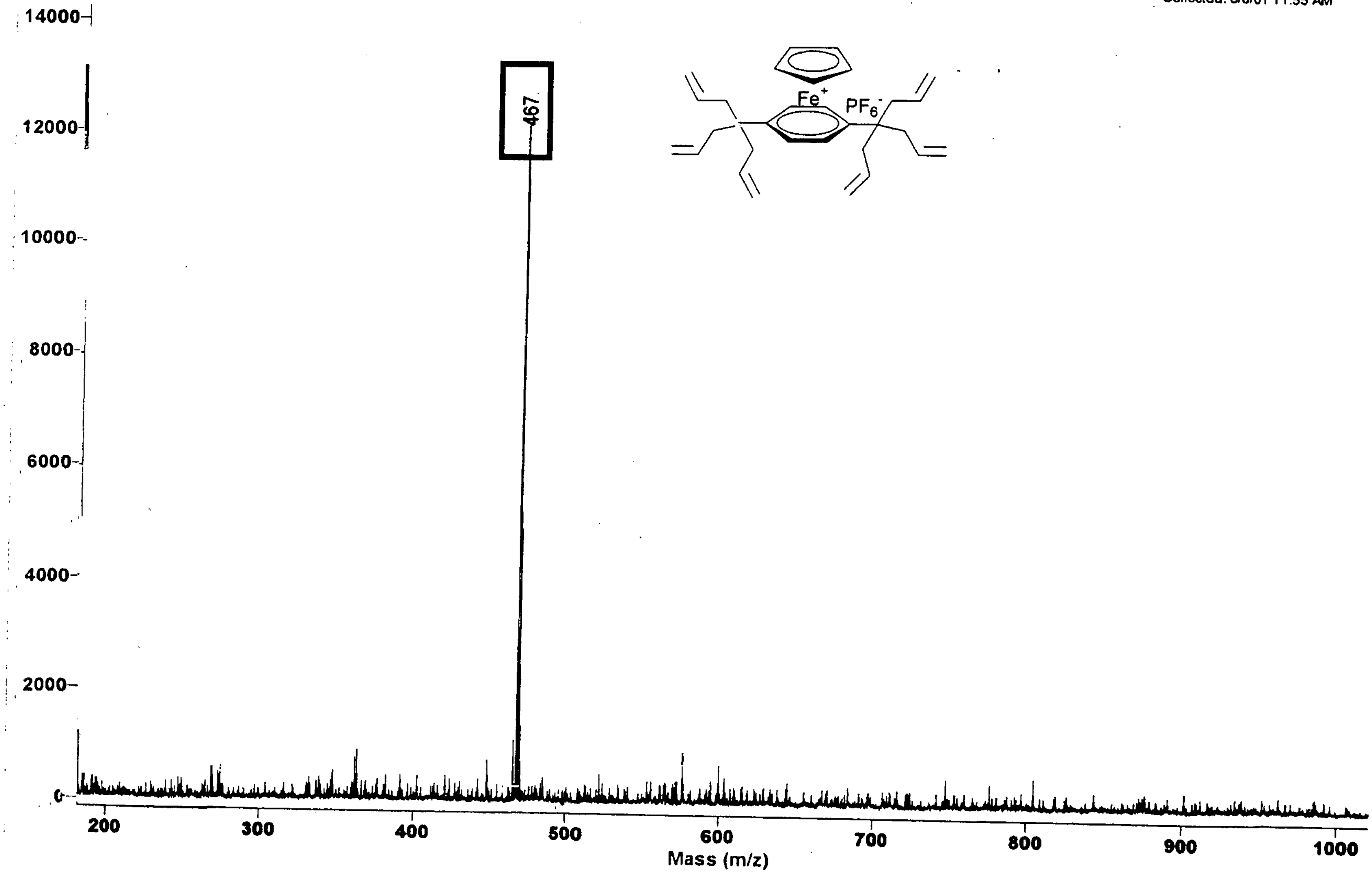
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast2505\08061004.ms
This File # 1 = C:\VOYAGER\DATA\JCB\AST2505\08061004.MS
Comment: HEXA - DHB

22

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 56

Laser : 2240
Scans Averaged: 118
Pressure: 8.86e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 6/8/01 11:55 AM



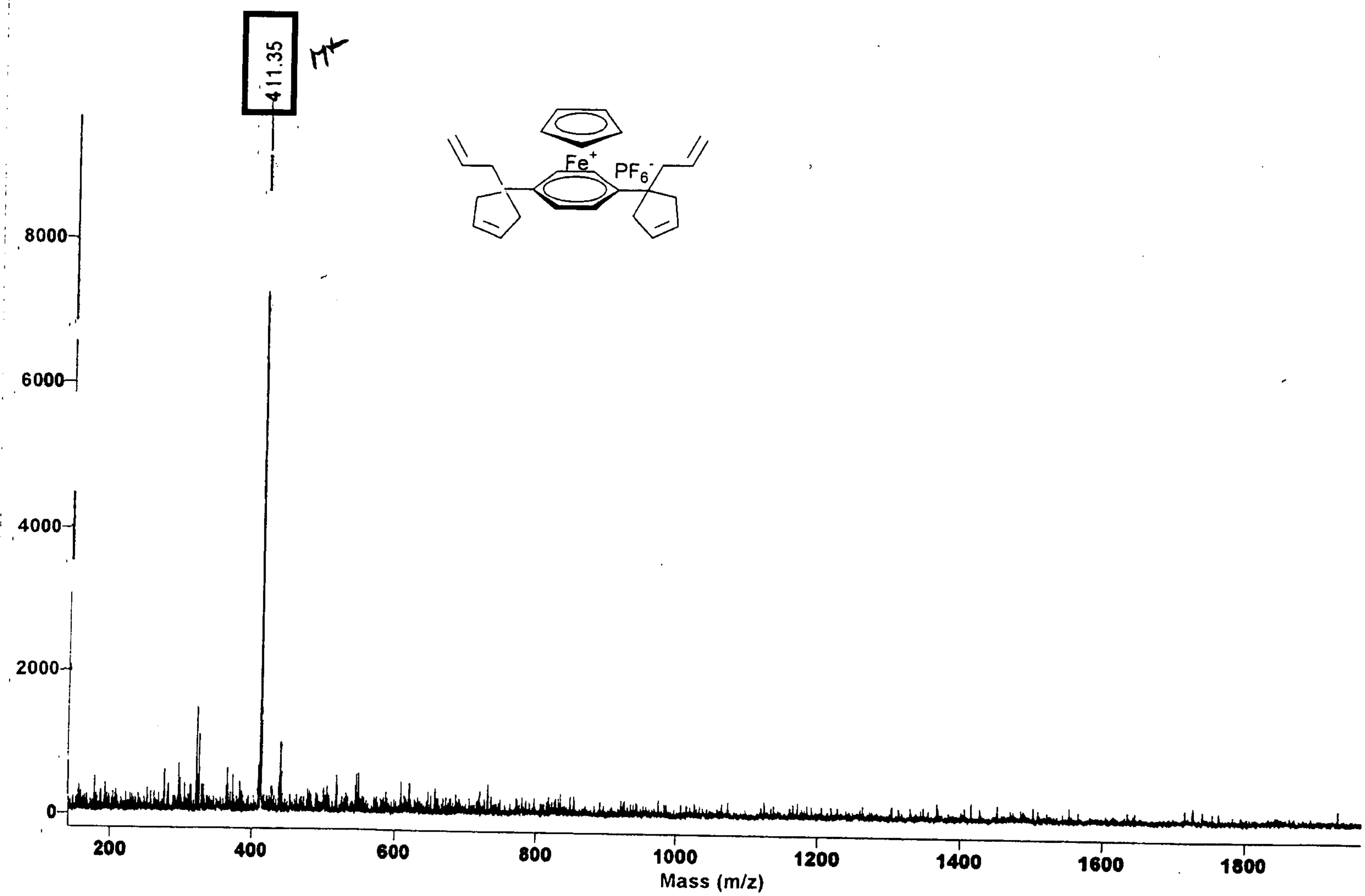
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast1004\12041012.ms
This File # 6 = C:\VOYAGER\DATA\JCB\AST1004\12041012.MS
Comment: 1403-2 - DHB

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 46

Laser : 2180
Scans Averaged: 186
Pressure: 5.39e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 4/12/01 10:52 AM

23



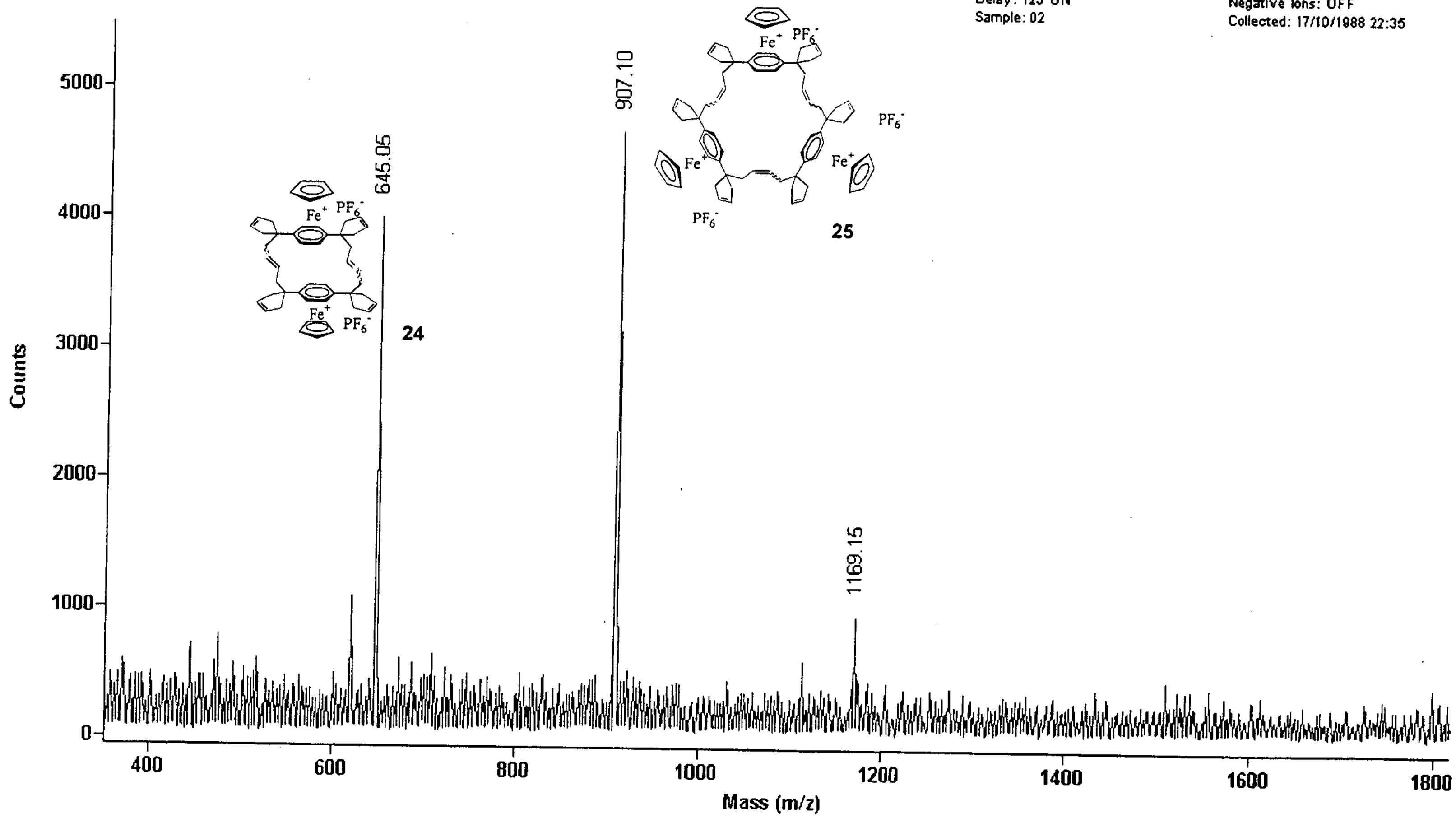
24 and 25

UPMC - LCSOB

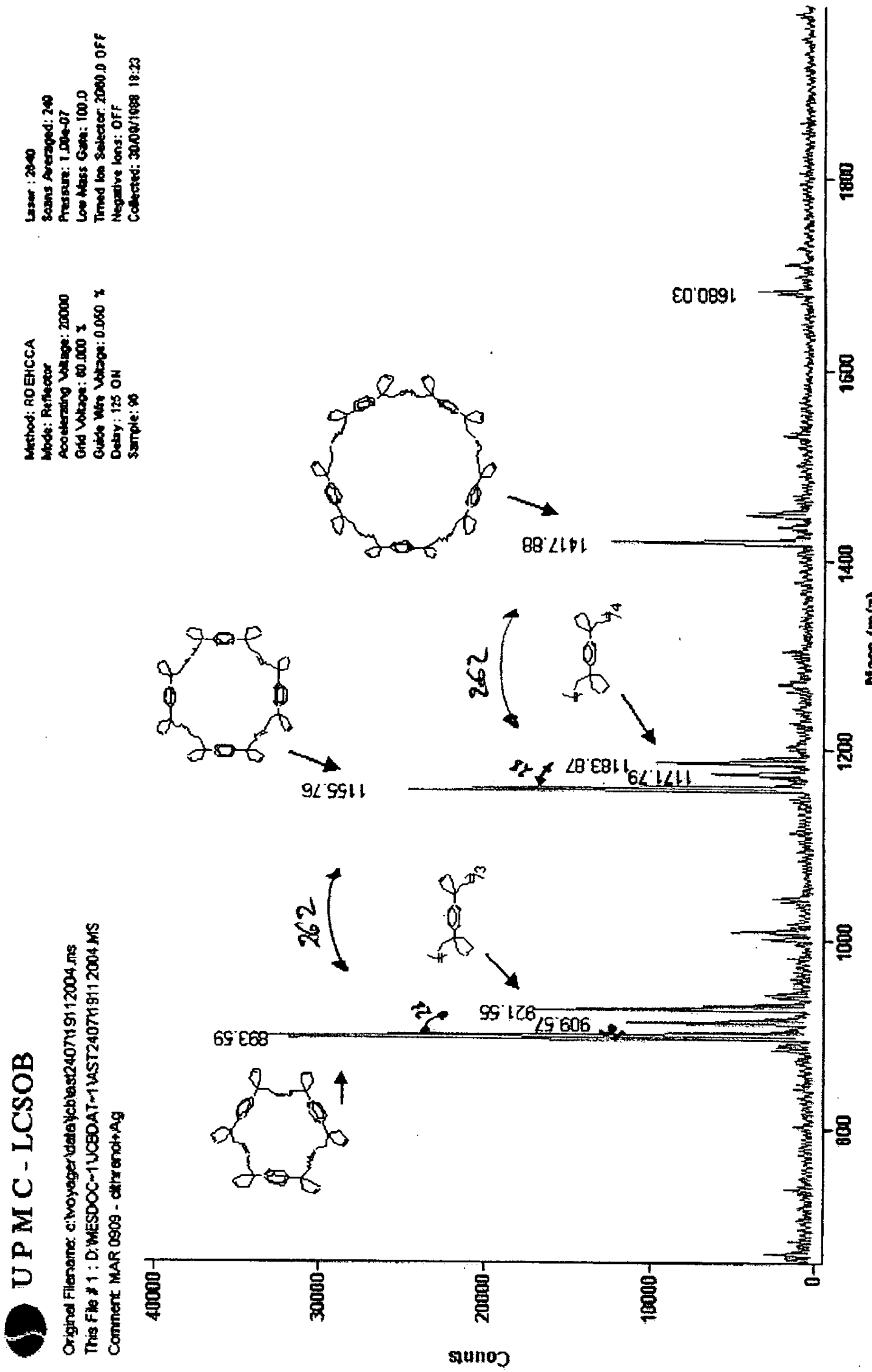
Original Filename: c:\voyager\data\jcb\ast2611\06122037.ms
This File # 1 : D:\MESDOC~1\JCBDAT~1\AST2611\06122037.MS
Comment: 1511 - DHB

Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 02

Laser : 2690
Scans Averaged: 187
Pressure: 2.62e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 17/10/1988 22:35



Metathesis of 26



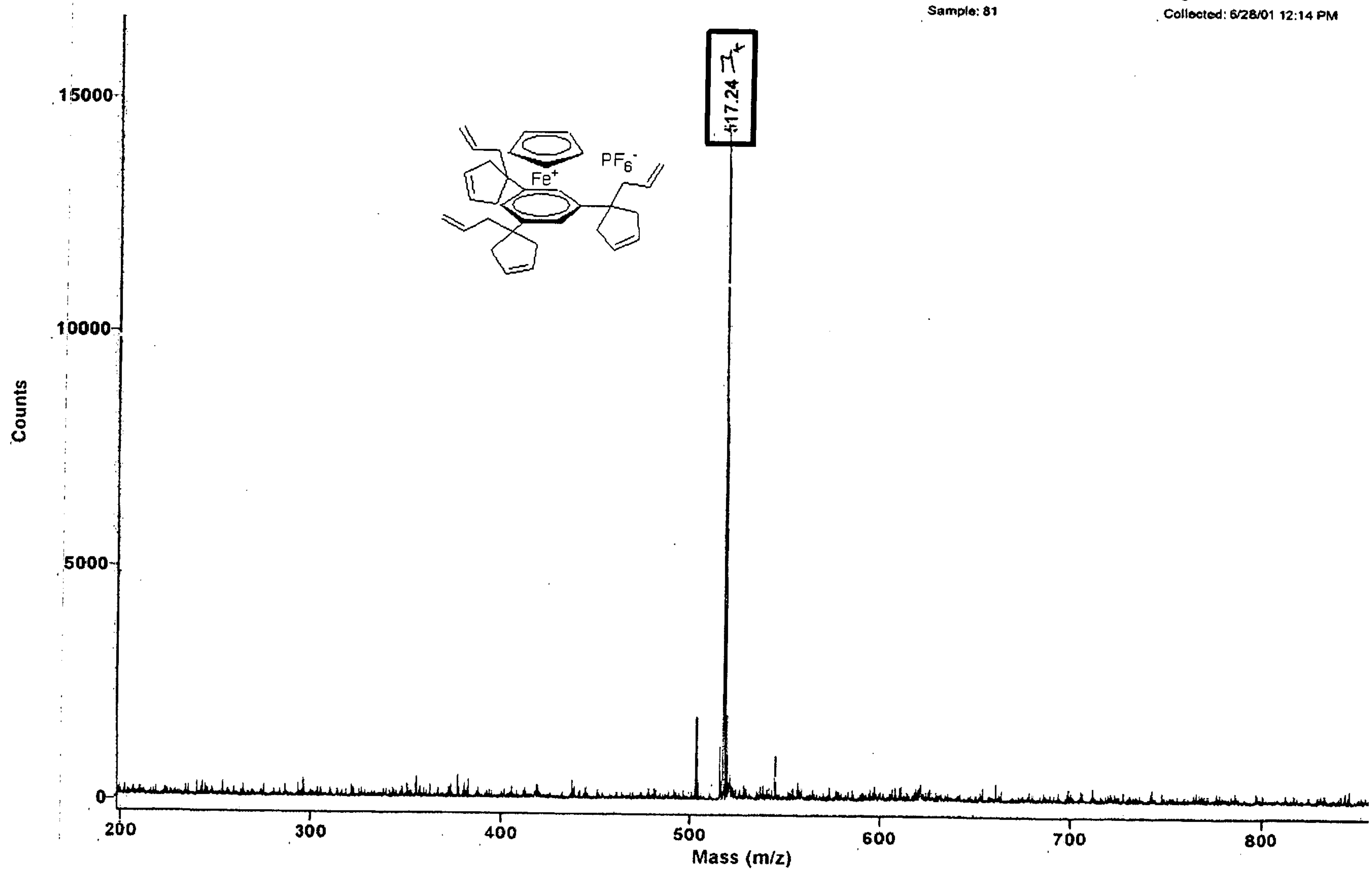
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast2606\28061016.ms
This File # 1 = C:\VOYAGER\DATA\JCB\AST2606\28061016.MS
Comment: MAR 506 - DHB

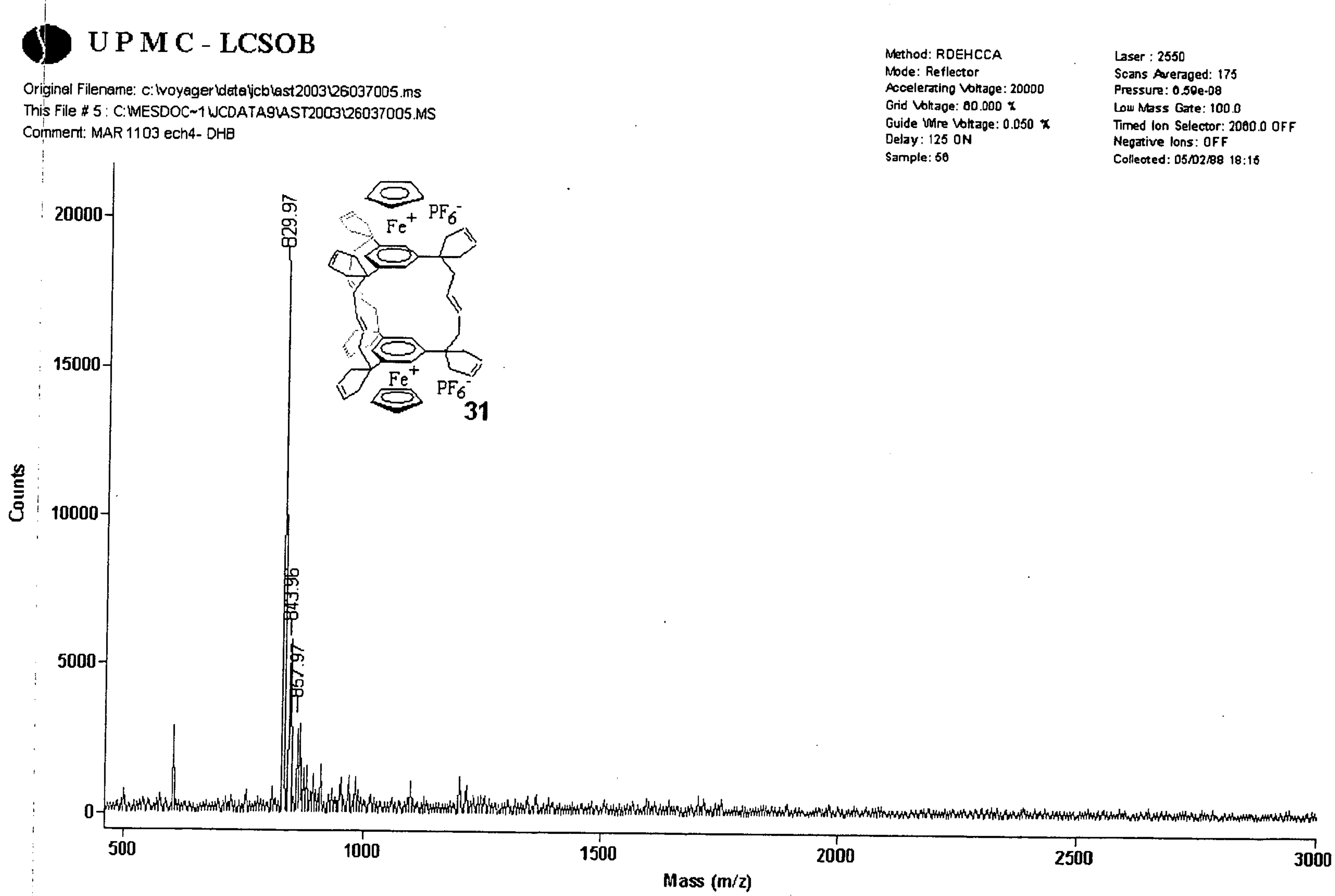
30

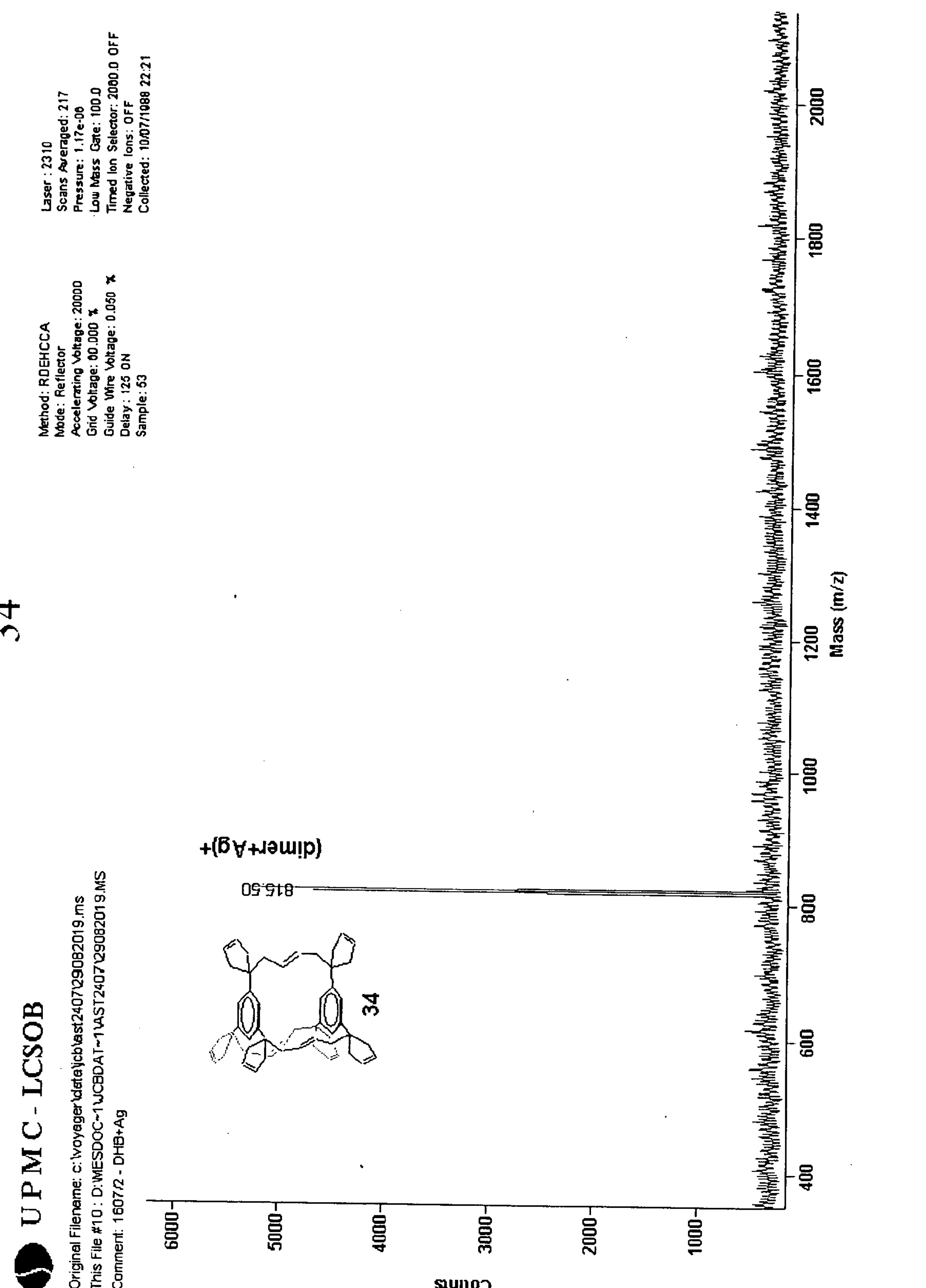
Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 81

Laser : 2280
Scans Averaged: 151
Pressure: 1.83e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 6/28/01 12:14 PM



31


UPMC - LCSOB
Original Filename: c:\voyager\data\jcb\ast2003\26037005.ms
This File # 5 : C:\MESDOC~1\JCDATA9\AST2003\26037005.MS
Comment: MAR 1103 ech4- DHB
Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 80.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 68
Laser : 2550
Scans Averaged: 175
Pressure: 0.59e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 05/02/88 18:16
829.97
843.96
857.97
Fe+
PF6-
31
Counts
20000
15000
10000
5000
0
500
1000
1500
2000
2500
3000
Mass (m/z)


34
UPMC - LCSOB
Original Filename: c:\voyager\data\jcb\ast2407\29082019.ms
This File #10 : D:\MESDOC~1\JCBDAT~1\AST2407\29082019.MS
Comment: 1607/2 - DHB+Ag
Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 80.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 53
Laser : 2310
Scans Averaged: 217
Pressure: 1.17e-06
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 10/07/1988 22:21
815.50
(dimer+Ag)+
34
Counts
6000
5000
4000
3000
2000
1000
400
600
800
1000
1200
1400
1600
1800
2000
Mass (m/z)

