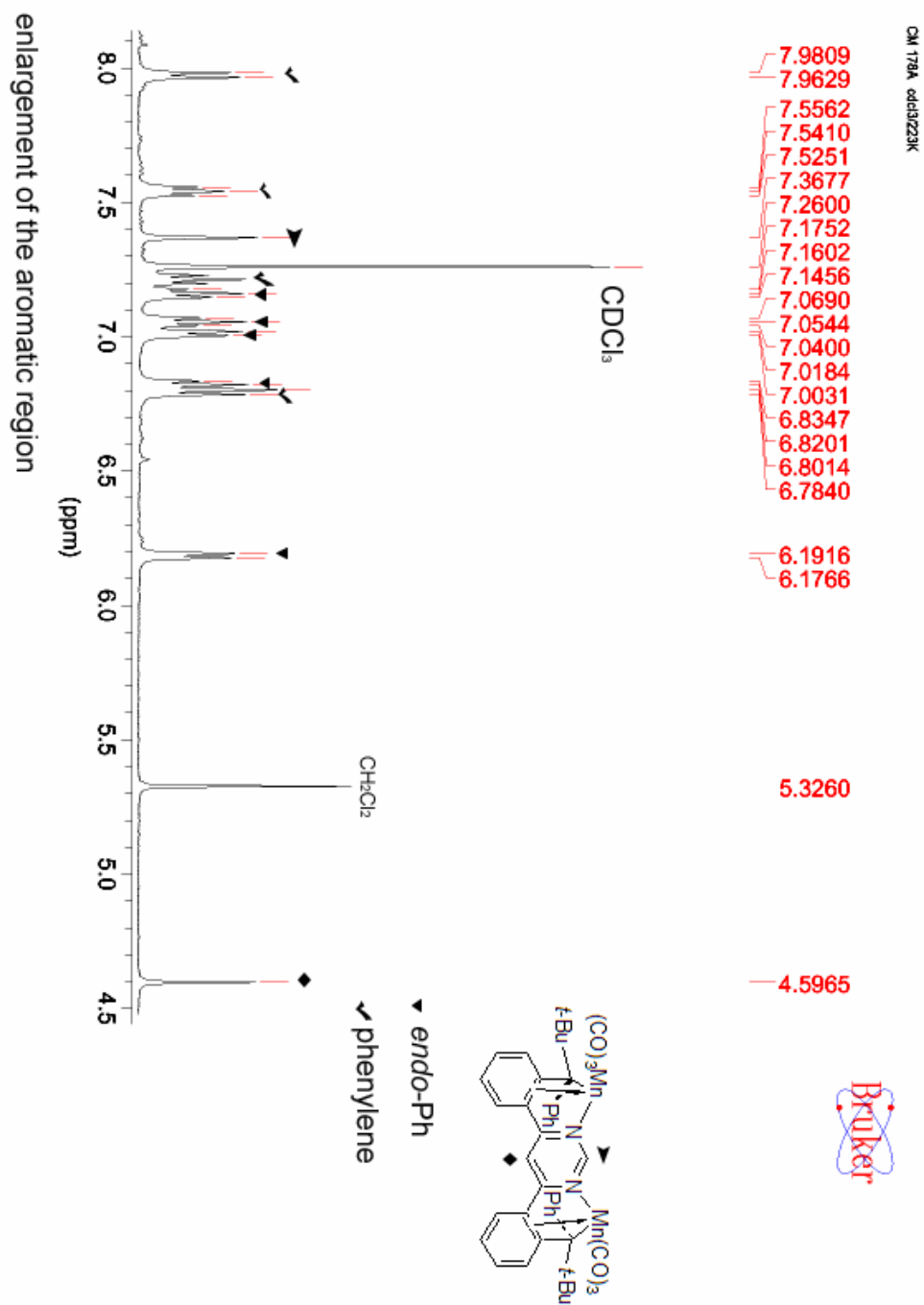


**New manganese-scaffolded organic triple-deckers based on
quinoxaline, pyrazine and pyrimidine cores.**

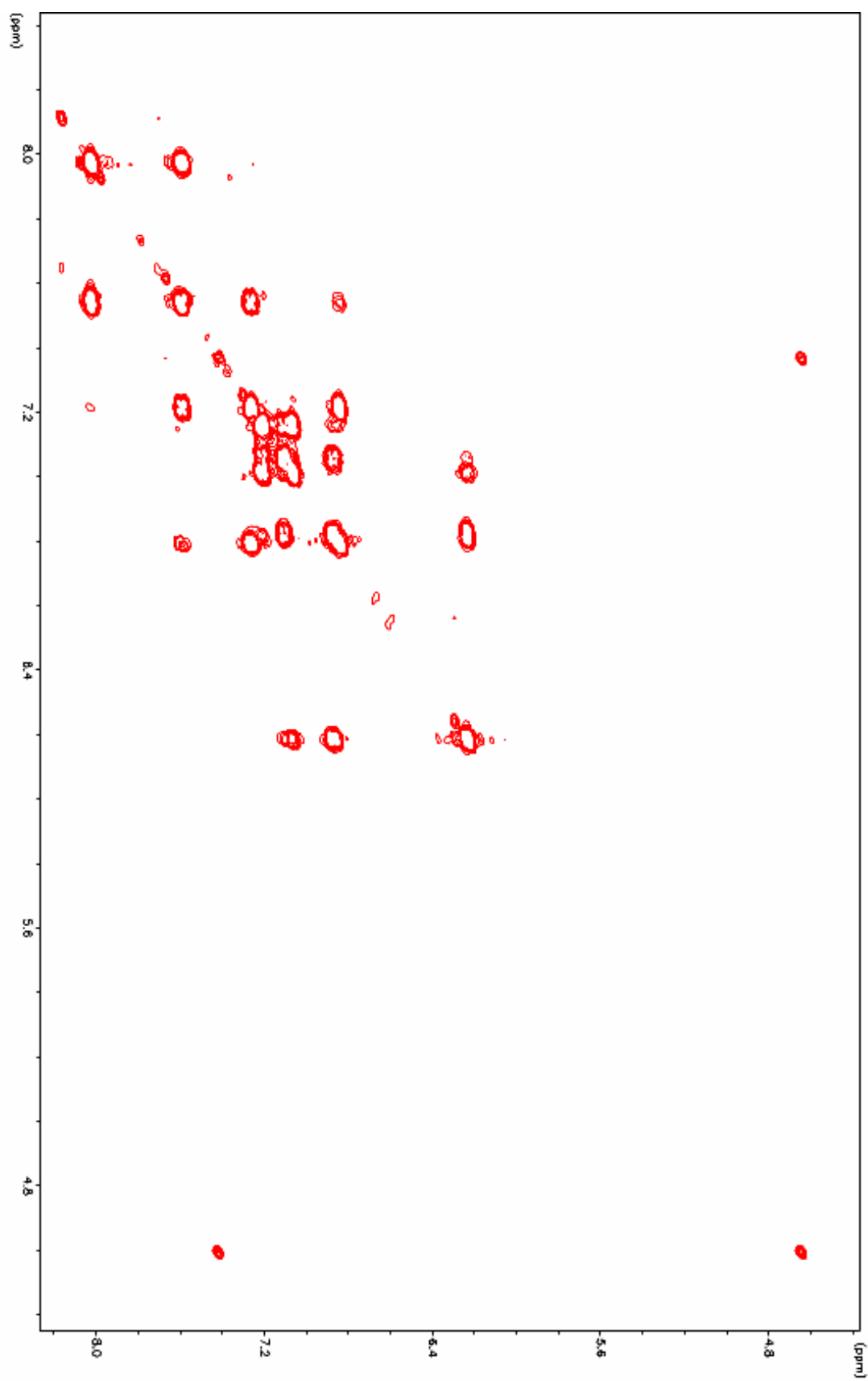
**Jean-Pierre Djukic,* Christophe Michon, Zoran Ratkovic, Nathalie Kyritsakas-Gruber,
André de Cian and Michel Pfeffer.**

*Institut de Chimie de Strasbourg, UMR 7177, Université Louis Pasteur, 4, rue Blaise Pascal,
F-67000 Strasbourg, France. E-mail : djukic@chimie.u-strasbg.fr; Fax : 33 (0) 390 24 50
01 ; Tel : 33 (0) 390 24 15 23*

