# New manganese-scaffolded organic triple-deckers based on quinoxaline, pyrazine and pyrimidine cores.

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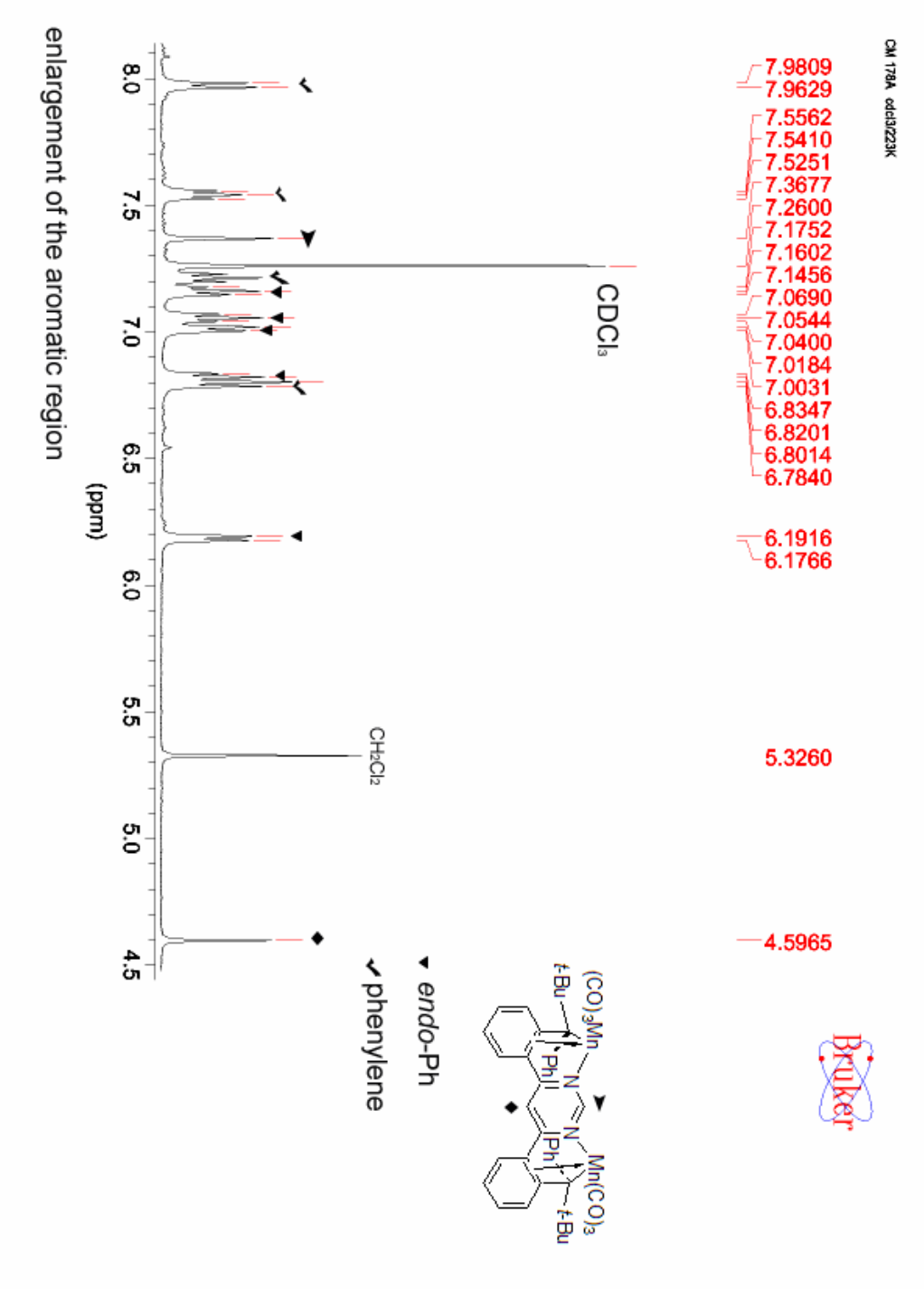
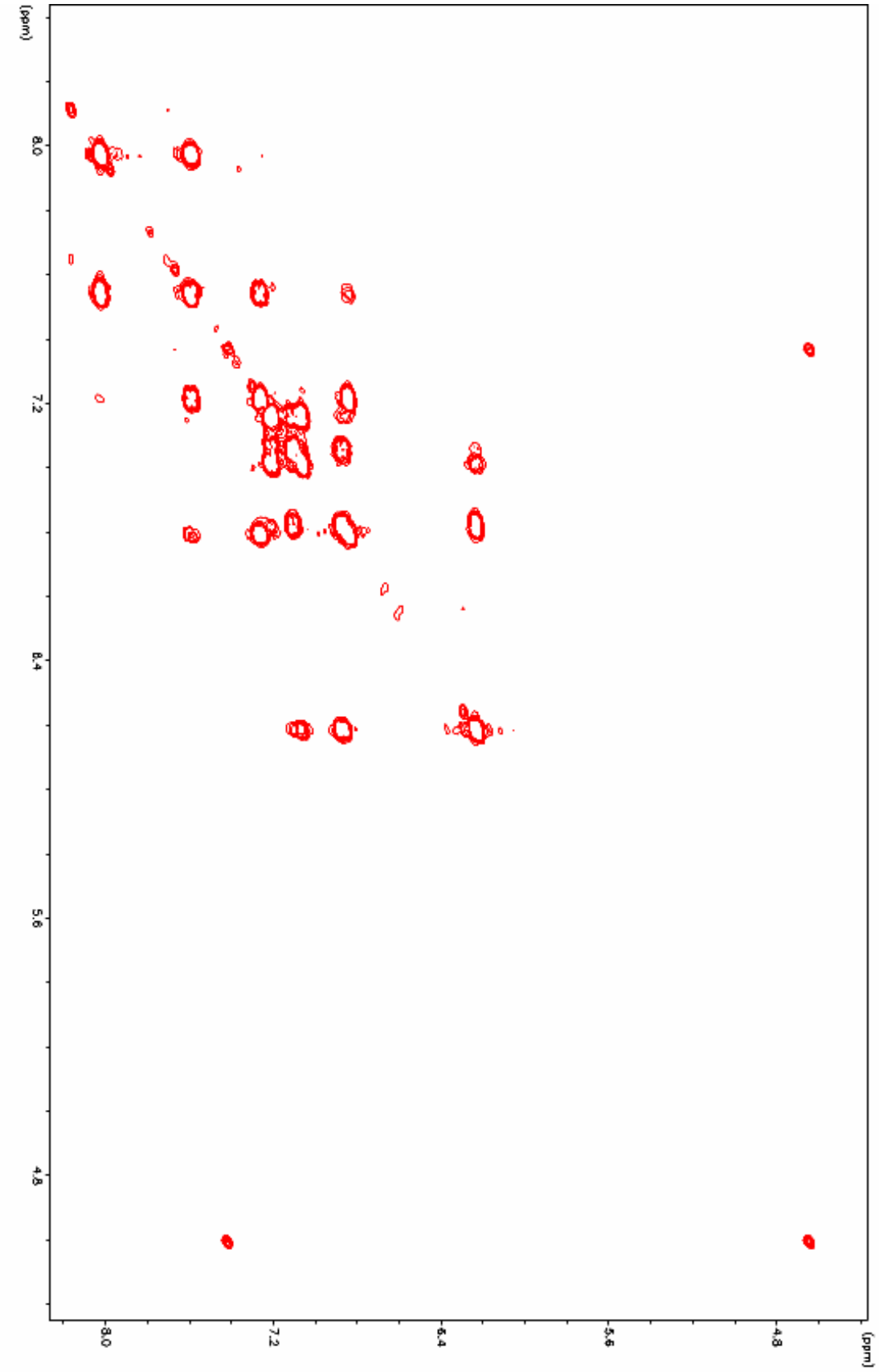
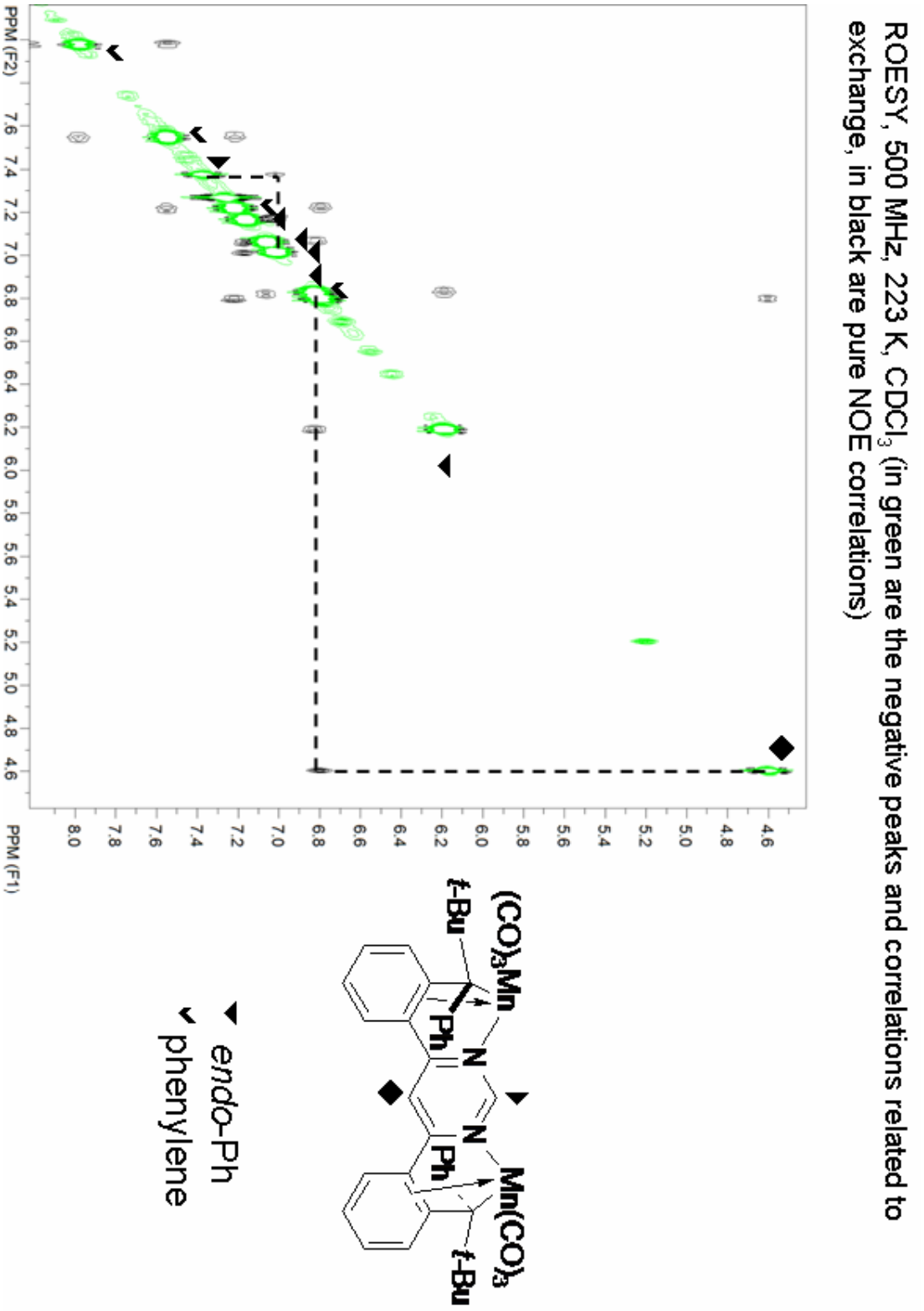
**Electronic Supporting Information**