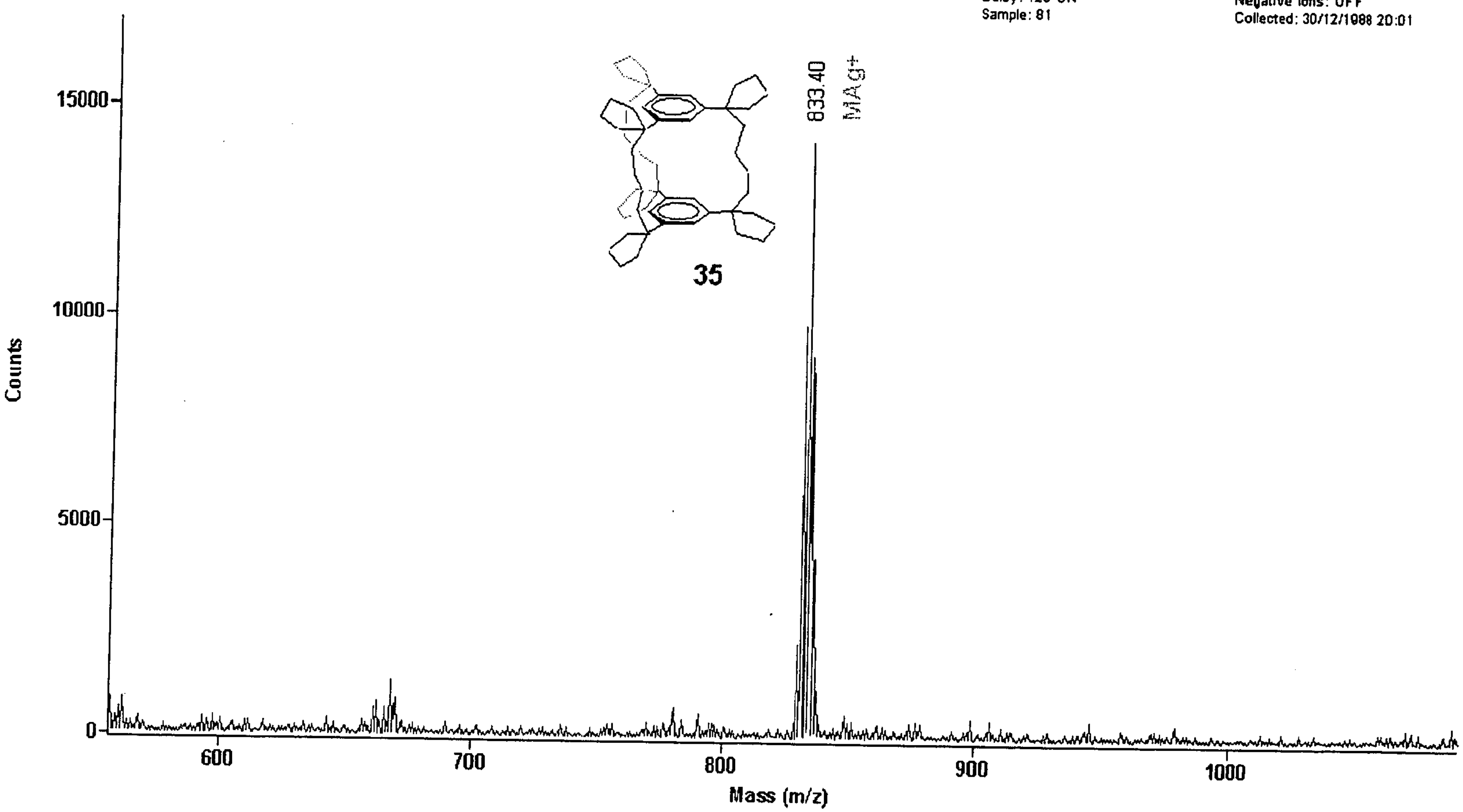
35

UPMC - LCSOB

Original Filename: c:\voyager\data\jcb\ast0601\18023013.ms
This File # 2 : D:\MESDOC~1\JCBDAT~1\AST0601\18023013.MS
Comment: MAR 1009 - dithranol+Ag

Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 80.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 81

Laser : 2300
Scans Averaged: 121
Pressure: 1.82e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2000.0 OFF
Negative Ions: OFF
Collected: 30/12/1988 20:01



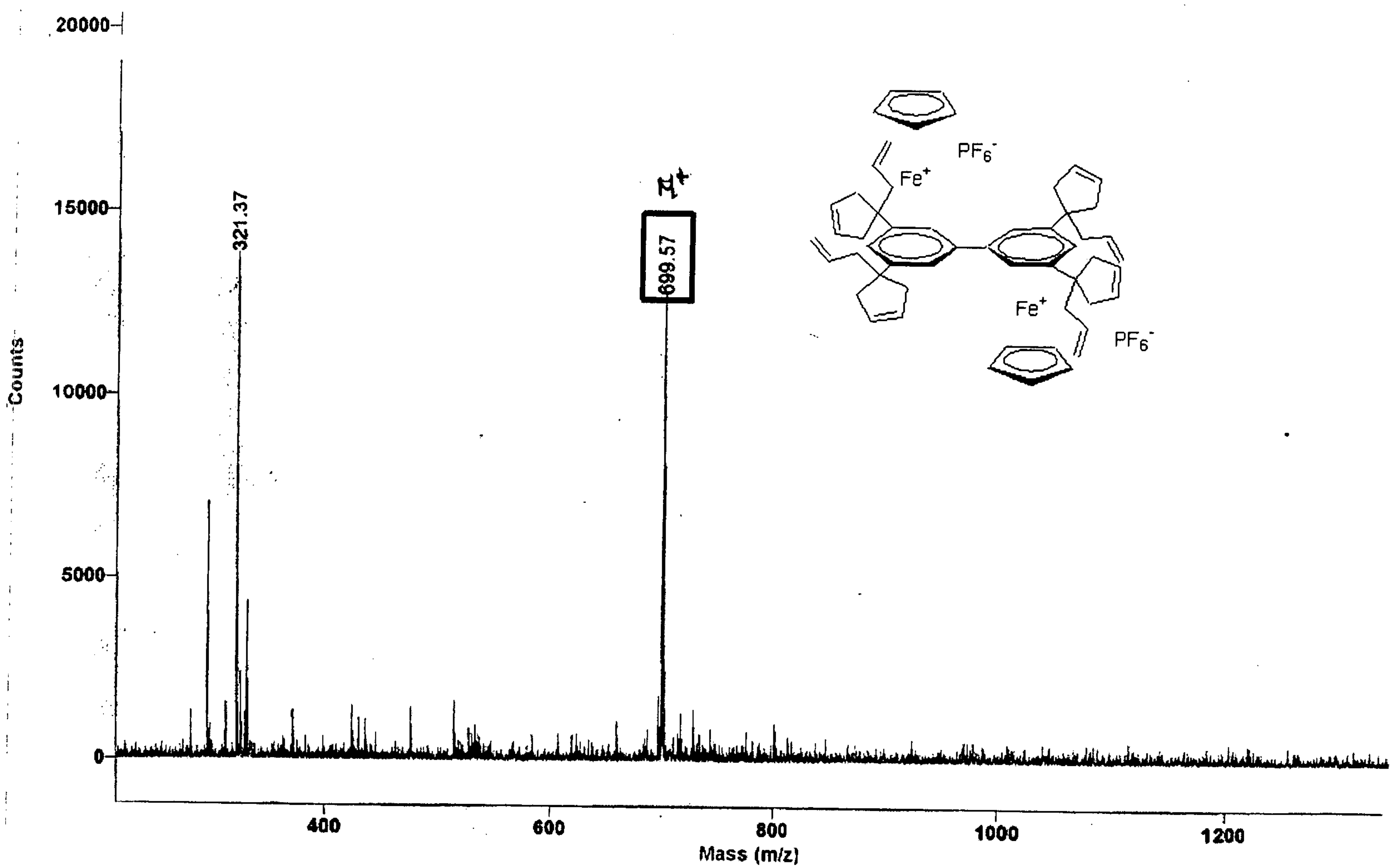
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast2606\28061032.ms
This File # 2 = C:\VOYAGER\DATA\JCB\AST2606\28061032.MS
Comment: MAR 2006 - DHB

38

Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 63

Laser : 2390
Scans Averaged: 136
Pressure: 9.44e-08
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 6/28/01 2:52 PM



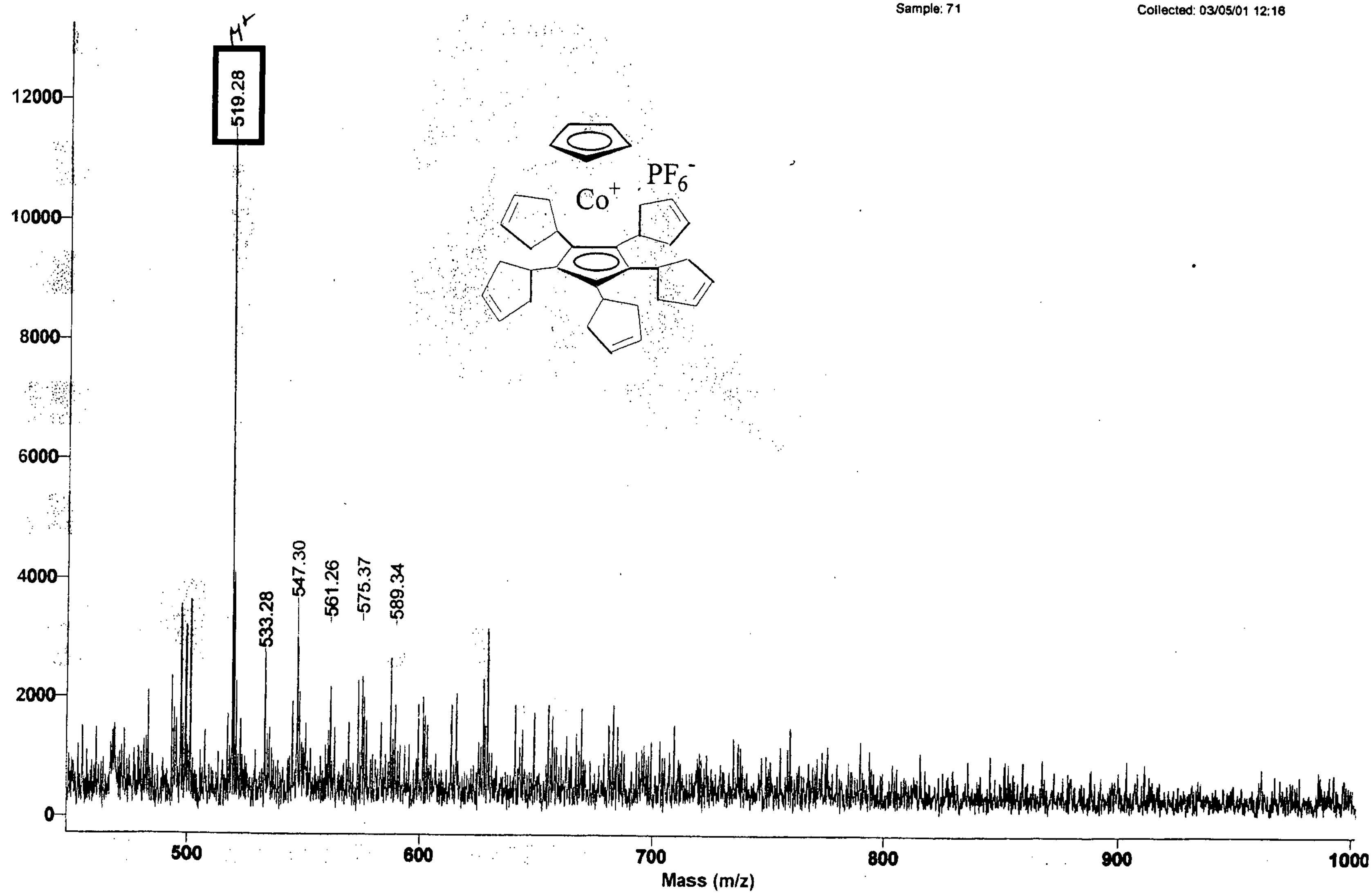
U P M C - LCSOB

Original Filename: c:\voyager\data\jcb\ast1004\03051010.ms
This File # 4 = C:\MESDOC~1\SAV030~1\JCB5DATA\AST1004\03051010.MS
Comment: Martinez 1204 - DHB

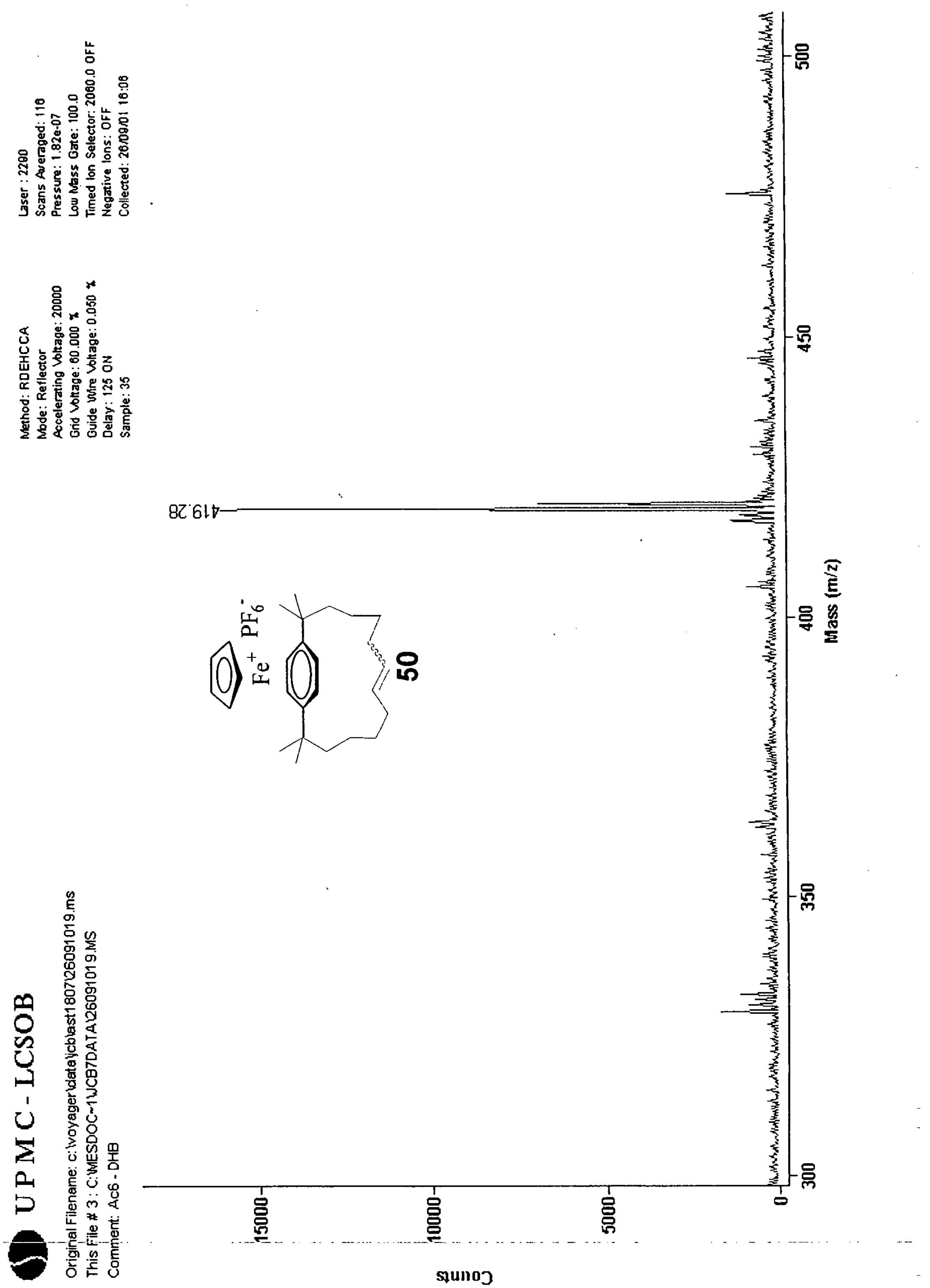
Method: RDEPNEW
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 60.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 71

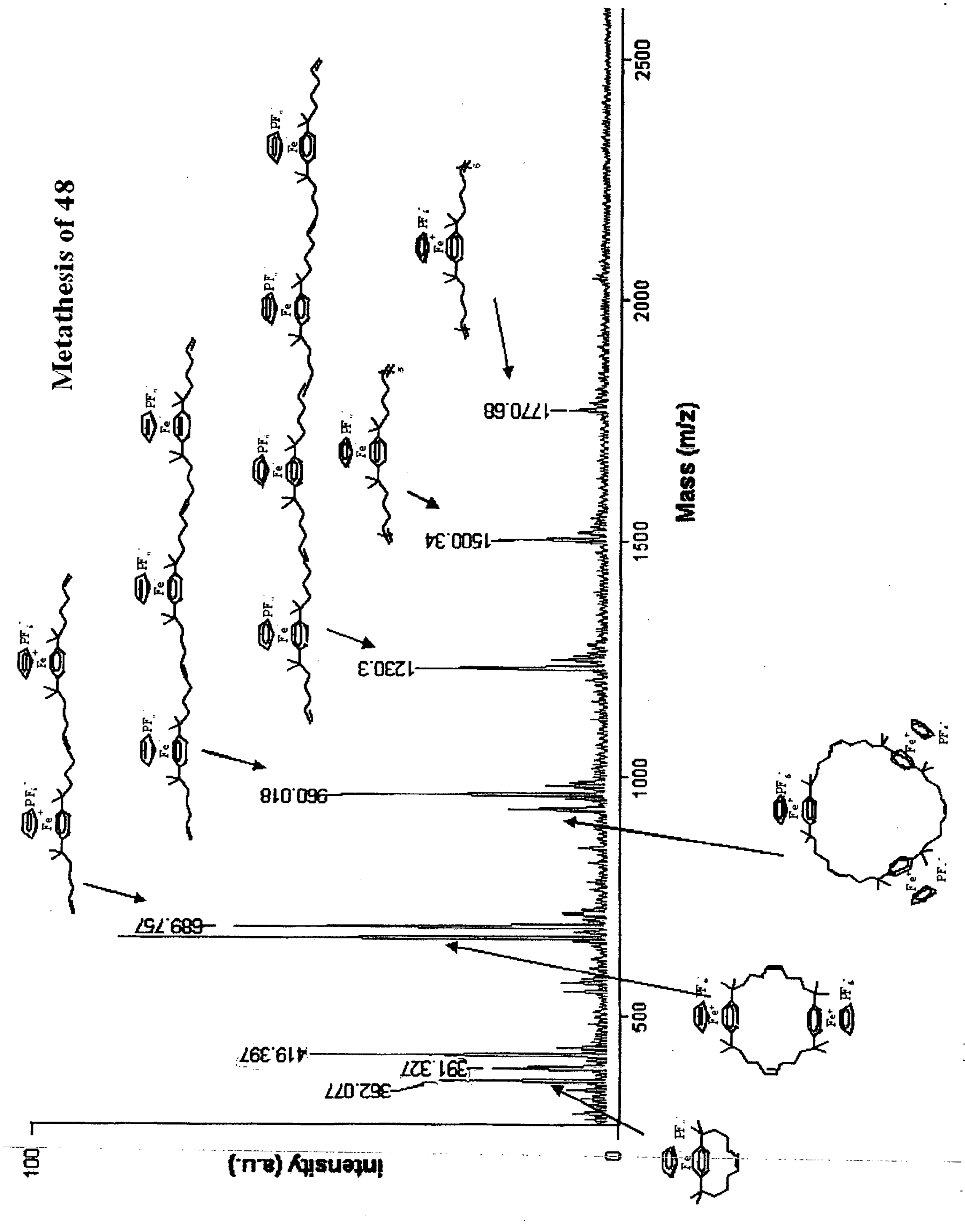
Laser : 2290
Scans Averaged: 256
Pressure: 1.91e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2060.0 OFF
Negative Ions: OFF
Collected: 03/05/01 12:16

41



50


UPMC - LCSOB
Original Filename: c:\voyager\data\jcb\ast1807\26091019.ms
This File # 3 : C:\MESDOC~1\JCB7DATA\26091019.MS
Comment: Ac6 - DHB
Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 80.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 35
Laser : 2280
Scans Averaged: 116
Pressure: 1.82e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2080.0 OFF
Negative Ions: OFF
Collected: 26/09/01 16:06
419.28
Fe+ PF6-
50
Counts
15000
10000
5000
0
300
350
400
450
500
Mass (m/z)


Metathesis of 48
Mass (m/z)
Intensity (a.u.)
362.077
391.327
419.397
689.757
960.018
1230.3
1500.34
1770.68
0
100
500
1000
1500
2000
2500

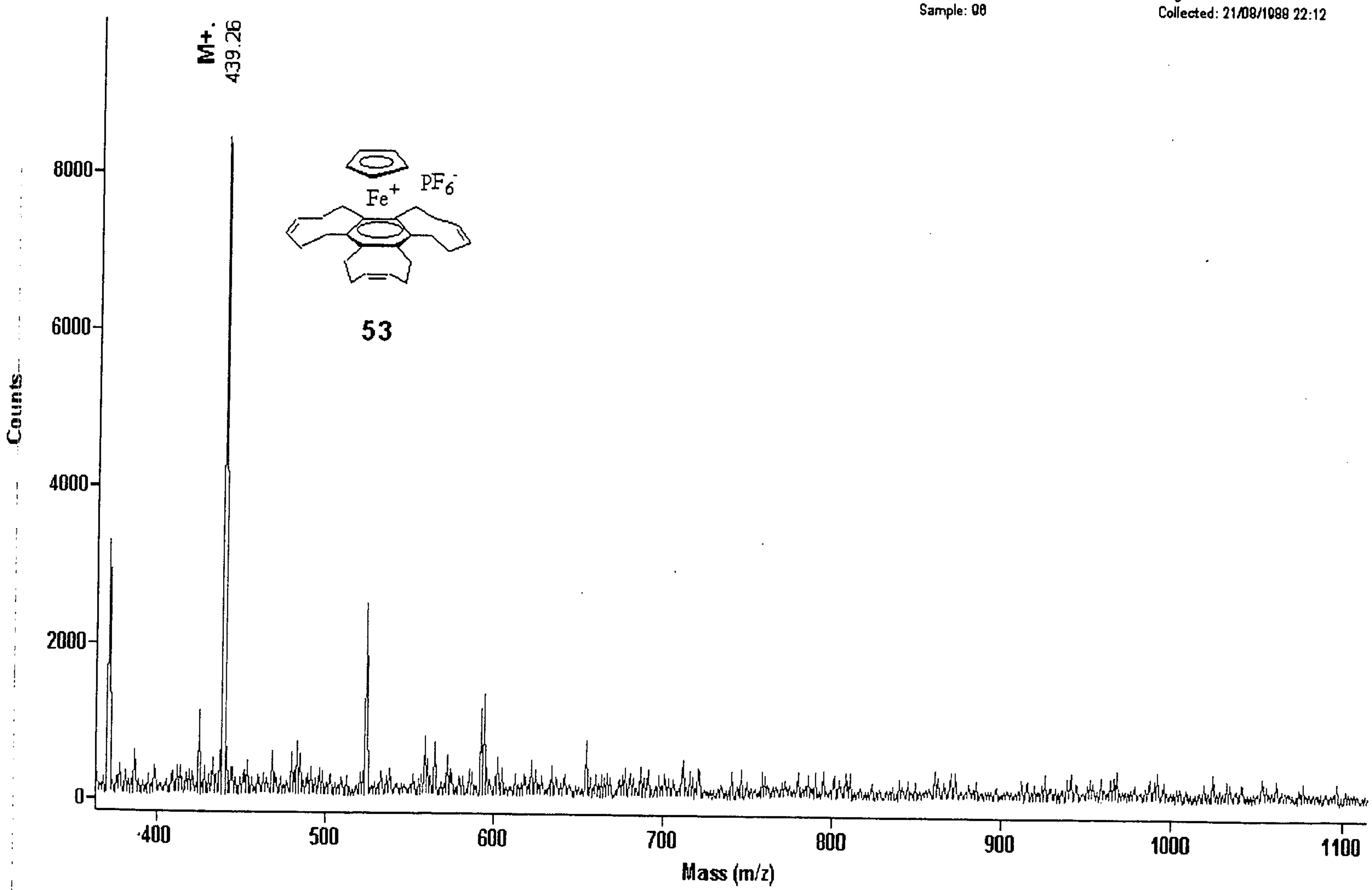
UPMC - LCSOB

Original Filename: c:\voyager\data\jcb\ast2407\10102007.ms
This File # 2 : D:\MESDOC~1\JCBDAT~1\AST2407\10102007.MS
Comment: 0110 S - DHB

53

Method: RDEHCCA
Mode: Reflector
Accelerating Voltage: 20000
Grid Voltage: 80.000 %
Guide Wire Voltage: 0.050 %
Delay: 125 ON
Sample: 98

Laser : 2340
Scans Averaged: 151
Pressure: 1.35e-07
Low Mass Gate: 100.0
Timed Ion Selector: 2080.0 OFF
Negative Ions: OFF
Collected: 21/08/1998 22:12



Complete crystallographic data including lists of atom coordinates, bond distances and angles, isotropic thermal parameters and anisotropic thermal parameters for complex **8**