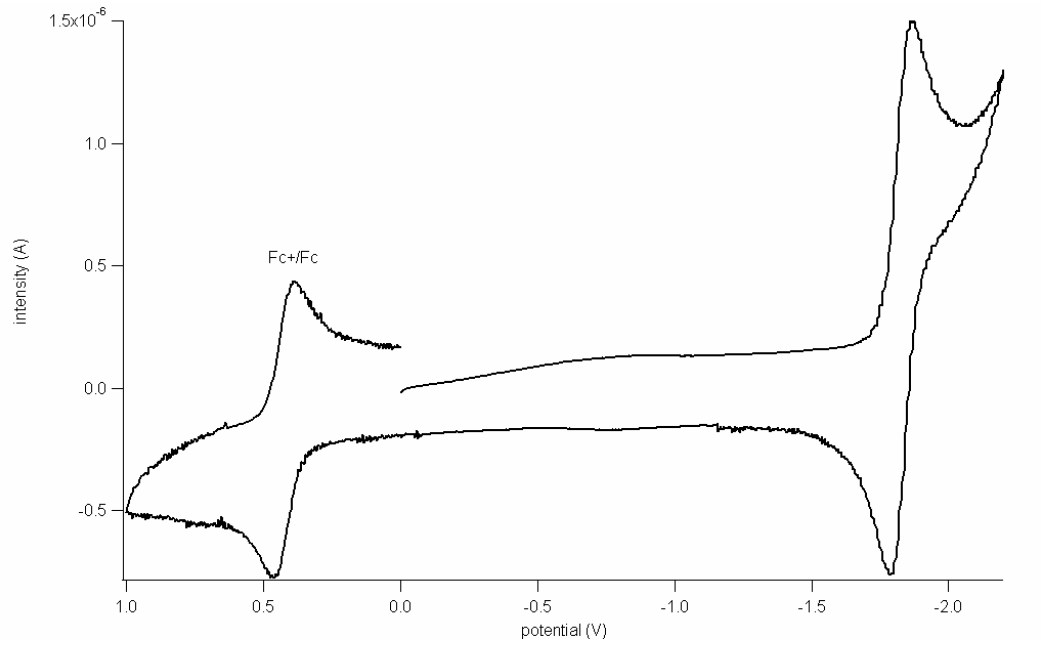

$^{1}$H NMR (500 MHz) spectrum of **3d** measured at 223 K in $CDCl_3$



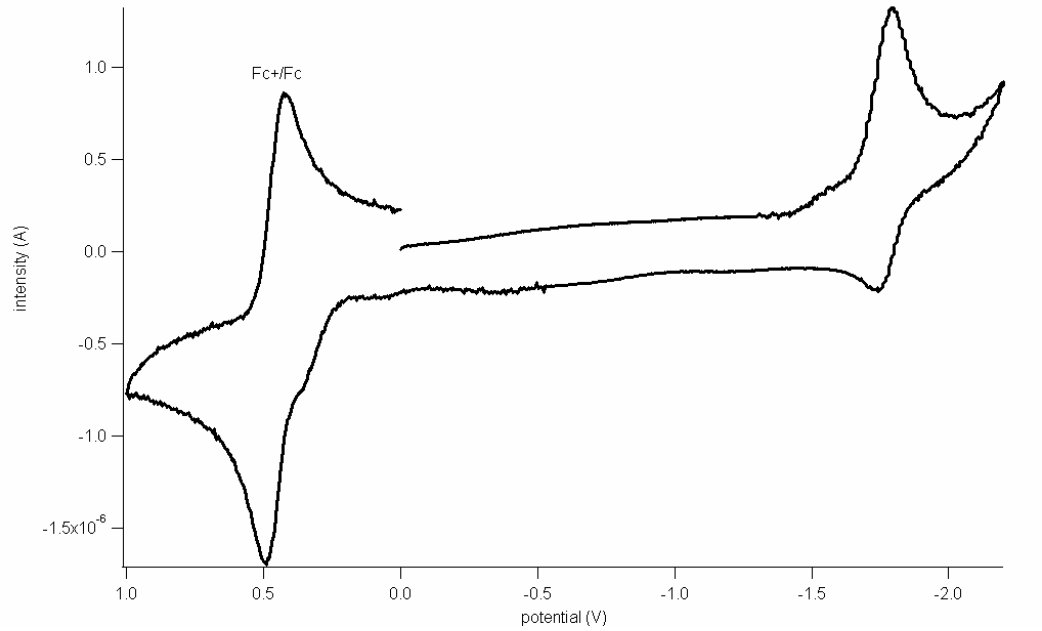

$^{1}$H-$^{1}$H COSY spectrum (500 MHz) of **3d** in $CDCl_3$ at 223 K



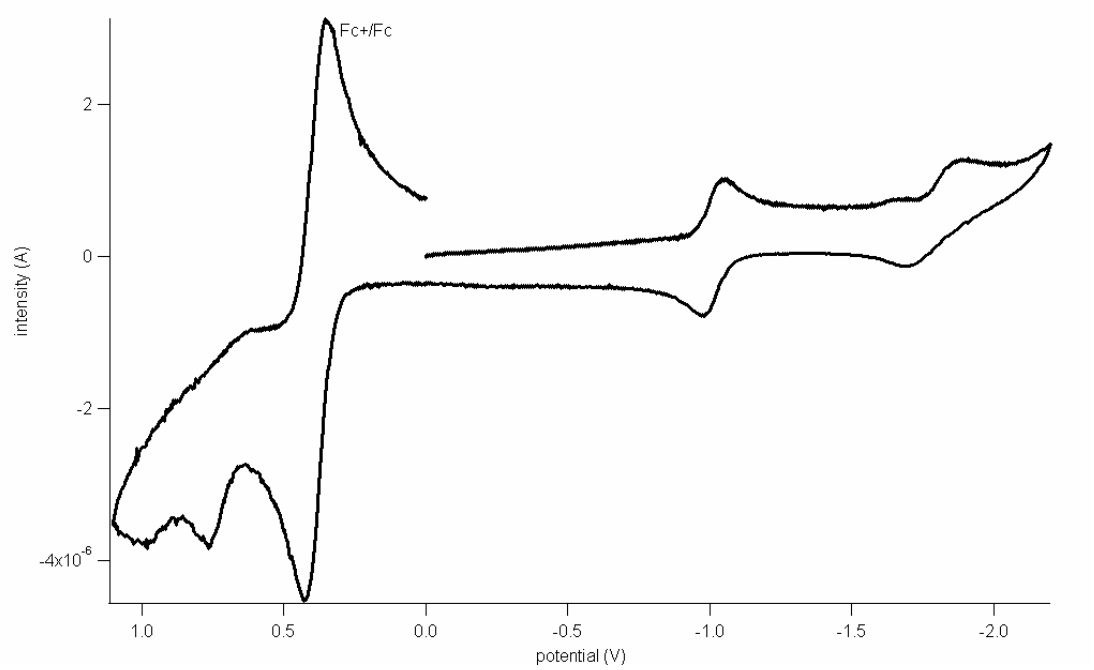

500 MHz $^{1}$H-$^{1}$H ROESY bi-dimensional spectrum of **3d** in $CDCl_3$ at 223 K.



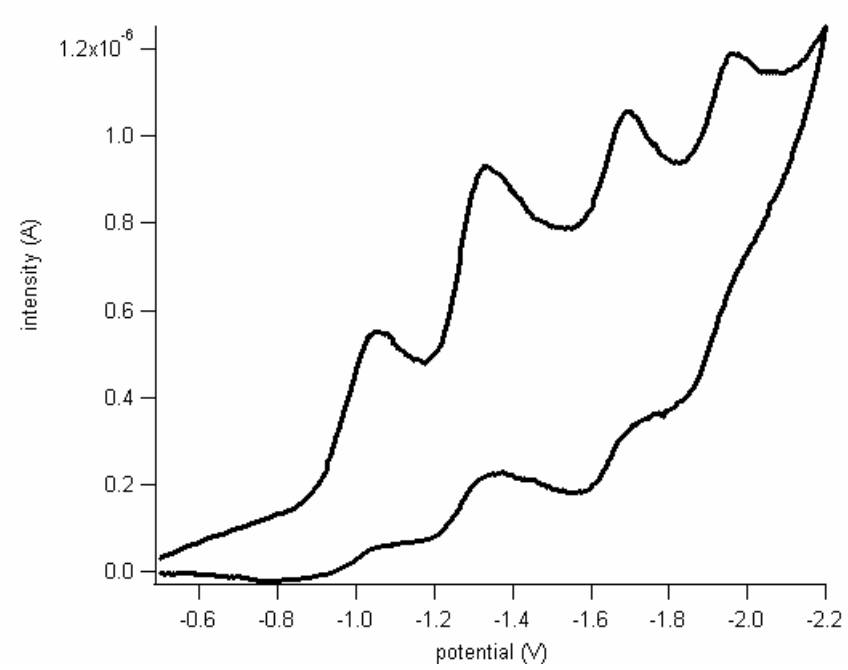

Room temperature cyclic voltammetry of 4,6-diphenylpyrimidine in MeCN ($10^{-4}$ M); scan rate 200 mV/s.



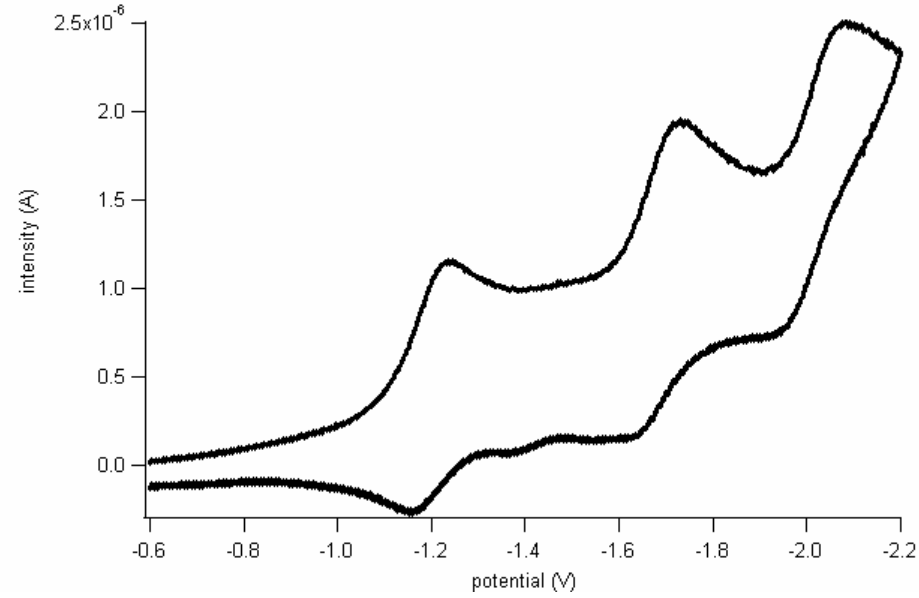

Room temperature cyclic voltammetry of 2,5-diphenylpyrazine in MeCN ($10^{-4}$ M); scan rate 200 mV/s.



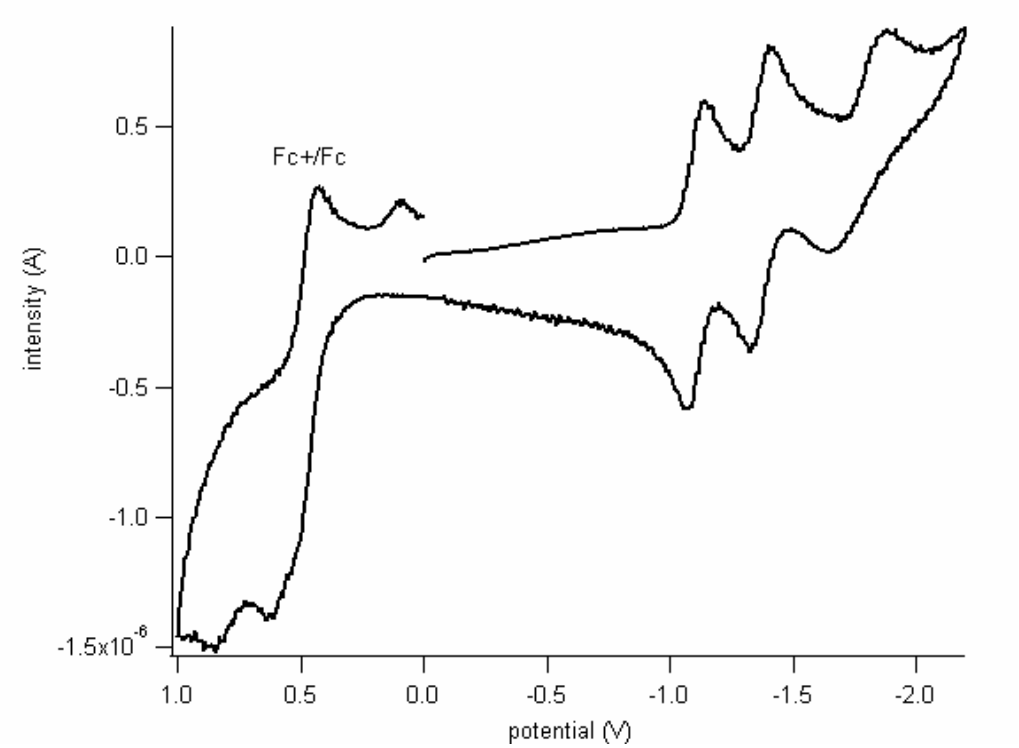

Room temperature cyclic voltammetry of **1c** in MeCN ($10^{-4}$ M); scan rate 400 mV/s.