Crystallographic data for complex 8

```
_chemical_compound_source              'synthesized at LCOO'
_chemical_name_systematic              ?
_chemical_name_common                  ?

_chemical_formula_analytical           ?
_chemical_formula_moiety               ?
_chemical_formula_structural           ?
_chemical_formula_sum                  'H17 C22 F6 P Fe'
_chemical_formula_weight                482.2

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
 H    H      0.000   0.000  'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
 C    C      0.002   0.002  'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
 F    F      0.010   0.570  'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
 P    P      0.090   0.095  'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'
 Fe   Fe     0.301   0.845  'International Tables Vol C Tables 4.2.6.8 and
6.1.1.4'

_cell_length_a                          19.8904(3)
_cell_length_b                          10.9561(1)
_cell_length_c                           9.3234(1)
_cell_angle_alpha                        90
_cell_angle_beta                         90.0555(5)
_cell_angle_gamma                        90
_cell_volume                            2031.77(7)
_cell_formula_units_Z                     4


_symmetry_cell_setting                 monoclinic
_symmetry_space_group_name_H-M         'P 21/n'
loop_
_symmetry_equiv_pos_as_xyz
'  x,        y,        z'
'  x+1/2, -y+1/2,  z+1/2'
' -x,       -y,       -z'
' -x+1/2,  y+1/2, -z+1/2'

_
_exptl_crystal_density_diffrn           1.576
_exptl_crystal_F_000                    976

_exptl_absorpt_coefficient_mu           0.840

_diffrn_ambient_temperature            295(1)
_diffrn_radiation_wavelength            0.71073
_diffrn_radiation_type                 MoK\a
_diffrn_radiation_source               'fine-focus sealed tube'
_diffrn_radiation_monochromator        graphite
_diffrn_radiation_detector             CCD
_diffrn_measurement_device             'Enraf-Nonius K-CCD'
```

```
_diffrn_measurement_method          '\w'


loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l

_diffrn_reflns_theta_min                 6.2
_diffrn_reflns_theta_max                 35

_reflns_number_total                8820
_reflns_number_observed             4751
_reflns_observed_criterion           >3sigma(I)
_reflns_limit_h_min                 -31
_reflns_limit_h_max                  31
_reflns_limit_k_min                   0
_reflns_limit_k_max                  17
_reflns_limit_l_min                   0
_reflns_limit_l_max                  15

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_B_iso_or_equiv
_atom_site_thermal_displace_type
Fe     Fe    0.09752(1)   0.28260(3)   0.27974(3)    2.95(1)    Bani
Pa     P    -0.09336(3)   0.23681(6)   0.82578(8)    4.68(3)    Bani
F1     F    -0.0352(1)    0.3318(2)    0.8150(4)    11.6(2)     Bani
F2     F    -0.1520(1)    0.1412(2)    0.8294(3)     9.7(1)     Bani
F3     F    -0.1471(5)    0.3414(8)    0.840(2)     10.1(5)     Bani
F4     F    -0.096(1)     0.226(1)     0.9882(9)    13.1(7)     Bani
F5     F    -0.0429(4)    0.1362(9)    0.814(2)     12.1(6)     Bani
F6     F    -0.0968(6)    0.258(1)     0.6626(7)    11.4(5)     Bani
F3'    F    -0.1422(6)    0.325(1)     0.759(2)     15.1(9)     Bani
F4'    F    -0.105(1)     0.292(2)     0.973(1)     17(1)       Bani
F5'    F    -0.0437(6)    0.147(1)     0.904(2)     12.5(7)     Bani
F6'    F    -0.0761(8)    0.170(2)     0.681(1)     15.3(8)     Bani

C11    C     0.165(1)     0.361(2)     0.139(3)      6.2(9)     Bani
C12    C     0.102(2)     0.347(2)     0.077(1)      7.0(9)     Bani
C13    C     0.085(1)     0.224(4)     0.078(2)      8(1)       Bani
C14    C     0.140(1)     0.163(1)     0.142(2)      4.8(5)     Bani
C15    C     0.1844(8)    0.250(3)     0.184(2)      6.1(7)     Bani
C11'   C     0.140(1)     0.369(1)     0.113(2)      4.7(5)     Bani
C12'   C     0.093(1)     0.290(3)     0.058(2)      6.4(8)     Bani
C13'   C     0.108(1)     0.176(2)     0.101(2)      6.4(8)     Bani
C14'   C     0.169(1)     0.179(2)     0.172(2)      5.9(7)     Bani
C15'   C     0.1940(8)    0.298(3)     0.180(2)      6.0(7)     Bani
C20    C     0.2118(1)    0.2565(2)    0.5781(2)     3.55(8)    Bani
C21    C     0.10156(9)   0.2209(2)    0.4944(2)     2.99(6)    Bani
C22    C     0.11296(8)   0.3483(2)    0.4906(2)     2.65(6)    Bani
C23    C     0.0695(1)    0.4270(2)    0.4147(2)     3.44(7)    Bani
C24    C     0.0130(1)    0.3768(3)    0.3463(3)     4.6(1)     Bani
C25    C     0.0010(1)    0.2510(3)    0.3509(3)     5.1(1)     Bani
C26    C     0.0454(1)    0.1713(2)    0.4230(2)     4.25(9)    Bani
C31    C     0.17609(9)   0.3802(2)    0.5726(2)     2.94(6)    Bani
C32    C     0.2169(1)    0.4858(2)    0.5059(2)     3.99(9)    Bani
```

```
C33    C    0.1977(1)    0.5943(2)    0.5921(3)    4.7(1)    Bani
C34    C    0.1642(1)    0.5658(2)    0.7081(3)    4.7(1)    Bani
C35    C    0.1544(1)    0.4307(2)    0.7229(2)    3.98(9)   Bani
C41    C    0.1567(1)    0.1584(2)    0.5794(2)    3.51(8)   Bani
C42    C    0.1779(1)    0.0322(2)    0.5209(3)    5.0(1)    Bani
C43    C    0.1526(2)   -0.0557(2)    0.6289(4)    6.5(2)    Bani
C44    C    0.1265(2)   -0.0037(3)    0.7410(3)    6.2(1)    Bani
C45    C    0.1286(1)    0.1307(2)    0.7333(2)    4.6(1)    Bani

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Fe    0.0397(1)    0.0436(2)    0.0287(1)    0.0012(1)    -0.00036(9)  -
0.0043(1)
Pa    0.0527(3)    0.0544(3)    0.0709(4)    -0.0051(3)    0.0013(3)
0.0130(3)
F1    0.097(2)    0.121(2)    0.223(3)    -0.057(1)    -0.043(2)    0.062(2)
F2    0.083(1)    0.077(1)    0.210(3)    -0.023(1)    0.017(2)    0.013(2)
F3    0.093(5)    0.062(3)    0.23(1)    0.020(3)    0.022(6)    -0.014(5)
F4    0.28(1)    0.158(9)    0.064(4)    0.01(1)    -0.006(6)    0.038(5)
F5    0.073(4)    0.090(4)    0.30(2)    0.041(4)    0.051(8)    0.027(9)
F6    0.23(1)    0.134(6)    0.069(3)    -0.001(7)    0.016(4)    0.011(4)
F3'    0.120(9)    0.120(9)    0.33(2)    -0.033(6)    -0.13(1)    0.13(1)
F4'    0.27(1)    0.22(1)    0.14(1)    0.04(1)    0.04(1)    -0.098(9)
F5'    0.121(7)    0.126(7)    0.23(1)    -0.004(5)    -0.070(8)    0.080(9)
F6'    0.22(1)    0.23(1)    0.136(7)    -0.09(1)    0.074(7)    -0.103(9)
C11    0.07(1)    0.09(1)    0.07(1)    -0.03(1)    0.042(8)    -0.020(8)
C12    0.13(2)    0.10(1)    0.033(5)    0.05(1)    0.011(7)    0.008(6)
C13    0.074(8)    0.19(3)    0.032(4)    -0.00(1)    0.001(4)    -0.035(9)
C14    0.068(9)    0.054(3)    0.062(8)    0.008(7)    0.021(6)    -0.018(4)
C15    0.041(5)    0.15(2)    0.042(3)    -0.026(8)    0.013(3)    -0.013(9)
C11'    0.071(9)    0.055(4)    0.052(7)    0.002(7)    0.020(7)    0.006(4)
C12'    0.074(6)    0.14(2)    0.031(4)    -0.01(1)    -0.008(4)    -0.002(8)
C13'    0.09(1)    0.09(1)    0.07(1)    -0.03(1)    0.027(8)    -0.043(8)
C14'    0.08(1)    0.09(1)    0.050(6)    0.033(9)    0.026(7)    0.008(6)
C15'    0.036(5)    0.15(2)    0.044(4)    -0.016(7)    0.016(3)    -0.021(7)
C20    0.042(1)    0.049(1)    0.0436(9)    0.0081(8)    -0.0029(7)
0.0026(8)
C21    0.0417(9)    0.0387(8)    0.0333(7)    -0.0026(7)    0.0074(6)    -
0.0020(7)
C22    0.0341(8)    0.0373(8)    0.0292(7)    0.0036(6)    0.0036(6)    -
0.0026(6)
C23    0.044(1)    0.047(1)    0.0396(9)    0.0133(8)    -0.0000(7)    -
0.0041(7)
C24    0.040(1)    0.078(2)    0.056(1)    0.015(1)    -0.0074(9)    -0.007(1)
C25    0.035(1)    0.096(2)    0.063(1)    -0.013(1)    -0.0042(9)    -0.011(1)
C26    0.052(1)    0.057(1)    0.052(1)    -0.019(1)    0.0072(9)    -0.007(1)
C31    0.0393(8)    0.0389(8)    0.0337(7)    -0.0005(7)    -0.0014(6)    -
0.0019(6)
C32    0.050(1)    0.049(1)    0.053(1)    -0.0095(9)    0.0015(9)    -
0.0009(9)
C33    0.058(1)    0.044(1)    0.077(2)    -0.007(1)    -0.004(1)    -0.010(1)
C34    0.055(1)    0.055(1)    0.068(1)    0.001(1)    -0.008(1)    -0.027(1)
C35    0.057(1)    0.058(1)    0.0364(9)    0.000(1)    -0.0035(8)    -
0.0096(8)
```

```
C41    0.057(1)    0.0374(9)    0.0389(9)    0.0067(8)    0.0060(8)
0.0044(7)
C42    0.084(2)    0.040(1)    0.067(1)    0.014(1)    0.008(1)    -0.000(1)
C43    0.110(2)    0.036(1)    0.100(2)    -0.004(1)    0.004(2)    0.013(1)
C44    0.113(3)    0.055(1)    0.069(2)    -0.019(2)    0.005(2)    0.020(1)
C45    0.075(2)    0.056(1)    0.042(1)    -0.001(1)    0.005(1)
0.0125(9)

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Fe    C11     2.07(2)    .    ?
Fe    C12     2.02(2)    .    ?
Fe    C13     2.00(3)    .    ?
Fe    C14     2.02(2)    .    ?
Fe    C15     1.98(2)    .    ?
Fe    C11'    2.01(2)    .    ?
Fe    C12'    2.07(2)    .    ?
Fe    C13'    2.05(2)    .    ?
Fe    C14'    2.08(2)    .    ?
Fe    C15'    2.14(2)    .    ?
Fe    C21     2.114(2)   .    ?
Fe    C22     2.116(2)   .    ?
Fe    C23     2.097(2)   .    ?
Fe    C24     2.068(2)   .    ?
Fe    C25     2.061(3)   .    ?
Fe    C26     2.085(2)   .    ?
Pa    F1      1.559(3)   .    ?
Pa    F2      1.568(3)   .    ?
Pa    F3      1.57(1)    .    ?
Pa    F4      1.52(1)    .    ?
Pa    F5      1.49(1)    .    ?
Pa    F6      1.54(1)    .    ?
Pa    F3'     1.50(1)    .    ?

Pa    F4'     1.52(2)    .    ?
Pa    F5'     1.57(1)    .    ?
Pa    F6'     1.57(2)    .    ?
F6    F6'     1.06(2)    .    ?
C11   C12     1.39(3)    .    ?
C11   C15     1.34(3)    .    ?
C11   C12'    1.80(3)    .    ?
C12   C13     1.39(4)    .    ?
C13   C14     1.41(3)    .    ?
C14   C15     1.36(3)    .    ?
C15   C11'    1.71(3)    .    ?
C11'  C12'    1.37(3)    .    ?
C11'  C15'    1.47(3)    .    ?
C12'  C13'    1.35(3)    .    ?
C13'  C14'    1.38(3)    .    ?
C14'  C15'    1.40(3)    .    ?
C20   C31     1.531(3)   .    ?
C20   C41     1.535(3)   .    ?
C21   C22     1.415(2)   .    ?
C21   C26     1.409(3)   .    ?
C21   C41     1.516(3)   .    ?
C22   C23     1.411(3)   .    ?
C22   C31     1.510(2)   .    ?
```

```
C23    C24      1.404(3)   .  ?
C24    C25      1.399(4)   .  ?
C25    C26      1.412(4)   .  ?
C31    C32      1.544(3)   .  ?
C31    C35      1.568(3)   .  ?
C32    C33      1.485(3)   .  ?
C33    C34      1.309(4)   .  ?
C34    C35      1.499(3)   .  ?
C41    C42      1.545(3)   .  ?
C41    C45      1.570(3)   .  ?
C42    C43      1.482(4)   .  ?
C43    C44      1.299(5)   .  ?
C44    C45      1.475(4)   .  ?

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C11    Fe    C12       40(1)     .  .  ?
C11    Fe    C13       67(1)     .  .  ?
C11    Fe    C14       66.0(8)   .  .  ?
C11    Fe    C15       38.7(9)   .  .  ?
C11    Fe    C11'      15.7(9)   .  .  ?
C11    Fe    C12'      51.5(9)   .  .  ?
C11    Fe    C13'      69.7(9)   .  .  ?
C11    Fe    C14'      58.3(9)   .  .  ?
C11    Fe    C15'      26.8(9)   .  .  ?
C11    Fe    C21      135.3(7)   .  .  ?
C11    Fe    C22      110.8(7)   .  .  ?
C11    Fe    C23      103.9(7)   .  .  ?
C11    Fe    C24      120.8(7)   .  .  ?
C11    Fe    C25      151.7(7)   .  .  ?
C11    Fe    C26      166.9(7)   .  .  ?
C12    Fe    C13       40(1)     .  .  ?
C12    Fe    C14       67.2(8)   .  .  ?
C12    Fe    C15       66.5(9)   .  .  ?
C12    Fe    C11'      24.7(9)   .  .  ?
C12    Fe    C12'      18.9(9)   .  .  ?
C12    Fe    C13'      55.4(9)   .  .  ?
C12    Fe    C14'      73.0(9)   .  .  ?
C12    Fe    C15'      61.7(9)   .  .  ?
C12    Fe    C21      175.0(7)   .  .  ?
C12    Fe    C22      138.1(7)   .  .  ?
C12    Fe    C23      108.1(7)   .  .  ?
C12    Fe    C24       98.2(7)   .  .  ?
C12    Fe    C25      113.7(7)   .  .  ?
C12    Fe    C26      145.7(7)   .  .  ?
C13    Fe    C14       41.1(9)   .  .  ?
C13    Fe    C15       68(1)     .  .  ?
C13    Fe    C11'      58.4(9)   .  .  ?
C13    Fe    C12'      22(1)     .  .  ?
C13    Fe    C13'      21(1)     .  .  ?
C13    Fe    C14'      57(1)     .  .  ?
C13    Fe    C15'      74(1)     .  .  ?
C13    Fe    C21      142.3(7)   .  .  ?
C13    Fe    C22      178.3(7)   .  .  ?
C13    Fe    C23      140.6(7)   .  .  ?
```

C13	Fe	C24	110.0(7)	.	.	?
C13	Fe	C25	97.7(8)	.	.	?
C13	Fe	C26	110.6(7)	.	.	?
C14	Fe	C15	39.7(8)	.	.	?
C14	Fe	C11'	68.7(7)	.	.	?
C14	Fe	C12'	53.7(8)	.	.	?
C14	Fe	C13'	21.4(8)	.	.	?
C14	Fe	C14'	18.6(8)	.	.	?
C14	Fe	C15'	53.1(8)	.	.	?
C14	Fe	C21	112.3(5)	.	.	?
C14	Fe	C22	138.7(5)	.	.	?
C14	Fe	C23	169.2(5)	.	.	?
C14	Fe	C24	148.7(5)	.	.	?
C14	Fe	C25	119.1(5)	.	.	?
C14	Fe	C26	103.7(5)	.	.	?
C15	Fe	C11'	50.7(8)	.	.	?
C15	Fe	C12'	66.0(9)	.	.	?
C15	Fe	C13'	55.9(9)	.	.	?
C15	Fe	C14'	23.8(9)	.	.	?
C15	Fe	C15'	15.0(9)	.	.	?
C15	Fe	C21	109.7(6)	.	.	?
C15	Fe	C22	110.8(6)	.	.	?
C15	Fe	C23	129.8(6)	.	.	?
C15	Fe	C24	159.4(6)	.	.	?
C15	Fe	C25	158.3(6)	.	.	?
C15	Fe	C26	128.2(6)	.	.	?
C11'	Fe	C12'	39.3(8)	.	.	?
C11'	Fe	C13'	66.1(9)	.	.	?
C11'	Fe	C14'	66.1(8)	.	.	?
C11'	Fe	C15'	41.2(9)	.	.	?
C11'	Fe	C21	150.3(6)	.	.	?
C11'	Fe	C22	119.9(6)	.	.	?
C11'	Fe	C23	102.8(6)	.	.	?
C11'	Fe	C24	109.9(6)	.	.	?
C11'	Fe	C25	136.2(6)	.	.	?
C11'	Fe	C26	169.0(6)	.	.	?
C12'	Fe	C13'	38.1(9)	.	.	?
C12'	Fe	C14'	64.4(9)	.	.	?
C12'	Fe	C15'	66.5(9)	.	.	?
C12'	Fe	C21	163.6(6)	.	.	?
C12'	Fe	C22	157.0(6)	.	.	?
C12'	Fe	C23	123.9(6)	.	.	?
C12'	Fe	C24	104.2(6)	.	.	?
C12'	Fe	C25	106.8(6)	.	.	?
C12'	Fe	C26	129.9(6)	.	.	?
C13'	Fe	C14'	39.1(9)	.	.	?
C13'	Fe	C15'	66.4(9)	.	.	?
C13'	Fe	C21	125.8(7)	.	.	?
C13'	Fe	C22	159.4(7)	.	.	?
C13'	Fe	C23	161.2(7)	.	.	?
C13'	Fe	C24	127.8(7)	.	.	?
C13'	Fe	C25	105.2(7)	.	.	?
C13'	Fe	C26	103.8(7)	.	.	?
C14'	Fe	C15'	38.7(9)	.	.	?
C14'	Fe	C21	104.9(6)	.	.	?
C14'	Fe	C22	122.4(6)	.	.	?
C14'	Fe	C23	152.1(6)	.	.	?
C14'	Fe	C24	166.9(6)	.	.	?
C14'	Fe	C25	134.5(6)	.	.	?
C14'	Fe	C26	109.3(6)	.	.	?

C15'	Fe	C21	113.8(7)	.	.	?
C15'	Fe	C22	104.3(7)	.	.	?
C15'	Fe	C23	116.1(7)	.	.	?
C15'	Fe	C24	145.1(7)	.	.	?
C15'	Fe	C25	171.5(7)	.	.	?
C15'	Fe	C26	140.4(7)	.	.	?
C21	Fe	C22	39.08(7)	.	.	?
C21	Fe	C23	71.52(7)	.	.	?
C21	Fe	C24	84.59(8)	.	.	?
C21	Fe	C25	71.10(9)	.	.	?
C21	Fe	C26	39.20(8)	.	.	?
C22	Fe	C23	39.13(7)	.	.	?
C22	Fe	C24	70.66(8)	.	.	?
C22	Fe	C25	83.83(9)	.	.	?
C22	Fe	C26	71.07(8)	.	.	?
C23	Fe	C24	39.38(9)	.	.	?
C23	Fe	C25	71.66(9)	.	.	?
C23	Fe	C26	85.66(8)	.	.	?
C24	Fe	C25	39.6(1)	.	.	?
C24	Fe	C26	72.24(9)	.	.	?
C25	Fe	C26	39.8(1)	.	.	?
F1	Pa	F2	177.5(1)	.	.	?
F1	Pa	F3	91.3(4)	.	.	?
F1	Pa	F4	98.2(5)	.	.	?
F1	Pa	F5	89.4(5)	.	.	?
F1	Pa	F6	82.4(4)	.	.	?
F1	Pa	F3'	91.3(6)	.	.	?
F1	Pa	F4'	84.6(6)	.	.	?
F1	Pa	F5'	89.0(5)	.	.	?
F1	Pa	F6'	95.3(6)	.	.	?
F2	Pa	F3	88.8(4)	.	.	?
F2	Pa	F4	84.3(5)	.	.	?
F2	Pa	F5	90.5(5)	.	.	?
F2	Pa	F6	95.1(4)	.	.	?
F2	Pa	F3'	87.6(6)	.	.	?
F2	Pa	F4'	97.6(6)	.	.	?
F2	Pa	F5'	92.2(5)	.	.	?
F2	Pa	F6'	82.6(6)	.	.	?
F3	Pa	F4	87.1(6)	.	.	?
F3	Pa	F5	179.1(6)	.	.	?
F3	Pa	F6	86.8(6)	.	.	?
F3	Pa	F3'	29.4(7)	.	.	?
F3	Pa	F4'	61.9(8)	.	.	?
F3	Pa	F5'	147.5(6)	.	.	?
F3	Pa	F6'	124.1(7)	.	.	?
F4	Pa	F5	92.3(7)	.	.	?
F4	Pa	F6	173.8(6)	.	.	?
F4	Pa	F3'	116.1(8)	.	.	?
F4	Pa	F4'	28.9(8)	.	.	?
F4	Pa	F5'	60.8(7)	.	.	?
F4	Pa	F6'	145.7(8)	.	.	?
F5	Pa	F6	93.9(6)	.	.	?
F5	Pa	F3'	151.2(7)	.	.	?
F5	Pa	F4'	117.6(8)	.	.	?
F5	Pa	F5'	31.9(7)	.	.	?
F5	Pa	F6'	56.4(7)	.	.	?
F6	Pa	F3'	57.8(7)	.	.	?
F6	Pa	F4'	145.7(7)	.	.	?
F6	Pa	F5'	125.4(6)	.	.	?
F6	Pa	F6'	39.9(7)	.	.	?
F3'	Pa	F4'	91.1(9)	.	.	?