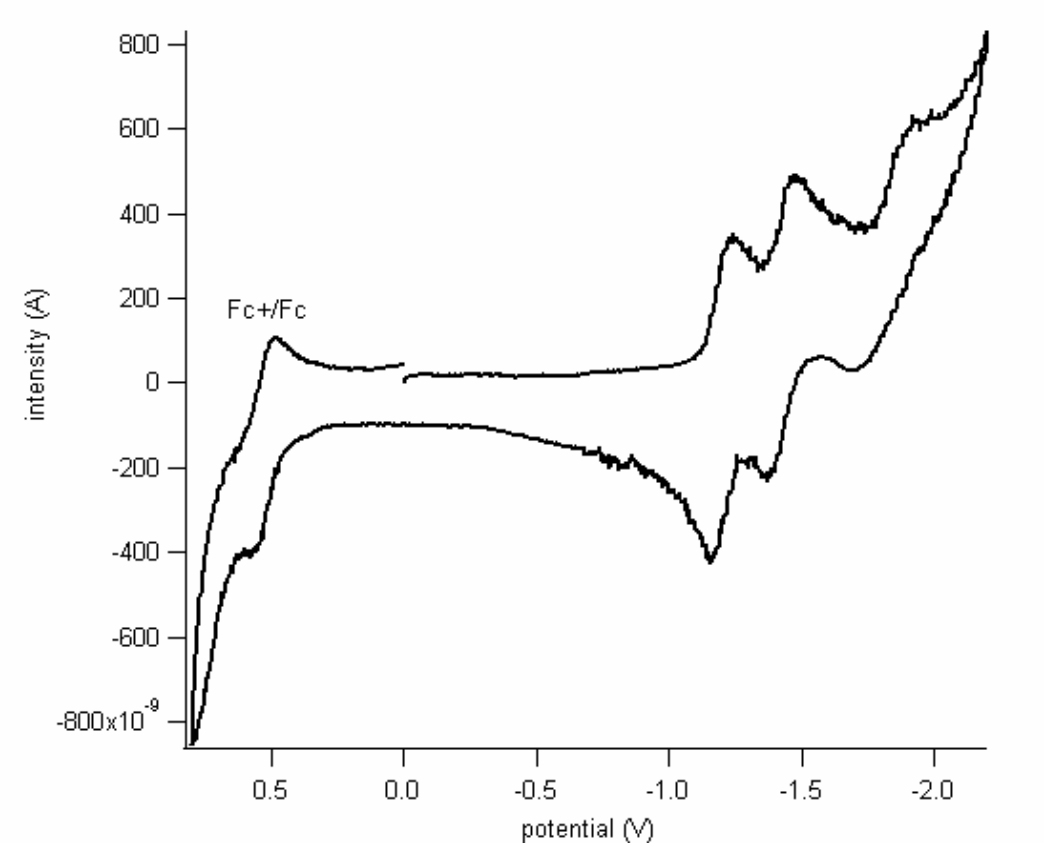

Room temperature cyclic voltammetry of **2b** in THF ($10^{-4}$ M); scan rate 50 mV/s.



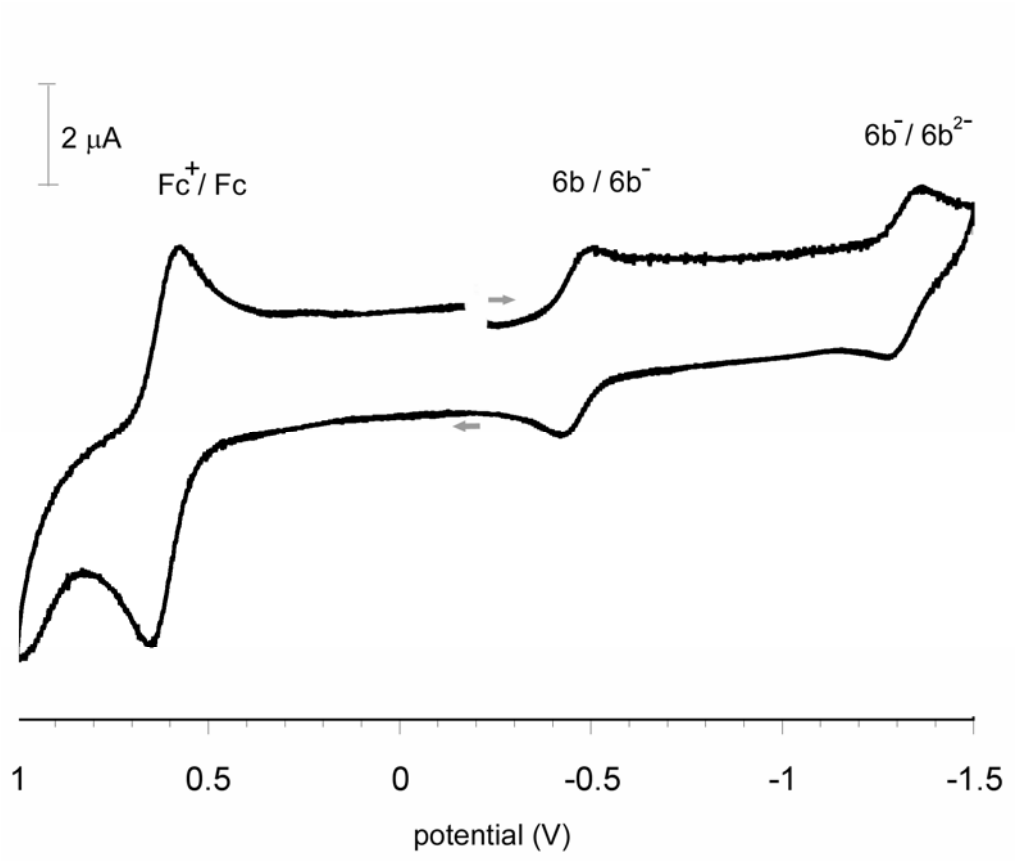

Room temperature cyclic voltammetry of **2c** in MeCN ($10^{-4}$ M); scan rate 400 mV/s.



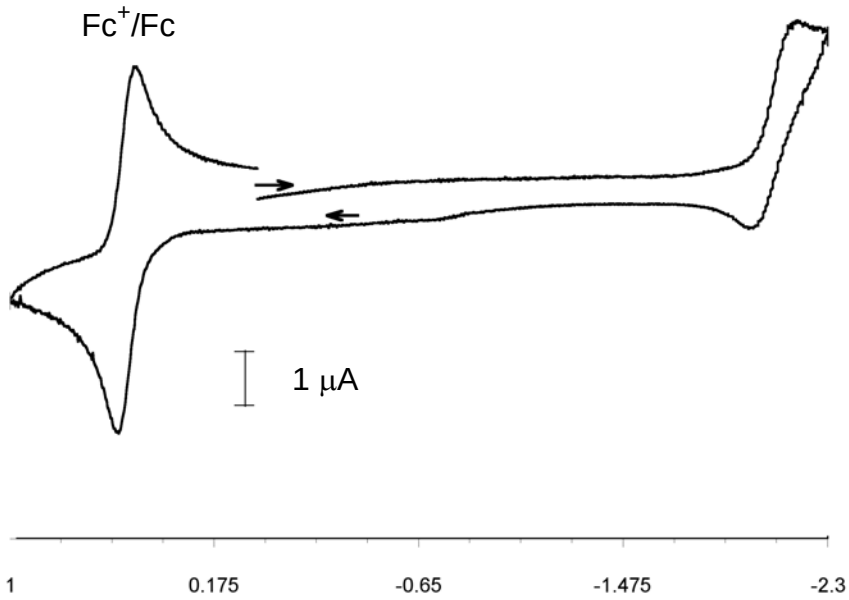

Room temperature cyclic voltammetry of **3b** in MeCN (10-4 M); scan rate 200 mV/s.



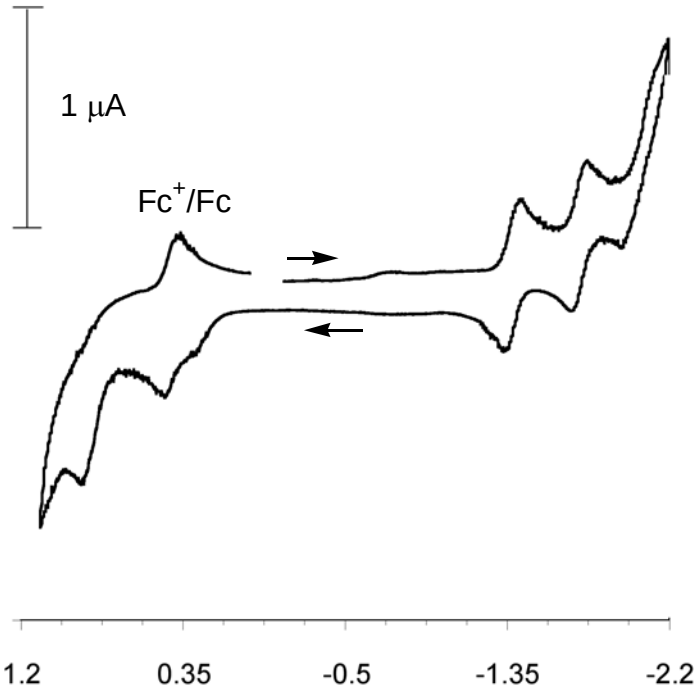

Room temperature cyclic voltammetry of **3d** in MeCN (10-4 M); scan rate 200 mV/s.




Room temperature cyclic voltammetry of **6b** in MeCN ($10^{-4}$ M); scan rate 80 mV/s.

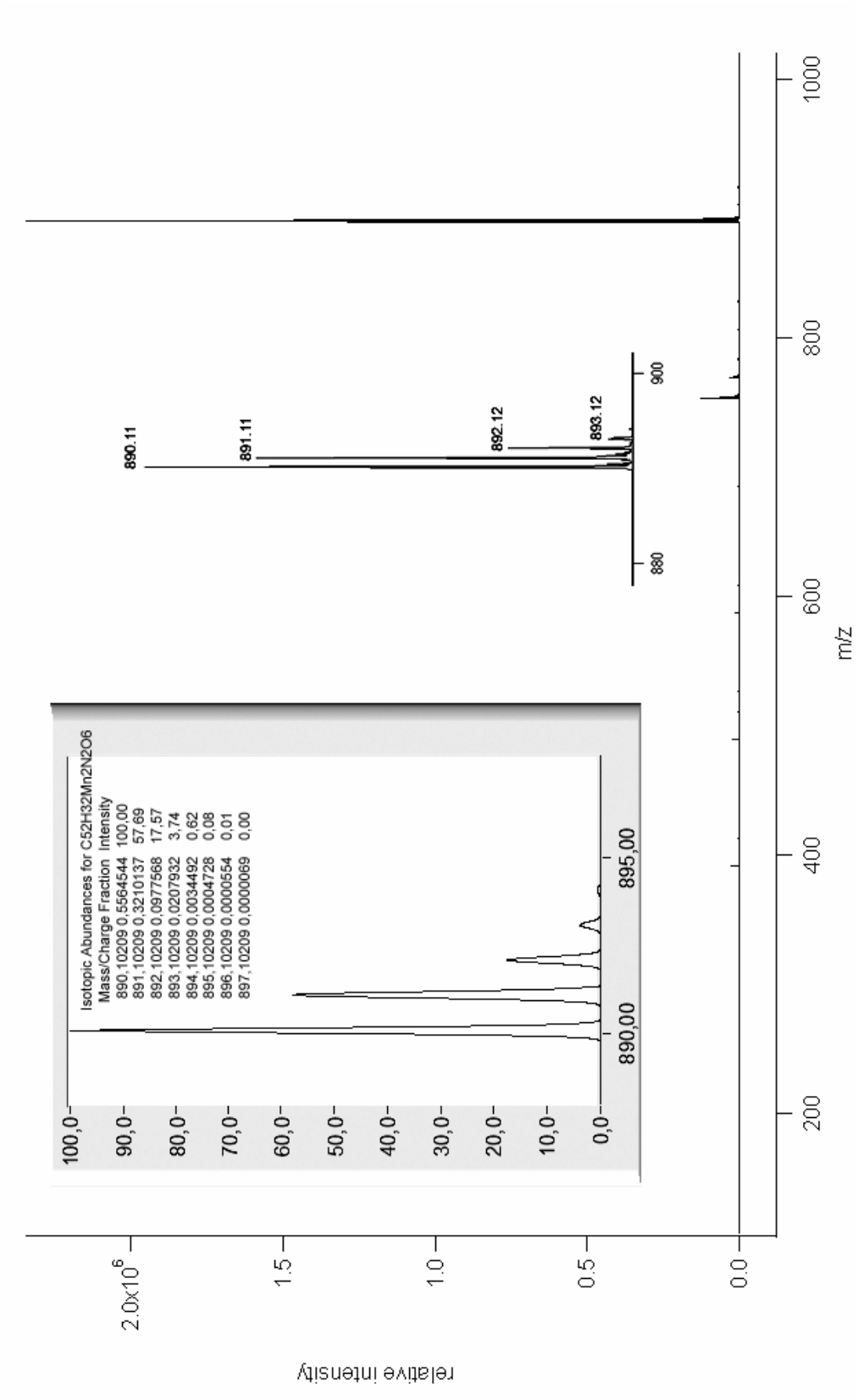



a)