F3'	Pa	F5'	176.8(8)	.	.	?
F3'	Pa	F6'	94.9(8)	.	.	?
F4'	Pa	F5'	85.8(8)	.	.	?
F4'	Pa	F6'	174.0(9)	.	.	?
F5'	Pa	F6'	88.2(8)	.	.	?
Pa	F6	F6'	72(1)	.	.	?
Pa	F6'	F6	68(1)	.	.	?
Fe	C11	C12	68(1)	.	.	?
Fe	C11	C15	67(1)	.	.	?
Fe	C11	C12'	64(1)	.	.	?
C12	C11	C15	107(2)	.	.	?
C12	C11	C12'	20(1)	.	.	?
C15	C11	C12'	88(2)	.	.	?
Fe	C12	C11	72(1)	.	.	?
Fe	C12	C13	69(1)	.	.	?
C11	C12	C13	109(2)	.	.	?
Fe	C13	C12	70(1)	.	.	?
Fe	C13	C14	70(1)	.	.	?
C12	C13	C14	106(2)	.	.	?
Fe	C14	C13	69(1)	.	.	?
Fe	C14	C15	68(1)	.	.	?
C13	C14	C15	107(2)	.	.	?
Fe	C15	C11	74(1)	.	.	?
Fe	C15	C14	72(1)	.	.	?
Fe	C15	C11'	66(1)	.	.	?
C11	C15	C14	111(2)	.	.	?
C11	C15	C11'	16(1)	.	.	?
C14	C15	C11'	95(2)	.	.	?
Fe	C11'	C15	64(1)	.	.	?
Fe	C11'	C12'	73(1)	.	.	?
Fe	C11'	C15'	74(1)	.	.	?
C15	C11'	C12'	91(2)	.	.	?
C15	C11'	C15'	18(1)	.	.	?
C12'	C11'	C15'	109(2)	.	.	?
Fe	C12'	C11	64(1)	.	.	?
Fe	C12'	C11'	68(1)	.	.	?
Fe	C12'	C13'	70(1)	.	.	?
C11	C12'	C11'	13(1)	.	.	?
C11	C12'	C13'	96(2)	.	.	?
C11'	C12'	C13'	109(2)	.	.	?
Fe	C13'	C12'	72(1)	.	.	?
Fe	C13'	C14'	72(1)	.	.	?
C12'	C13'	C14'	108(2)	.	.	?
Fe	C14'	C13'	69(1)	.	.	?
Fe	C14'	C15'	73(1)	.	.	?
C13'	C14'	C15'	111(2)	.	.	?
Fe	C15'	C11'	65(1)	.	.	?
Fe	C15'	C14'	68(1)	.	.	?
C11'	C15'	C14'	102(2)	.	.	?
C31	C20	C41	106.8(2)	.	.	?
Fe	C21	C22	70.5(1)	.	.	?
Fe	C21	C26	69.3(1)	.	.	?
Fe	C21	C41	131.8(1)	.	.	?
C22	C21	C26	119.7(2)	.	.	?
C22	C21	C41	110.1(2)	.	.	?
C26	C21	C41	130.2(2)	.	.	?
Fe	C22	C21	70.4(1)	.	.	?
Fe	C22	C23	69.7(1)	.	.	?
Fe	C22	C31	132.0(1)	.	.	?
C21	C22	C23	121.2(2)	.	.	?

```
C21    C22    C31    110.4(1)   .   .   ?
C23    C22    C31    128.4(2)   .   .   ?
Fe     C23    C22     71.1(1)   .   .   ?
Fe     C23    C24     69.2(1)   .   .   ?
C22    C23    C24    118.6(2)   .   .   ?
Fe     C24    C23     71.4(1)   .   .   ?
Fe     C24    C25     69.9(1)   .   .   ?
C23    C24    C25    120.6(2)   .   .   ?
Fe     C25    C24     70.5(2)   .   .   ?
Fe     C25    C26     71.0(1)   .   .   ?
C24    C25    C26    121.1(2)   .   .   ?
Fe     C26    C21     71.5(1)   .   .   ?
Fe     C26    C25     69.2(1)   .   .   ?
C21    C26    C25    118.8(2)   .   .   ?
C20    C31    C22    101.4(1)   .   .   ?
C20    C31    C32    115.6(2)   .   .   ?
C20    C31    C35    114.2(2)   .   .   ?
C22    C31    C32    114.0(2)   .   .   ?
C22    C31    C35    107.7(1)   .   .   ?
C32    C31    C35    103.9(2)   .   .   ?
C31    C32    C33    104.3(2)   .   .   ?
C32    C33    C34    112.8(2)   .   .   ?
C33    C34    C35    112.2(2)   .   .   ?
C31    C35    C34    103.3(2)   .   .   ?
C20    C41    C21    101.3(2)   .   .   ?
C20    C41    C42    115.4(2)   .   .   ?
C20    C41    C45    113.4(2)   .   .   ?
C21    C41    C42    114.7(2)   .   .   ?
C21    C41    C45    107.9(2)   .   .   ?
C42    C41    C45    104.3(2)   .   .   ?
C41    C42    C43    104.4(2)   .   .   ?
C42    C43    C44    113.5(3)   .   .   ?
C43    C44    C45    112.8(3)   .   .   ?
C41    C45    C44    104.3(2)   .   .   ?

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
C12    Fe    C11    C12        0(2)   .   .   .   .   ?
C12    Fe    C11    C15     -120(2)   .   .   .   .   ?
C12    Fe    C11    C12'     -21(2)   .   .   .   .   ?
C13    Fe    C11    C12       38(2)   .   .   .   .   ?
C13    Fe    C11    C15      -83(2)   .   .   .   .   ?
C13    Fe    C11    C12'      17(1)   .   .   .   .   ?
C14    Fe    C11    C12       83(2)   .   .   .   .   ?
C14    Fe    C11    C15      -38(2)   .   .   .   .   ?
C14    Fe    C11    C12'      62(1)   .   .   .   .   ?
C15    Fe    C11    C12      120(2)   .   .   .   .   ?
C15    Fe    C11    C15        0(2)   .   .   .   .   ?
C15    Fe    C11    C12'      99(2)   .   .   .   .   ?
C11'   Fe    C11    C12      -14(3)   .   .   .   .   ?
C11'   Fe    C11    C15     -134(3)   .   .   .   .   ?
C11'   Fe    C11    C12'     -35(2)   .   .   .   .   ?
```

C12'	Fe	C11	C12	21(2)	.	.	.	.	?
C12'	Fe	C11	C15	-99(2)	.	.	.	.	?
C12'	Fe	C11	C12'	0(1)	.	.	.	.	?
C13'	Fe	C11	C12	60(2)	.	.	.	.	?
C13'	Fe	C11	C15	-60(2)	.	.	.	.	?
C13'	Fe	C11	C12'	39(1)	.	.	.	.	?
C14'	Fe	C11	C12	102(2)	.	.	.	.	?
C14'	Fe	C11	C15	-18(2)	.	.	.	.	?
C14'	Fe	C11	C12'	81(1)	.	.	.	.	?
C15'	Fe	C11	C12	137(2)	.	.	.	.	?
C15'	Fe	C11	C15	17(2)	.	.	.	.	?
C15'	Fe	C11	C12'	116(2)	.	.	.	.	?
C21	Fe	C11	C12	-179(2)	.	.	.	.	?
C21	Fe	C11	C15	60(2)	.	.	.	.	?
C21	Fe	C11	C12'	160(1)	.	.	.	.	?
C22	Fe	C11	C12	-142(2)	.	.	.	.	?
C22	Fe	C11	C15	98(2)	.	.	.	.	?
C22	Fe	C11	C12'	-163(1)	.	.	.	.	?
C23	Fe	C11	C12	-102(2)	.	.	.	.	?
C23	Fe	C11	C15	138(2)	.	.	.	.	?
C23	Fe	C11	C12'	-123(1)	.	.	.	.	?
C24	Fe	C11	C12	-63(2)	.	.	.	.	?
C24	Fe	C11	C15	177(2)	.	.	.	.	?
C24	Fe	C11	C12'	-84(1)	.	.	.	.	?
C25	Fe	C11	C12	-24(2)	.	.	.	.	?
C25	Fe	C11	C15	-145(2)	.	.	.	.	?
C25	Fe	C11	C12'	-45(1)	.	.	.	.	?
C26	Fe	C11	C12	122(2)	.	.	.	.	?
C26	Fe	C11	C15	2(2)	.	.	.	.	?
C26	Fe	C11	C12'	101(1)	.	.	.	.	?
C11	Fe	C12	C11	0(2)	.	.	.	.	?
C11	Fe	C12	C13	119(2)	.	.	.	.	?
C13	Fe	C12	C11	-119(2)	.	.	.	.	?
C13	Fe	C12	C13	0(2)	.	.	.	.	?
C14	Fe	C12	C11	-79(2)	.	.	.	.	?
C14	Fe	C12	C13	40(2)	.	.	.	.	?
C15	Fe	C12	C11	-36(2)	.	.	.	.	?
C15	Fe	C12	C13	83(2)	.	.	.	.	?
C11'	Fe	C12	C11	9(2)	.	.	.	.	?
C11'	Fe	C12	C13	128(2)	.	.	.	.	?
C12'	Fe	C12	C11	-120(2)	.	.	.	.	?
C12'	Fe	C12	C13	-1(2)	.	.	.	.	?
C13'	Fe	C12	C11	-100(2)	.	.	.	.	?
C13'	Fe	C12	C13	19(2)	.	.	.	.	?
C14'	Fe	C12	C11	-61(2)	.	.	.	.	?
C14'	Fe	C12	C13	59(2)	.	.	.	.	?
C15'	Fe	C12	C11	-20(2)	.	.	.	.	?
C15'	Fe	C12	C13	99(2)	.	.	.	.	?
C21	Fe	C12	C11	6(2)	.	.	.	.	?
C21	Fe	C12	C13	125(2)	.	.	.	.	?
C22	Fe	C12	C11	59(2)	.	.	.	.	?
C22	Fe	C12	C13	179(2)	.	.	.	.	?
C23	Fe	C12	C11	90(2)	.	.	.	.	?
C23	Fe	C12	C13	-150(2)	.	.	.	.	?
C24	Fe	C12	C11	129(2)	.	.	.	.	?
C24	Fe	C12	C13	-111(2)	.	.	.	.	?
C25	Fe	C12	C11	168(2)	.	.	.	.	?
C25	Fe	C12	C13	-73(2)	.	.	.	.	?
C26	Fe	C12	C11	-160(2)	.	.	.	.	?
C26	Fe	C12	C13	-41(2)	.	.	.	.	?

C11	Fe	C13	C12	-37(2)	.	.	.	.	.	?
C11	Fe	C13	C14	79(2)	.	.	.	.	.	?
C12	Fe	C13	C12	0(2)	.	.	.	.	.	?
C12	Fe	C13	C14	116(2)	.	.	.	.	.	?
C14	Fe	C13	C12	-116(2)	.	.	.	.	.	?
C14	Fe	C13	C14	0(2)	.	.	.	.	.	?
C15	Fe	C13	C12	-79(2)	.	.	.	.	.	?
C15	Fe	C13	C14	37(2)	.	.	.	.	.	?
C11'	Fe	C13	C12	-23(2)	.	.	.	.	.	?
C11'	Fe	C13	C14	93(1)	.	.	.	.	.	?
C12'	Fe	C13	C12	1(2)	.	.	.	.	.	?
C12'	Fe	C13	C14	117(2)	.	.	.	.	.	?
C13'	Fe	C13	C12	-129(2)	.	.	.	.	.	?
C13'	Fe	C13	C14	-13(2)	.	.	.	.	.	?
C14'	Fe	C13	C12	-103(2)	.	.	.	.	.	?
C14'	Fe	C13	C14	13(2)	.	.	.	.	.	?
C15'	Fe	C13	C12	-65(2)	.	.	.	.	.	?
C15'	Fe	C13	C14	51(2)	.	.	.	.	.	?
C21	Fe	C13	C12	-173(2)	.	.	.	.	.	?
C21	Fe	C13	C14	-57(1)	.	.	.	.	.	?
C22	Fe	C13	C12	-31(2)	.	.	.	.	.	?
C22	Fe	C13	C14	84(2)	.	.	.	.	.	?
C23	Fe	C13	C12	47(2)	.	.	.	.	.	?
C23	Fe	C13	C14	163(1)	.	.	.	.	.	?
C24	Fe	C13	C12	79(2)	.	.	.	.	.	?
C24	Fe	C13	C14	-165(1)	.	.	.	.	.	?
C25	Fe	C13	C12	118(2)	.	.	.	.	.	?
C25	Fe	C13	C14	-126(1)	.	.	.	.	.	?
C26	Fe	C13	C12	157(2)	.	.	.	.	.	?
C26	Fe	C13	C14	-87(1)	.	.	.	.	.	?
C11	Fe	C14	C13	-83(2)	.	.	.	.	.	?
C11	Fe	C14	C15	37(1)	.	.	.	.	.	?
C12	Fe	C14	C13	-39(2)	.	.	.	.	.	?
C12	Fe	C14	C15	80(1)	.	.	.	.	.	?
C13	Fe	C14	C13	0(2)	.	.	.	.	.	?
C13	Fe	C14	C15	119(2)	.	.	.	.	.	?
C15	Fe	C14	C13	-119(2)	.	.	.	.	.	?
C15	Fe	C14	C15	0(2)	.	.	.	.	.	?
C11'	Fe	C14	C13	-66(1)	.	.	.	.	.	?
C11'	Fe	C14	C15	54(1)	.	.	.	.	.	?
C12'	Fe	C14	C13	-24(2)	.	.	.	.	.	?
C12'	Fe	C14	C15	95(1)	.	.	.	.	.	?
C13'	Fe	C14	C13	13(2)	.	.	.	.	.	?
C13'	Fe	C14	C15	132(2)	.	.	.	.	.	?
C14'	Fe	C14	C13	-144(2)	.	.	.	.	.	?
C14'	Fe	C14	C15	-25(2)	.	.	.	.	.	?
C15'	Fe	C14	C13	-110(2)	.	.	.	.	.	?
C15'	Fe	C14	C15	9(1)	.	.	.	.	.	?
C21	Fe	C14	C13	146(1)	.	.	.	.	.	?
C21	Fe	C14	C15	-94(1)	.	.	.	.	.	?
C22	Fe	C14	C13	-177(1)	.	.	.	.	.	?
C22	Fe	C14	C15	-58(1)	.	.	.	.	.	?
C23	Fe	C14	C13	-105(1)	.	.	.	.	.	?
C23	Fe	C14	C15	14(1)	.	.	.	.	.	?
C24	Fe	C14	C13	28(1)	.	.	.	.	.	?
C24	Fe	C14	C15	147(1)	.	.	.	.	.	?
C25	Fe	C14	C13	66(1)	.	.	.	.	.	?
C25	Fe	C14	C15	-174(1)	.	.	.	.	.	?
C26	Fe	C14	C13	106(1)	.	.	.	.	.	?
C26	Fe	C14	C15	-135(1)	.	.	.	.	.	?
C11	Fe	C15	C11	0(2)	.	.	.	.	.	?

C11	Fe	C15	C14	-119(2)	.	.	.	.	?
C11	Fe	C15	C11'	-15(2)	.	.	.	.	?
C12	Fe	C15	C11	37(2)	.	.	.	.	?
C12	Fe	C15	C14	-82(1)	.	.	.	.	?
C12	Fe	C15	C11'	22(1)	.	.	.	.	?
C13	Fe	C15	C11	81(2)	.	.	.	.	?
C13	Fe	C15	C14	-38(1)	.	.	.	.	?
C13	Fe	C15	C11'	66(1)	.	.	.	.	?
C14	Fe	C15	C11	119(2)	.	.	.	.	?
C14	Fe	C15	C14	0(1)	.	.	.	.	?
C14	Fe	C15	C11'	105(1)	.	.	.	.	?
C11'	Fe	C15	C11	15(2)	.	.	.	.	?
C11'	Fe	C15	C14	-105(1)	.	.	.	.	?
C11'	Fe	C15	C11'	0(1)	.	.	.	.	?
C12'	Fe	C15	C11	58(2)	.	.	.	.	?
C12'	Fe	C15	C14	-61(1)	.	.	.	.	?
C12'	Fe	C15	C11'	43(1)	.	.	.	.	?
C13'	Fe	C15	C11	100(2)	.	.	.	.	?
C13'	Fe	C15	C14	-19(1)	.	.	.	.	?
C13'	Fe	C15	C11'	85(1)	.	.	.	.	?
C14'	Fe	C15	C11	138(2)	.	.	.	.	?
C14'	Fe	C15	C14	19(2)	.	.	.	.	?
C14'	Fe	C15	C11'	124(2)	.	.	.	.	?
C15'	Fe	C15	C11	-31(3)	.	.	.	.	?
C15'	Fe	C15	C14	-150(3)	.	.	.	.	?
C15'	Fe	C15	C11'	-45(3)	.	.	.	.	?
C21	Fe	C15	C11	-139(1)	.	.	.	.	?
C21	Fe	C15	C14	101(1)	.	.	.	.	?
C21	Fe	C15	C11'	-154(1)	.	.	.	.	?
C22	Fe	C15	C11	-98(1)	.	.	.	.	?
C22	Fe	C15	C14	143(1)	.	.	.	.	?
C22	Fe	C15	C11'	-112(1)	.	.	.	.	?
C23	Fe	C15	C11	-58(1)	.	.	.	.	?
C23	Fe	C15	C14	-177(1)	.	.	.	.	?
C23	Fe	C15	C11'	-72(1)	.	.	.	.	?
C24	Fe	C15	C11	-8(1)	.	.	.	.	?
C24	Fe	C15	C14	-127(1)	.	.	.	.	?
C24	Fe	C15	C11'	-22(1)	.	.	.	.	?
C25	Fe	C15	C11	132(1)	.	.	.	.	?
C25	Fe	C15	C14	13(1)	.	.	.	.	?
C25	Fe	C15	C11'	118(1)	.	.	.	.	?
C26	Fe	C15	C11	-179(1)	.	.	.	.	?
C26	Fe	C15	C14	61(1)	.	.	.	.	?
C26	Fe	C15	C11'	166(1)	.	.	.	.	?
C11	Fe	C11'	C15	35(3)	.	.	.	.	?
C11	Fe	C11'	C12'	135(3)	.	.	.	.	?
C11	Fe	C11'	C15'	19(3)	.	.	.	.	?
C12	Fe	C11'	C15	-123(2)	.	.	.	.	?
C12	Fe	C11'	C12'	-23(2)	.	.	.	.	?
C12	Fe	C11'	C15'	-139(2)	.	.	.	.	?
C13	Fe	C11'	C15	-86(1)	.	.	.	.	?
C13	Fe	C11'	C12'	13(2)	.	.	.	.	?
C13	Fe	C11'	C15'	-103(2)	.	.	.	.	?
C14	Fe	C11'	C15	-42(1)	.	.	.	.	?
C14	Fe	C11'	C12'	58(1)	.	.	.	.	?
C14	Fe	C11'	C15'	-58(1)	.	.	.	.	?
C15	Fe	C11'	C15	0(1)	.	.	.	.	?
C15	Fe	C11'	C12'	100(1)	.	.	.	.	?
C15	Fe	C11'	C15'	-16(1)	.	.	.	.	?
C12'	Fe	C11'	C15	-100(1)	.	.	.	.	?
C12'	Fe	C11'	C12'	0(2)	.	.	.	.	?

C12'	Fe	C11'	C15'	-116(2)	. . . . .	?
C13'	Fe	C11'	C15	-65(1)	. . . . .	?
C13'	Fe	C11'	C12'	35(1)	. . . . .	?
C13'	Fe	C11'	C15'	-81(1)	. . . . .	?
C14'	Fe	C11'	C15	-22(1)	. . . . .	?
C14'	Fe	C11'	C12'	78(1)	. . . . .	?
C14'	Fe	C11'	C15'	-38(1)	. . . . .	?
C15'	Fe	C11'	C15	16(1)	. . . . .	?
C15'	Fe	C11'	C12'	116(2)	. . . . .	?
C15'	Fe	C11'	C15'	0(2)	. . . . .	?
C21	Fe	C11'	C15	56(1)	. . . . .	?
C21	Fe	C11'	C12'	156(1)	. . . . .	?
C21	Fe	C11'	C15'	40(1)	. . . . .	?
C22	Fe	C11'	C15	93(1)	. . . . .	?
C22	Fe	C11'	C12'	-167(1)	. . . . .	?
C22	Fe	C11'	C15'	77(1)	. . . . .	?
C23	Fe	C11'	C15	131(1)	. . . . .	?
C23	Fe	C11'	C12'	-129(1)	. . . . .	?
C23	Fe	C11'	C15'	115(1)	. . . . .	?
C24	Fe	C11'	C15	172(1)	. . . . .	?
C24	Fe	C11'	C12'	-88(1)	. . . . .	?
C24	Fe	C11'	C15'	156(1)	. . . . .	?
C25	Fe	C11'	C15	-152(1)	. . . . .	?
C25	Fe	C11'	C12'	-52(1)	. . . . .	?
C25	Fe	C11'	C15'	-168(1)	. . . . .	?
C26	Fe	C11'	C15	-89(1)	. . . . .	?
C26	Fe	C11'	C12'	11(1)	. . . . .	?
C26	Fe	C11'	C15'	-105(1)	. . . . .	?
C11	Fe	C12'	C11	0(1)	. . . . .	?
C11	Fe	C12'	C11'	-14(2)	. . . . .	?
C11	Fe	C12'	C13'	107(2)	. . . . .	?
C12	Fe	C12'	C11	45(2)	. . . . .	?
C12	Fe	C12'	C11'	31(2)	. . . . .	?
C12	Fe	C12'	C13'	152(3)	. . . . .	?
C13	Fe	C12'	C11	-133(2)	. . . . .	?
C13	Fe	C12'	C11'	-147(2)	. . . . .	?
C13	Fe	C12'	C13'	-26(2)	. . . . .	?
C14	Fe	C12'	C11	-87(1)	. . . . .	?
C14	Fe	C12'	C11'	-101(1)	. . . . .	?
C14	Fe	C12'	C13'	21(2)	. . . . .	?
C15	Fe	C12'	C11	-42(1)	. . . . .	?
C15	Fe	C12'	C11'	-57(1)	. . . . .	?
C15	Fe	C12'	C13'	65(2)	. . . . .	?
C11'	Fe	C12'	C11	14(1)	. . . . .	?
C11'	Fe	C12'	C11'	0(2)	. . . . .	?
C11'	Fe	C12'	C13'	121(2)	. . . . .	?
C13'	Fe	C12'	C11	-107(2)	. . . . .	?
C13'	Fe	C12'	C11'	-121(2)	. . . . .	?
C13'	Fe	C12'	C13'	0(2)	. . . . .	?
C14'	Fe	C12'	C11	-69(1)	. . . . .	?
C14'	Fe	C12'	C11'	-83(1)	. . . . .	?
C14'	Fe	C12'	C13'	39(2)	. . . . .	?
C15'	Fe	C12'	C11	-26(1)	. . . . .	?
C15'	Fe	C12'	C11'	-40(1)	. . . . .	?
C15'	Fe	C12'	C13'	81(2)	. . . . .	?
C21	Fe	C12'	C11	-121(1)	. . . . .	?
C21	Fe	C12'	C11'	-135(1)	. . . . .	?
C21	Fe	C12'	C13'	-13(1)	. . . . .	?
C22	Fe	C12'	C11	44(1)	. . . . .	?
C22	Fe	C12'	C11'	30(1)	. . . . .	?

C22	Fe	C12'	C13'	152(1)	. . . . .	?
C23	Fe	C12'	C11	81(1)	. . . . .	?
C23	Fe	C12'	C11'	66(1)	. . . . .	?
C23	Fe	C12'	C13'	-172(1)	. . . . .	?
C24	Fe	C12'	C11	118(1)	. . . . .	?
C24	Fe	C12'	C11'	104(1)	. . . . .	?
C24	Fe	C12'	C13'	-135(1)	. . . . .	?
C25	Fe	C12'	C11	159(1)	. . . . .	?
C25	Fe	C12'	C11'	145(1)	. . . . .	?
C25	Fe	C12'	C13'	-93(1)	. . . . .	?
C26	Fe	C12'	C11	-163(1)	. . . . .	?
C26	Fe	C12'	C11'	-177(1)	. . . . .	?
C26	Fe	C12'	C13'	-56(1)	. . . . .	?
C11	Fe	C13'	C12'	-53(2)	. . . . .	?
C11	Fe	C13'	C14'	64(2)	. . . . .	?
C12	Fe	C13'	C12'	-11(2)	. . . . .	?
C12	Fe	C13'	C14'	107(2)	. . . . .	?
C13	Fe	C13'	C12'	27(3)	. . . . .	?
C13	Fe	C13'	C14'	144(3)	. . . . .	?
C14	Fe	C13'	C12'	-129(2)	. . . . .	?
C14	Fe	C13'	C14'	-11(2)	. . . . .	?
C15	Fe	C13'	C12'	-94(2)	. . . . .	?
C15	Fe	C13'	C14'	23(2)	. . . . .	?
C11'	Fe	C13'	C12'	-36(2)	. . . . .	?
C11'	Fe	C13'	C14'	81(2)	. . . . .	?
C12'	Fe	C13'	C12'	0(2)	. . . . .	?
C12'	Fe	C13'	C14'	117(2)	. . . . .	?
C14'	Fe	C13'	C12'	-117(2)	. . . . .	?
C14'	Fe	C13'	C14'	0(2)	. . . . .	?
C15'	Fe	C13'	C12'	-82(2)	. . . . .	?
C15'	Fe	C13'	C14'	36(2)	. . . . .	?
C21	Fe	C13'	C12'	175(1)	. . . . .	?
C21	Fe	C13'	C14'	-67(1)	. . . . .	?
C22	Fe	C13'	C12'	-148(1)	. . . . .	?
C22	Fe	C13'	C14'	-31(1)	. . . . .	?
C23	Fe	C13'	C12'	20(1)	. . . . .	?
C23	Fe	C13'	C14'	137(1)	. . . . .	?
C24	Fe	C13'	C12'	61(1)	. . . . .	?
C24	Fe	C13'	C14'	178(1)	. . . . .	?
C25	Fe	C13'	C12'	98(1)	. . . . .	?
C25	Fe	C13'	C14'	-145(1)	. . . . .	?
C26	Fe	C13'	C12'	139(1)	. . . . .	?
C26	Fe	C13'	C14'	-104(1)	. . . . .	?
C11	Fe	C14'	C13'	-96(2)	. . . . .	?
C11	Fe	C14'	C15'	25(2)	. . . . .	?
C12	Fe	C14'	C13'	-56(2)	. . . . .	?
C12	Fe	C14'	C15'	66(2)	. . . . .	?
C13	Fe	C14'	C13'	-14(2)	. . . . .	?
C13	Fe	C14'	C15'	107(2)	. . . . .	?
C14	Fe	C14'	C13'	13(2)	. . . . .	?
C14	Fe	C14'	C15'	134(2)	. . . . .	?
C15	Fe	C14'	C13'	-126(2)	. . . . .	?
C15	Fe	C14'	C15'	-5(2)	. . . . .	?
C11'	Fe	C14'	C13'	-81(2)	. . . . .	?
C11'	Fe	C14'	C15'	40(2)	. . . . .	?
C12'	Fe	C14'	C13'	-38(2)	. . . . .	?
C12'	Fe	C14'	C15'	84(2)	. . . . .	?
C13'	Fe	C14'	C13'	0(2)	. . . . .	?
C13'	Fe	C14'	C15'	121(2)	. . . . .	?
C15'	Fe	C14'	C13'	-121(2)	. . . . .	?
C15'	Fe	C14'	C15'	0(2)	. . . . .	?

C21	Fe	C14'	C13'	129(1)	. . . . . ?
C21	Fe	C14'	C15'	-110(1)	. . . . . ?
C22	Fe	C14'	C13'	168(1)	. . . . . ?
C22	Fe	C14'	C15'	-71(1)	. . . . . ?
C23	Fe	C14'	C13'	-152(1)	. . . . . ?
C23	Fe	C14'	C15'	-31(1)	. . . . . ?
C24	Fe	C14'	C13'	-6(1)	. . . . . ?
C24	Fe	C14'	C15'	115(1)	. . . . . ?
C25	Fe	C14'	C13'	51(1)	. . . . . ?
C25	Fe	C14'	C15'	172(1)	. . . . . ?
C26	Fe	C14'	C13'	88(1)	. . . . . ?
C26	Fe	C14'	C15'	-150(1)	. . . . . ?
C11	Fe	C15'	C11'	-11(2)	. . . . . ?
C11	Fe	C15'	C14'	-128(2)	. . . . . ?
C12	Fe	C15'	C11'	18(2)	. . . . . ?
C12	Fe	C15'	C14'	-98(2)	. . . . . ?
C13	Fe	C15'	C11'	60(2)	. . . . . ?
C13	Fe	C15'	C14'	-56(2)	. . . . . ?
C14	Fe	C15'	C11'	100(1)	. . . . . ?
C14	Fe	C15'	C14'	-17(2)	. . . . . ?
C15	Fe	C15'	C11'	123(3)	. . . . . ?
C15	Fe	C15'	C14'	7(3)	. . . . . ?
C11'	Fe	C15'	C11'	0(2)	. . . . . ?
C11'	Fe	C15'	C14'	-116(2)	. . . . . ?
C12'	Fe	C15'	C11'	38(1)	. . . . . ?
C12'	Fe	C15'	C14'	-78(2)	. . . . . ?
C13'	Fe	C15'	C11'	80(2)	. . . . . ?
C13'	Fe	C15'	C14'	-36(2)	. . . . . ?
C14'	Fe	C15'	C11'	116(2)	. . . . . ?
C14'	Fe	C15'	C14'	0(2)	. . . . . ?
C21	Fe	C15'	C11'	-160(1)	. . . . . ?
C21	Fe	C15'	C14'	84(1)	. . . . . ?
C22	Fe	C15'	C11'	-119(1)	. . . . . ?
C22	Fe	C15'	C14'	124(1)	. . . . . ?
C23	Fe	C15'	C11'	-79(1)	. . . . . ?
C23	Fe	C15'	C14'	164(1)	. . . . . ?
C24	Fe	C15'	C11'	-43(1)	. . . . . ?
C24	Fe	C15'	C14'	-159(1)	. . . . . ?
C25	Fe	C15'	C11'	77(1)	. . . . . ?
C25	Fe	C15'	C14'	-40(2)	. . . . . ?
C26	Fe	C15'	C11'	163(1)	. . . . . ?
C26	Fe	C15'	C14'	47(1)	. . . . . ?
C11	Fe	C21	C22	64(1)	. . . . . ?
C11	Fe	C21	C26	-162(1)	. . . . . ?
C11	Fe	C21	C41	-36(1)	. . . . . ?
C12	Fe	C21	C22	58(8)	. . . . . ?
C12	Fe	C21	C26	-167(8)	. . . . . ?
C12	Fe	C21	C41	-41(8)	. . . . . ?
C13	Fe	C21	C22	178(1)	. . . . . ?
C13	Fe	C21	C26	-48(1)	. . . . . ?
C13	Fe	C21	C41	78(1)	. . . . . ?
C14	Fe	C21	C22	141.5(5)	. . . . . ?
C14	Fe	C21	C26	-84.4(5)	. . . . . ?
C14	Fe	C21	C41	41.6(5)	. . . . . ?
C15	Fe	C21	C22	99.0(7)	. . . . . ?
C15	Fe	C21	C26	-126.9(7)	. . . . . ?
C15	Fe	C21	C41	-0.9(7)	. . . . . ?
C11'	Fe	C21	C22	56(1)	. . . . . ?
C11'	Fe	C21	C26	-170(1)	. . . . . ?
C11'	Fe	C21	C41	-44(1)	. . . . . ?