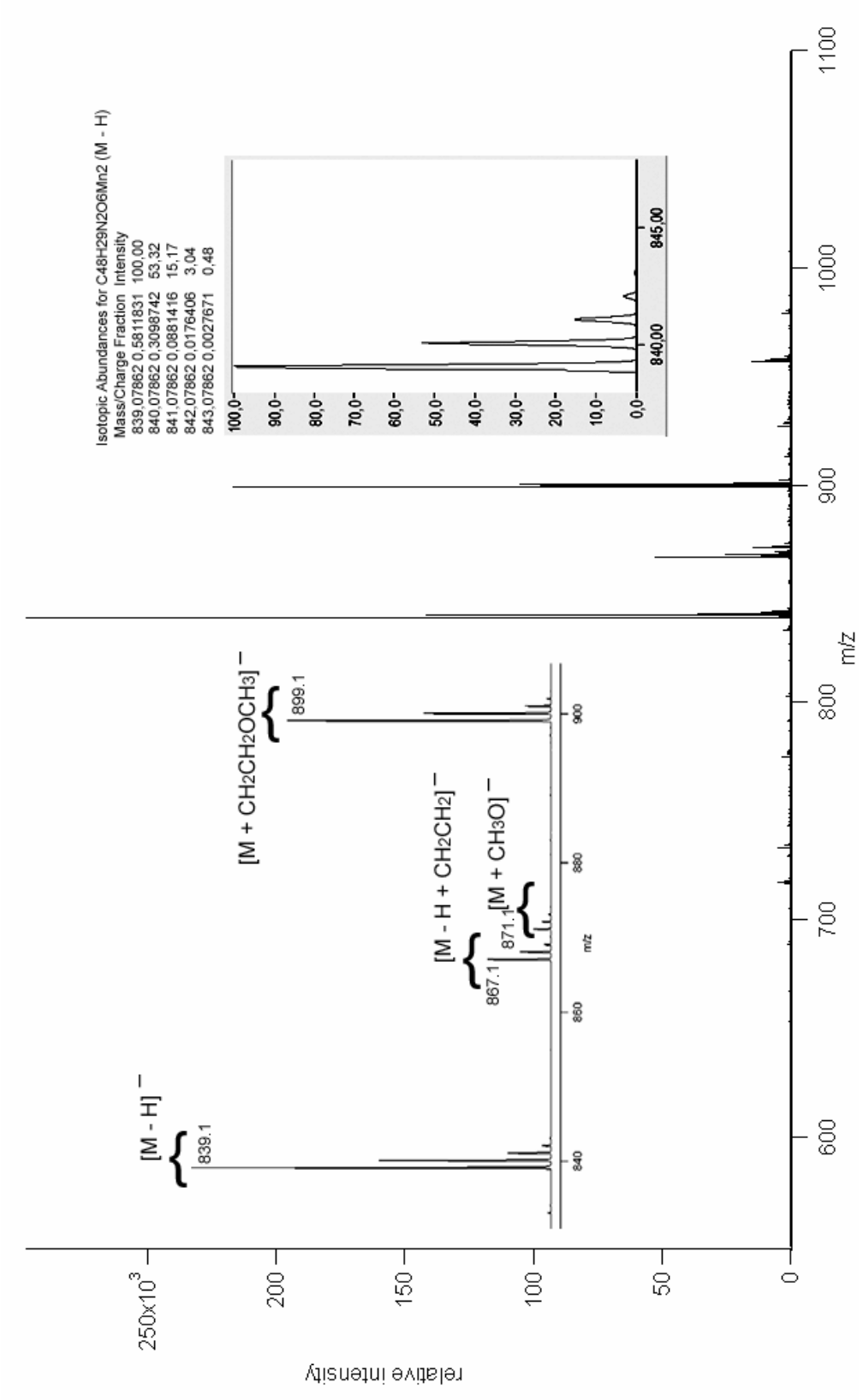



b)

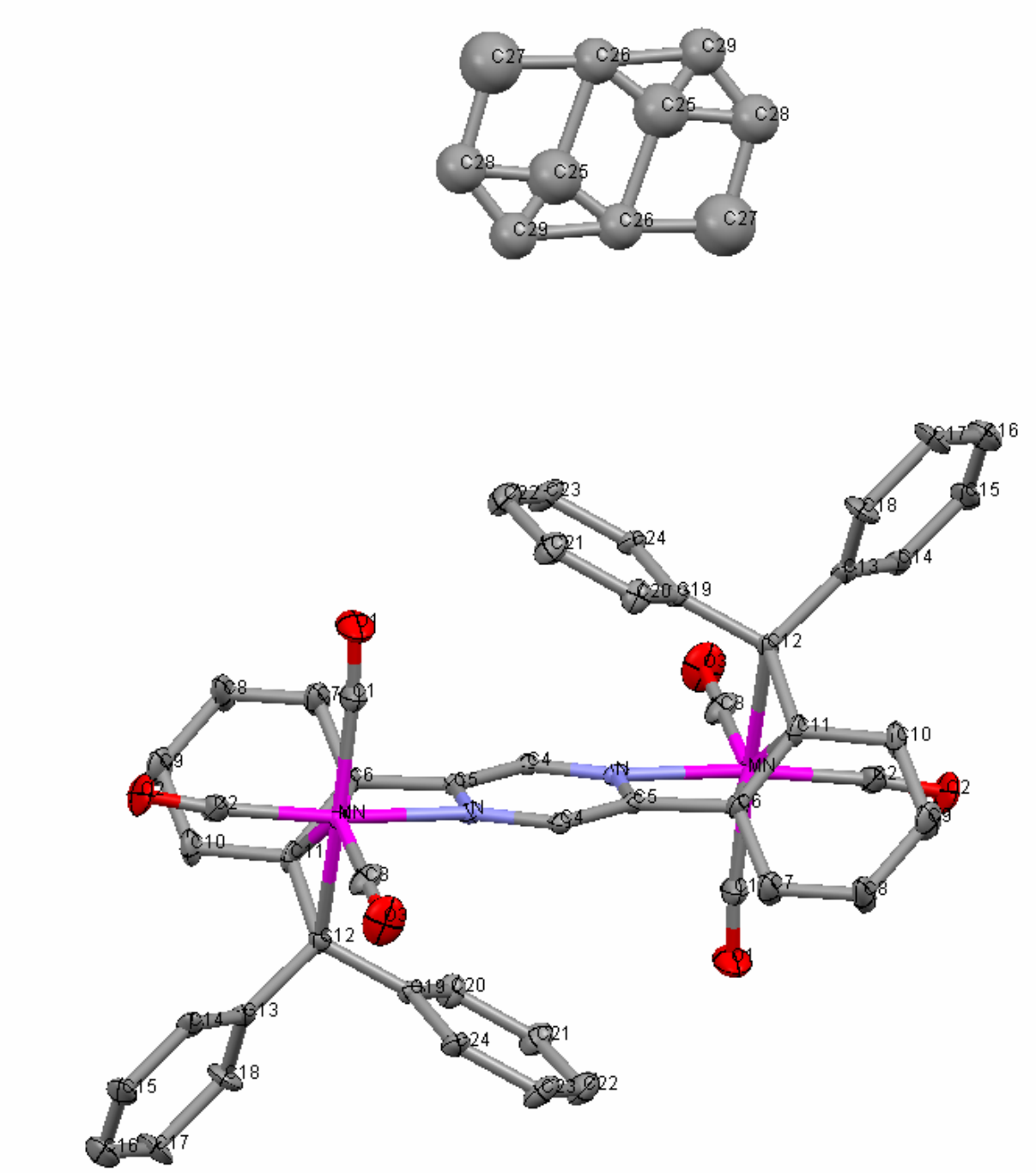
a) Room temperature cyclic voltammetry of **7** in MeCN; scan rate 800 mV/s. b) Room temperature cyclic voltammetry of **8** in MeCN; scan rate 100 mV/s.




Negative mode electrospray mass spectrum of a 1,2-dimethoxyethane solution of [**1b**]$^{\cdot-}$.




Negative mode electrospray mass spectrum of a solution of [**3b**]$^{\cdot-}$ in 1,2-dimethoxyethane: four major peaks are detected and assigned to products of degradation of the radical anion by de-hydrogenation and reaction with the solvent.




CSD Mercury 1.4 drawing of the structure of **2b**, ellipsoids are drawn at 30 % probability level.

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_audit_creation_date                4-06-02

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_publ_contact_author_address        # Address of author for correspondance
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_publ_contact_author_phone         'xxxxxxxxxx'
_publ_contact_author_fax           'xxxxxxxxxx'
_publ_contact_author_email         xxx@xx.xx.xx

_publ_requested_journal            'Acta Crystallographica C'
_publ_contact_letter
;
     Please consider this CIF submission for publication as a new structure
     paper in Acta Crystallographica Section C. The figures, chemical
     structure diagram (scheme), Transfert of Copyright Agreement form and
     structure factors will be sent on receipt of your acknowledgement
letter
;

_publ_requested_category            FM
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# 2. PROCESSING SUMMARY (IUCr Office Use Only)

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_journal_date_to_coeditor         ?
_journal_date_from_coeditor       ?
_journal_date_accepted            ?

_journal_date_printers_first      ?
_journal_date_printers_final      ?
_journal_date_proofs_out          ?
_journal_date_proofs_in           ?
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_journal_coeditor_code            ?
_journal_coeditor_notes
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_journal_techeditor_code          ?
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_journal_suppl_publ_pages         ?

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# 3. TITLE AND AUTHOR LIST

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; ?
;

# The loop structure below should contain the names  and addresses of all
# authors, in the required order  of publication. Repeat as necessary.

loop_
_publ_author_name
_publ_author_address
'Dupont Karl'           #<--'Last name, first name'
; Research School of Chemistry
 National Laboratory
 Ouchnock
 Islandia
;


# 4. TEXT
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_publ_section_exptl_prep
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; ?
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_publ_section_references
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Burla, M.C., Camalli, M., Cascarano, G.,Giacovazzo, C., Polidori, G.,
Spagna, R. &Viterbo, D. (1989).  SIR.  J. Appl. Cryst. 22, 389-393.

OpenMoleN, Interactive Intelligent Structure  solution (1997)
Nonius B.V., Delft, The Netherlands.

KappaCCD Operation Manual (1997), Nonius B.V., Delft, The Nederlands.

Otwinowski, Z. & Minor, W. (1997), Methods in Enzymology, 276, 307-326.

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_publ_section_figure_captions
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 # If more than one structure is reported, sections 5-10 should be filled
in
 # per structure. For each data set, replace the ? in the data_? line below
 # by a unique identifier.


data_4b

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# 5. CHEMICAL DATA

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_chemical_formula_structural       ?
_chemical_formula_analytical       ?
_chemical_formula_sum              'C60 H40 Mn2 N2 O6'
_chemical_formula_weight           994.87
_chemical_melting_point            ?
_chemical_compound_source          ?