C12'	Fe	C21	C22	171(2)	.	.	.	.	?
C12'	Fe	C21	C26	-55(2)	.	.	.	.	?
C12'	Fe	C21	C41	71(2)	.	.	.	.	?
C13'	Fe	C21	C22	160.6(8)	.	.	.	.	?
C13'	Fe	C21	C26	-65.3(8)	.	.	.	.	?
C13'	Fe	C21	C41	60.7(8)	.	.	.	.	?
C14'	Fe	C21	C22	123.5(7)	.	.	.	.	?
C14'	Fe	C21	C26	-102.4(7)	.	.	.	.	?
C14'	Fe	C21	C41	23.6(7)	.	.	.	.	?
C15'	Fe	C21	C22	83.5(7)	.	.	.	.	?
C15'	Fe	C21	C26	-142.4(7)	.	.	.	.	?
C15'	Fe	C21	C41	-16.4(7)	.	.	.	.	?
C22	Fe	C21	C22	0.0(1)	.	.	.	.	?
C22	Fe	C21	C26	134.1(1)	.	.	.	.	?
C22	Fe	C21	C41	-99.9(2)	.	.	.	.	?
C23	Fe	C21	C22	-27.6(1)	.	.	.	.	?
C23	Fe	C21	C26	106.5(1)	.	.	.	.	?
C23	Fe	C21	C41	-127.5(1)	.	.	.	.	?
C24	Fe	C21	C22	-65.7(1)	.	.	.	.	?
C24	Fe	C21	C26	68.4(1)	.	.	.	.	?
C24	Fe	C21	C41	-165.6(2)	.	.	.	.	?
C25	Fe	C21	C22	-104.0(1)	.	.	.	.	?
C25	Fe	C21	C26	30.1(2)	.	.	.	.	?
C25	Fe	C21	C41	156.1(2)	.	.	.	.	?
C26	Fe	C21	C22	-134.1(1)	.	.	.	.	?
C26	Fe	C21	C26	0.0(2)	.	.	.	.	?
C26	Fe	C21	C41	126.0(2)	.	.	.	.	?
C11	Fe	C22	C21	-137.6(7)	.	.	.	.	?
C11	Fe	C22	C23	86.6(7)	.	.	.	.	?
C11	Fe	C22	C31	-37.3(7)	.	.	.	.	?
C12	Fe	C22	C21	-174(1)	.	.	.	.	?
C12	Fe	C22	C23	51(1)	.	.	.	.	?
C12	Fe	C22	C31	-73(1)	.	.	.	.	?
C13	Fe	C22	C21	-143(25)	.	.	.	.	?
C13	Fe	C22	C23	81(25)	.	.	.	.	?
C13	Fe	C22	C31	-43(25)	.	.	.	.	?
C14	Fe	C22	C21	-60.7(7)	.	.	.	.	?
C14	Fe	C22	C23	163.5(7)	.	.	.	.	?
C14	Fe	C22	C31	39.6(7)	.	.	.	.	?
C15	Fe	C22	C21	-96.0(7)	.	.	.	.	?
C15	Fe	C22	C23	128.2(7)	.	.	.	.	?
C15	Fe	C22	C31	4.2(7)	.	.	.	.	?
C11'	Fe	C22	C21	-151.8(6)	.	.	.	.	?
C11'	Fe	C22	C23	72.4(6)	.	.	.	.	?
C11'	Fe	C22	C31	-51.5(6)	.	.	.	.	?
C12'	Fe	C22	C21	-173(2)	.	.	.	.	?
C12'	Fe	C22	C23	51(2)	.	.	.	.	?
C12'	Fe	C22	C31	-73(2)	.	.	.	.	?
C13'	Fe	C22	C21	-50(2)	.	.	.	.	?
C13'	Fe	C22	C23	174(2)	.	.	.	.	?
C13'	Fe	C22	C31	50(2)	.	.	.	.	?
C14'	Fe	C22	C21	-72.7(8)	.	.	.	.	?
C14'	Fe	C22	C23	151.5(8)	.	.	.	.	?
C14'	Fe	C22	C31	27.6(8)	.	.	.	.	?
C15'	Fe	C22	C21	-110.2(7)	.	.	.	.	?
C15'	Fe	C22	C23	113.9(7)	.	.	.	.	?
C15'	Fe	C22	C31	-10.0(7)	.	.	.	.	?
C21	Fe	C22	C21	0.0(1)	.	.	.	.	?
C21	Fe	C22	C23	-135.8(1)	.	.	.	.	?
C21	Fe	C22	C31	100.2(1)	.	.	.	.	?
C23	Fe	C22	C21	135.8(1)	.	.	.	.	?

C23	Fe	C22	C23	0.0(1)	.	.	.	.	?
C23	Fe	C22	C31	-123.9(2)	.	.	.	.	?
C24	Fe	C22	C21	105.9(1)	.	.	.	.	?
C24	Fe	C22	C23	-29.9(1)	.	.	.	.	?
C24	Fe	C22	C31	-153.9(1)	.	.	.	.	?
C25	Fe	C22	C21	67.4(1)	.	.	.	.	?
C25	Fe	C22	C23	-68.4(1)	.	.	.	.	?
C25	Fe	C22	C31	167.7(1)	.	.	.	.	?
C26	Fe	C22	C21	28.7(1)	.	.	.	.	?
C26	Fe	C22	C23	-107.1(1)	.	.	.	.	?
C26	Fe	C22	C31	128.9(1)	.	.	.	.	?
C11	Fe	C23	C22	-106.0(7)	.	.	.	.	?
C11	Fe	C23	C24	122.0(7)	.	.	.	.	?
C12	Fe	C23	C22	-147.1(7)	.	.	.	.	?
C12	Fe	C23	C24	80.8(7)	.	.	.	.	?
C13	Fe	C23	C22	-177(1)	.	.	.	.	?
C13	Fe	C23	C24	51(1)	.	.	.	.	?
C14	Fe	C23	C22	-85(3)	.	.	.	.	?
C14	Fe	C23	C24	143(3)	.	.	.	.	?
C15	Fe	C23	C22	-73.0(8)	.	.	.	.	?
C15	Fe	C23	C24	154.9(8)	.	.	.	.	?
C11'	Fe	C23	C22	-122.1(6)	.	.	.	.	?
C11'	Fe	C23	C24	105.8(6)	.	.	.	.	?
C12'	Fe	C23	C22	-158.6(7)	.	.	.	.	?
C12'	Fe	C23	C24	69.3(7)	.	.	.	.	?
C13'	Fe	C23	C22	-174(2)	.	.	.	.	?
C13'	Fe	C23	C24	54(2)	.	.	.	.	?
C14'	Fe	C23	C22	-59(1)	.	.	.	.	?
C14'	Fe	C23	C24	168(1)	.	.	.	.	?
C15'	Fe	C23	C22	-80.5(7)	.	.	.	.	?
C15'	Fe	C23	C24	147.5(7)	.	.	.	.	?
C21	Fe	C23	C22	27.6(1)	.	.	.	.	?
C21	Fe	C23	C24	-104.5(1)	.	.	.	.	?
C22	Fe	C23	C22	0.0(1)	.	.	.	.	?
C22	Fe	C23	C24	-132.1(2)	.	.	.	.	?
C24	Fe	C23	C22	132.1(2)	.	.	.	.	?
C24	Fe	C23	C24	0.0(2)	.	.	.	.	?
C25	Fe	C23	C22	103.2(1)	.	.	.	.	?
C25	Fe	C23	C24	-28.9(2)	.	.	.	.	?
C26	Fe	C23	C22	65.0(1)	.	.	.	.	?
C26	Fe	C23	C24	-67.1(2)	.	.	.	.	?
C11	Fe	C24	C23	-73.5(8)	.	.	.	.	?
C11	Fe	C24	C25	152.6(8)	.	.	.	.	?
C12	Fe	C24	C23	-108.5(7)	.	.	.	.	?
C12	Fe	C24	C25	117.5(7)	.	.	.	.	?
C13	Fe	C24	C23	-148.5(8)	.	.	.	.	?
C13	Fe	C24	C25	77.5(8)	.	.	.	.	?
C14	Fe	C24	C23	-167.5(9)	.	.	.	.	?
C14	Fe	C24	C25	58.6(9)	.	.	.	.	?
C15	Fe	C24	C23	-68(2)	.	.	.	.	?
C15	Fe	C24	C25	158(2)	.	.	.	.	?
C11'	Fe	C24	C23	-86.0(6)	.	.	.	.	?
C11'	Fe	C24	C25	140.0(6)	.	.	.	.	?
C12'	Fe	C24	C23	-126.8(6)	.	.	.	.	?
C12'	Fe	C24	C25	99.2(6)	.	.	.	.	?
C13'	Fe	C24	C23	-160.7(8)	.	.	.	.	?
C13'	Fe	C24	C25	65.4(8)	.	.	.	.	?
C14'	Fe	C24	C23	-156(3)	.	.	.	.	?
C14'	Fe	C24	C25	70(3)	.	.	.	.	?
C15'	Fe	C24	C23	-58(1)	.	.	.	.	?

C15'	Fe	C24	C25	168(1)	.	.	.	.	.	?
C21	Fe	C24	C23	67.3(1)	.	.	.	.	.	?
C21	Fe	C24	C25	-66.7(2)	.	.	.	.	.	?
C22	Fe	C24	C23	29.8(1)	.	.	.	.	.	?
C22	Fe	C24	C25	-104.2(2)	.	.	.	.	.	?
C23	Fe	C24	C23	-0.0(2)	.	.	.	.	.	?
C23	Fe	C24	C25	-134.0(2)	.	.	.	.	.	?
C25	Fe	C24	C23	134.0(2)	.	.	.	.	.	?
C25	Fe	C24	C25	0.0(2)	.	.	.	.	.	?
C26	Fe	C24	C23	105.4(2)	.	.	.	.	.	?
C26	Fe	C24	C25	-28.6(2)	.	.	.	.	.	?
C11	Fe	C25	C24	-57(1)	.	.	.	.	.	?
C11	Fe	C25	C26	169(1)	.	.	.	.	.	?
C12	Fe	C25	C24	-73.4(8)	.	.	.	.	.	?
C12	Fe	C25	C26	152.0(8)	.	.	.	.	.	?
C13	Fe	C25	C24	-112.2(8)	.	.	.	.	.	?
C13	Fe	C25	C26	113.2(8)	.	.	.	.	.	?
C14	Fe	C25	C24	-149.6(6)	.	.	.	.	.	?
C14	Fe	C25	C26	75.8(6)	.	.	.	.	.	?
C15	Fe	C25	C24	-159(2)	.	.	.	.	.	?
C15	Fe	C25	C26	66(2)	.	.	.	.	.	?
C11'	Fe	C25	C24	-60.7(8)	.	.	.	.	.	?
C11'	Fe	C25	C26	164.7(8)	.	.	.	.	.	?
C12'	Fe	C25	C24	-92.2(6)	.	.	.	.	.	?
C12'	Fe	C25	C26	133.2(6)	.	.	.	.	.	?
C13'	Fe	C25	C24	-131.9(7)	.	.	.	.	.	?
C13'	Fe	C25	C26	93.5(7)	.	.	.	.	.	?
C14'	Fe	C25	C24	-162.5(9)	.	.	.	.	.	?
C14'	Fe	C25	C26	62.9(9)	.	.	.	.	.	?
C15'	Fe	C25	C24	-129(4)	.	.	.	.	.	?
C15'	Fe	C25	C26	97(4)	.	.	.	.	.	?
C21	Fe	C25	C24	104.9(2)	.	.	.	.	.	?
C21	Fe	C25	C26	-29.7(2)	.	.	.	.	.	?
C22	Fe	C25	C24	66.9(2)	.	.	.	.	.	?
C22	Fe	C25	C26	-67.7(2)	.	.	.	.	.	?
C23	Fe	C25	C24	28.8(2)	.	.	.	.	.	?
C23	Fe	C25	C26	-105.8(2)	.	.	.	.	.	?
C24	Fe	C25	C24	0.0(2)	.	.	.	.	.	?
C24	Fe	C25	C26	-134.6(2)	.	.	.	.	.	?
C26	Fe	C25	C24	134.6(2)	.	.	.	.	.	?
C26	Fe	C25	C26	0.0(2)	.	.	.	.	.	?
C11	Fe	C26	C21	72(3)	.	.	.	.	.	?
C11	Fe	C26	C25	-156(3)	.	.	.	.	.	?
C12	Fe	C26	C21	178(1)	.	.	.	.	.	?
C12	Fe	C26	C25	-50(1)	.	.	.	.	.	?
C13	Fe	C26	C21	151.1(8)	.	.	.	.	.	?
C13	Fe	C26	C25	-76.7(8)	.	.	.	.	.	?
C14	Fe	C26	C21	108.6(5)	.	.	.	.	.	?
C14	Fe	C26	C25	-119.3(5)	.	.	.	.	.	?
C15	Fe	C26	C21	73.4(8)	.	.	.	.	.	?
C15	Fe	C26	C25	-154.5(8)	.	.	.	.	.	?
C11'	Fe	C26	C21	153(3)	.	.	.	.	.	?
C11'	Fe	C26	C25	-74(3)	.	.	.	.	.	?
C12'	Fe	C26	C21	162.4(8)	.	.	.	.	.	?
C12'	Fe	C26	C25	-65.4(8)	.	.	.	.	.	?
C13'	Fe	C26	C21	130.6(7)	.	.	.	.	.	?
C13'	Fe	C26	C25	-97.2(7)	.	.	.	.	.	?
C14'	Fe	C26	C21	90.1(7)	.	.	.	.	.	?
C14'	Fe	C26	C25	-137.8(7)	.	.	.	.	.	?
C15'	Fe	C26	C21	61(1)	.	.	.	.	.	?
C15'	Fe	C26	C25	-167(1)	.	.	.	.	.	?