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     _atom_type_description
     _atom_type_scat_dispersion_real
     _atom_type_scat_dispersion_imag
     _atom_type_scat_source
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 H  ?  0.000  0.000 International_Tables_Vol_IV_Table_2.3.1
 Mn ?  0.295  0.729 International_Tables_Vol_IV_Table_2.3.1
 N  ?  0.004  0.003 International_Tables_Vol_IV_Table_2.3.1
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 # 6. CRYSTAL DATA

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     -x,-y,-z
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_cell_length_b                    10.4576(3)
_cell_length_c                    15.1807(6)
_cell_angle_alpha                 88.237(5)
_cell_angle_beta                  85.895(5)
_cell_angle_gamma                 73.054(5)
_cell_volume                      1408.97(8)
_cell_formula_units_Z             1
_cell_measurement_temperature     294
_cell_measurement_reflns_used     ?
_cell_measurement_theta_min       ?
_cell_measurement_theta_max       ?
_cell_special_details
;
Cell parameters refined using Scalepack part of DENZO
 Z. Otwinowski, W. Minor, 1997
;

_exptl_crystal_description        prism
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# 7. EXPERIMENTAL DATA

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_diffrn_measurement_device_type    KappaCCD
_diffrn_measurement_method         '\p scans'

_diffrn_measurement_details
;
   7762 reflections were collected using program Collect
 ("Collect" Data collection software, Nonius B.V., 1998)
 The conditions were as follow : crystal to detector distance =  36. mm.
 Scan angle =  2.0 deg 1 scans of   50 sec per frame.
 Data collection was divided into  2 set(s)
 with the following starting angles and number of frames :

 Set 1 Theta =    6.30 Omega =    0.00 Kappa =    0.00   91 frames
 Set 2 Theta =   -6.30 Kappa = -111.00 Phi   =    0.00   24 frames
 Friedel pairs were averaged. Internal R = 0.04
;

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_diffrn_standards_interval_count   ?
_diffrn_standards_interval_time    ?
_diffrn_standards_decay_%          0

_diffrn_reflns_number              7762
_diffrn_reflns_av_R_equivalents    0.040
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_diffrn_reflns_limit_h_min         -11
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_diffrn_reflns_limit_k_min         -13
_diffrn_reflns_limit_k_max         8
_diffrn_reflns_limit_l_min         -17
_diffrn_reflns_limit_l_max         19
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_computing_structure_refinement    LSFM_OpenMoleN_(_1997)
_computing_molecular_graphics      ?
_computing_publication_material    CIFGEN_IN_OpenMoleN_(_1997)
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# 8. REFINEMENT DATA


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# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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MN  0.9315(1)  0.0042(1)  0.28605(8)  0.0198(5)  1.000  Uani  ? ?  Mn
C1  1.089(1)  -0.150(1)  0.2690(7)  0.033(5)  1.000  Uani  ? ?  C
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O1  1.180(1)  -0.2414(9)  0.2521(6)  0.058(5)  1.000  Uani  ? ?  O
C2  0.941(1)  0.024(1)  0.1662(7)  0.032(5)  1.000  Uani  ? ?  C
O2  0.9568(9)  0.026(1)  0.0925(5)  0.042(5)  1.000  Uani  ? ?  O
C3  0.783(1)  -0.075(1)  0.2798(7)  0.036(5)  1.000  Uani  ? ?  C
O3  0.6875(8)  -0.1208(8)  0.2776(6)  0.065(4)  1.000  Uani  ? ?  O
N  0.9496(7)  -0.0117(6)  0.4183(5)  0.019(3)  1.000  Uani  ? ?  N
C4  0.9112(8)  -0.0805(8)  0.4868(6)  0.019(4)  1.000  Uani  ? ?  C
C5  1.0368(8)  0.0694(8)  0.4313(6)  0.019(4)  1.000  Uani  ? ?  C
C6  1.0625(9)  0.1415(9)  0.3480(6)  0.024(4)  1.000  Uani  ? ?  C
C7  1.212(1)  0.143(1)  0.3265(7)  0.041(5)  1.000  Uani  ? ?  C
C8  1.244(1)  0.216(1)  0.2538(7)  0.051(5)  1.000  Uani  ? ?  C
C9  1.127(1)  0.281(1)  0.1983(8)  0.047(5)  1.000  Uani  ? ?  C
C10  0.982(1)  0.284(1)  0.2198(7)  0.037(5)  1.000  Uani  ? ?  C
C11  0.9434(9)  0.2098(8)  0.2976(6)  0.027(4)  1.000  Uani  ? ?  C
C12  0.7854(8)  0.2026(8)  0.3124(6)  0.021(4)  1.000  Uani  ? ?  C
C13  0.6742(9)  0.284(1)  0.2491(6)  0.025(4)  1.000  Uani  ? ?  C
C14  0.6259(9)  0.232(1)  0.1758(6)  0.026(4)  1.000  Uani  ? ?  C
C15  0.528(1)  0.313(1)  0.1220(7)  0.036(5)  1.000  Uani  ? ?  C
C16  0.474(1)  0.447(1)  0.1369(8)  0.047(6)  1.000  Uani  ? ?  C
C17  0.513(2)  0.507(2)  0.2108(9)  0.065(7)  1.000  Uani  ? ?  C
C18  0.618(1)  0.423(1)  0.2662(8)  0.043(6)  1.000  Uani  ? ?  C
C19  0.7099(8)  0.2182(8)  0.4043(6)  0.021(4)  1.000  Uani  ? ?  C
C20  0.749(1)  0.2893(9)  0.4689(7)  0.032(4)  1.000  Uani  ? ?  C
C21  0.677(1)  0.304(1)  0.5547(7)  0.037(5)  1.000  Uani  ? ?  C
C22  0.562(1)  0.241(1)  0.5749(7)  0.042(5)  1.000  Uani  ? ?  C
C23  0.520(1)  0.174(1)  0.5100(7)  0.037(5)  1.000  Uani  ? ?  C
C24  0.5918(9)  0.162(1)  0.4246(6)  0.027(4)  1.000  Uani  ? ?  C
C25  0.051(4)  0.460(4)  0.547(3)  0.11(1)  0.500  Uiso  ? ?  C
C26  0.124(1)  0.435(1)  0.4787(8)  0.077(3)  1.000  Uiso  ? ?  C
C27  -0.119(6)  0.539(6)  0.621(4)  0.14(2)  0.500  Uiso  ? ?  C
C28  0.040(4)  0.444(4)  0.637(3)  0.09(1)  0.500  Uiso  ? ?  C
C29  0.143(4)  0.408(4)  0.581(3)  0.08(1)  0.500  Uiso  ? ?  C


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MN  0.0191(5)  0.0265(6)  0.0152(5)  -0.0051(4)  0.0011(5)  -0.0013(5)  Mn
C1  0.036(5)  0.043(5)  0.024(5)  0.002(4)  -0.001(4)  0.001(4)  C
O1  0.070(5)  0.057(5)  0.048(5)  0.034(4)  0.007(4)  -0.002(4)  O
C2  0.023(4)  0.059(6)  0.024(4)  -0.008(4)  -0.005(4)  0.001(4)  C
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O2  0.064(5)  0.086(6)  0.014(3)  -0.008(4)  0.003(3)  -0.004(4)  O
C3  0.038(4)  0.037(5)  0.033(5)  -0.012(4)  0.011(4)  -0.013(4)  C
O3  0.064(3)  0.078(4)  0.056(5)  -0.056(2)  -0.008(3)  -0.010(4)  O
N  0.016(3)  0.020(3)  0.021(3)  -0.008(2)  0.000(3)  -0.003(3)  N
C4  0.016(3)  0.017(3)  0.024(4)  -0.002(3)  0.000(3)  0.002(3)  C
C5  0.016(3)  0.020(4)  0.021(4)  -0.004(3)  0.002(3)  0.004(3)  C
C6  0.018(4)  0.036(4)  0.021(4)  -0.009(3)  -0.002(3)  0.008(3)  C
C7  0.029(4)  0.059(6)  0.039(5)  -0.021(4)  -0.005(4)  0.022(5)  C
C8  0.030(4)  0.090(6)  0.049(6)  -0.026(4)  -0.007(4)  0.046(5)  C
C9  0.041(4)  0.059(5)  0.042(6)  -0.030(4)  0.003(4)  0.020(4)  C
C10  0.044(4)  0.047(5)  0.025(4)  -0.025(3)  -0.006(4)  0.017(4)  C
C11  0.031(4)  0.031(4)  0.021(4)  -0.017(3)  0.004(3)  0.007(3)  C
C12  0.016(3)  0.027(4)  0.023(4)  -0.007(3)  -0.005(3)  0.007(3)  C
C13  0.015(3)  0.043(5)  0.025(4)  -0.005(3)  -0.000(3)  0.008(4)  C
C14  0.014(3)  0.051(5)  0.024(4)  -0.013(3)  -0.005(3)  0.007(4)  C
C15  0.019(4)  0.065(6)  0.038(5)  -0.010(4)  -0.011(4)  0.019(5)  C
C16  0.033(5)  0.071(7)  0.044(6)  -0.002(5)  -0.014(4)  0.014(6)  C
C17  0.041(6)  0.11(1)  0.062(7)  0.024(6)  -0.015(5)  0.045(6)  C
C18  0.035(5)  0.044(6)  0.053(6)  0.015(5)  -0.009(5)  0.020(5)  C
C19  0.016(3)  0.025(4)  0.023(4)  -0.006(3)  -0.001(3)  -0.002(3)  C
C20  0.038(4)  0.029(4)  0.030(5)  -0.016(3)  0.001(4)  -0.004(4)  C
C21  0.039(5)  0.043(5)  0.032(5)  -0.013(4)  0.004(4)  -0.012(4)  C
C22  0.038(5)  0.055(6)  0.034(5)  -0.015(4)  0.009(4)  -0.007(5)  C
C23  0.029(4)  0.048(5)  0.037(5)  -0.021(3)  0.012(4)  -0.016(4)  C
C24  0.017(4)  0.040(5)  0.029(5)  -0.006(3)  0.002(3)  0.002(4)  C

# 10. MOLECULAR GEOMETRY



loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
MN  C1  1.841(9)  .  .  ?
MN  C2  1.82(1)  .  .  ?
MN  C3  1.82(1)  .  .  ?
C1  O1  1.11(1)  .  .  ?
C2  O2  1.12(1)  .  .  ?
C3  O3  1.12(1)  .  .  ?
N  C4  1.33(1)  .  .  ?
N  C5  1.36(1)  .  .  ?
C5  C6  1.49(1)  .  .  ?
C6  C7  1.42(1)  .  .  ?
```

```
C6  C11  1.40(1)  . .  ?
C7  C8  1.38(2)  . .  ?
C8  C9  1.42(1)  . .  ?
C9  C10  1.36(1)  . .  ?
C10  C11  1.47(1)  . .  ?
C11  C12  1.49(1)  . .  ?
C12  C13  1.51(1)  . .  ?
C12  C19  1.51(1)  . .  ?
C13  C14  1.41(1)  . .  ?
C13  C18  1.42(1)  . .  ?
C14  C15  1.36(1)  . .  ?
C15  C16  1.36(2)  . .  ?
C16  C17  1.42(2)  . .  ?
C17  C18  1.42(2)  . .  ?
C19  C20  1.38(1)  . .  ?
C19  C24  1.40(1)  . .  ?
C20  C21  1.41(1)  . .  ?
C21  C22  1.43(2)  . .  ?
C22  C23  1.37(2)  . .  ?
C23  C24  1.41(1)  . .  ?
C25  C25  1.83(6)  . 2_566  ?
C25  C26  1.19(4)  . .  ?
C25  C26  1.74(4)  . 2_566  ?
C25  C27  1.87(7)  . .  ?
C25  C28  1.37(6)  . .  ?
C25  C29  1.03(5)  . .  ?
C26  C27  1.53(6)  . 2_566  ?
C26  C29  1.59(4)  . .  ?
C27  C28  1.55(6)  . .  ?
C28  C29  1.22(5)  . .  ?

loop_
     _geom_contact_atom_site_label_1
     _geom_contact_atom_site_label_2
     _geom_contact_distance
     _geom_contact_site_symmetry_1
     _geom_contact_site_symmetry_2
     _geom_contact_publ_flag
     ?   ?   ?   ?   ?   ?

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_2
```

```
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
C1  MN  C2  86.4(4)  . .  .  ?
C1  MN  C3  95.8(5)  . .  .  ?
C2  MN  C3  90.1(5)  . .  .  ?
MN  C1  O1  174(1)  . .  .  ?
MN  C2  O2  173.9(9)  . .  .  ?
MN  C3  O3  177.5(8)  . .  .  ?
C4  N  C5  118.8(7)  . .  .  ?
N  C5  C6  110.8(8)  . .  .  ?
C5  C6  C7  116.0(8)  . .  .  ?
C5  C6  C11  121.5(8)  . .  .  ?
C7  C6  C11  122.4(9)  . .  .  ?
C6  C7  C8  119.6(9)  . .  .  ?
C7  C8  C9  119(1)  . .  .  ?
C8  C9  C10  121(1)  . .  .  ?
C9  C10  C11  120.7(9)  . .  .  ?
C6  C11  C10  116.4(8)  . .  .  ?
C6  C11  C12  124.8(8)  . .  .  ?
C10  C11  C12  118.6(7)  . .  .  ?
C11  C12  C13  116.0(8)  . .  .  ?
C11  C12  C19  119.8(8)  . .  .  ?
C13  C12  C19  108.4(6)  . .  .  ?
C12  C13  C14  125.3(8)  . .  .  ?
C12  C13  C18  115.7(9)  . .  .  ?
C14  C13  C18  119.0(9)  . .  .  ?
C13  C14  C15  120.9(9)  . .  .  ?
C14  C15  C16  120(1)  . .  .  ?
C15  C16  C17  121(1)  . .  .  ?
C16  C17  C18  117(1)  . .  .  ?
C13  C18  C17  119(1)  . .  .  ?
C12  C19  C20  122.6(8)  . .  .  ?
C12  C19  C24  119.1(8)  . .  .  ?
C20  C19  C24  118.3(8)  . .  .  ?
C19  C20  C21  122(1)  . .  .  ?
C20  C21  C22  118(1)  . .  .  ?
C21  C22  C23  119(1)  . .  .  ?
C22  C23  C24  121(1)  . .  .  ?
C19  C24  C23  120.6(9)  . .  .  ?
C25  C25  C26  66(2)  2_566 .  .  ?
C25  C25  C26  38(1)  2_566 .  2_566  ?
C25  C25  C27  88(2)  2_566 .  .  ?
C25  C25  C28  143(3)  2_566 .  .  ?
C25  C25  C29  157(4)  2_566 .  .  ?
C26  C25  C26  105(2)  . .  2_566  ?
C26  C25  C27  155(3)  . .  .  ?
C26  C25  C28  149(3)  . .  .  ?
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C26  C25  C29  90(3)  . .  .  ?
C26  C25  C27  49(2)  2_566 .  .  ?
C26  C25  C28  104(2)  2_566 .  .  ?
C26  C25  C29  162(4)  2_566 .  .  ?
C27  C25  C28  54(2)  . .  .  ?
C27  C25  C29  113(4)  . .  .  ?
C28  C25  C29  58(3)  . .  .  ?
C25  C26  C25  74(2)  . .  2_566  ?
C25  C26  C27  143(2)  . .  2_566  ?
C25  C26  C29  40(2)  . .  .  ?
C25  C26  C27  69(2)  2_566 .  2_566  ?
C25  C26  C29  114(1)  2_566 .  .  ?
C27  C26  C29  175(2)  2_566 .  .  ?
C25  C27  C26  60(2)  . .  2_566  ?
C25  C27  C28  46(2)  . .  .  ?
C26  C27  C28  106(3)  2_566 .  .  ?
C25  C28  C27  79(3)  . .  .  ?
C25  C28  C29  46(2)  . .  .  ?
C27  C28  C29  125(3)  . .  .  ?
C25  C29  C26  48(2)  . .  .  ?
C25  C29  C28  74(3)  . .  .  ?
C26  C29  C28  123(3)  . .  .  ?
```