Electronic Supporting Information

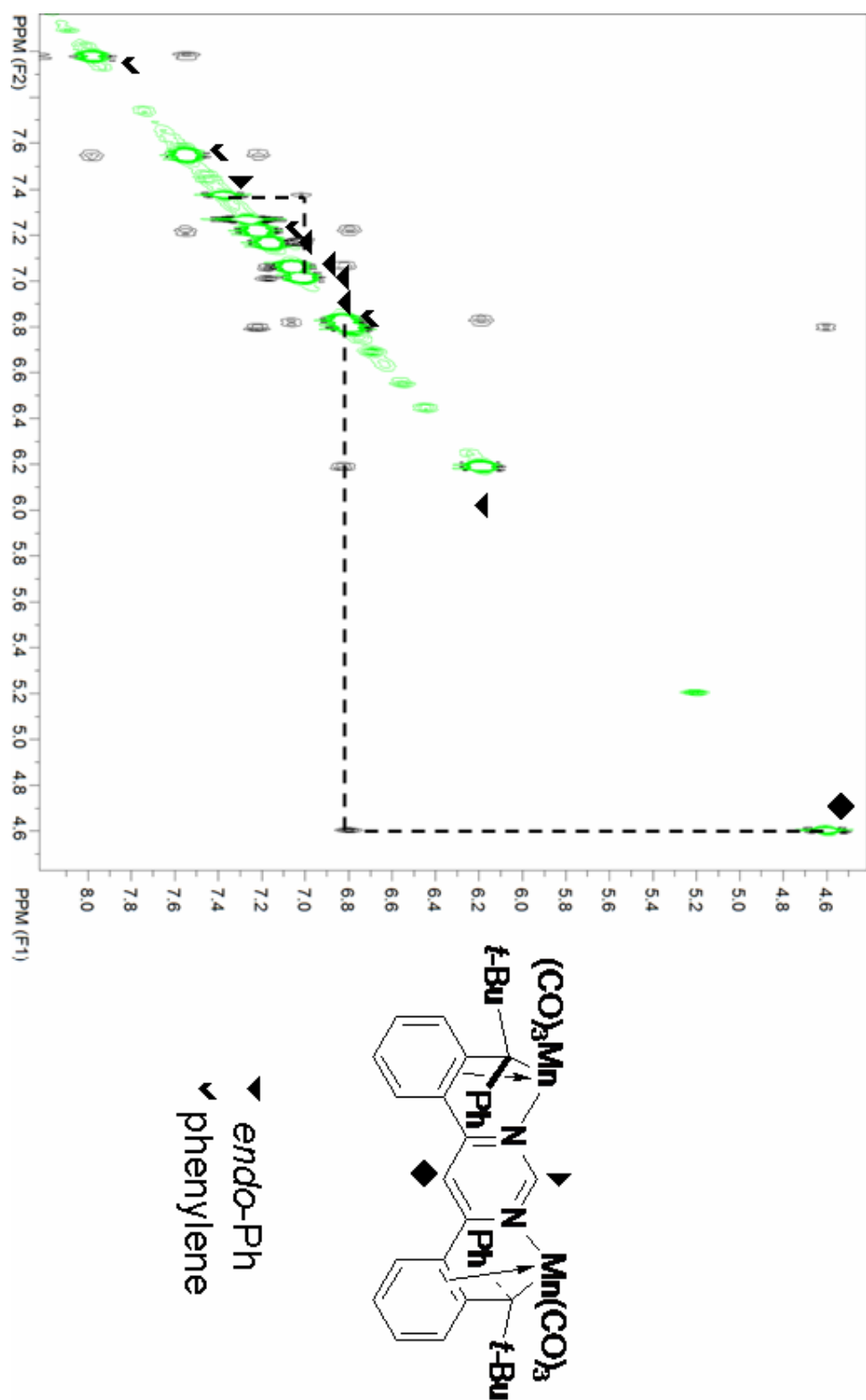


¹H NMR (500 MHz) spectrum of **3d** measured at 223 K in CDCl₃

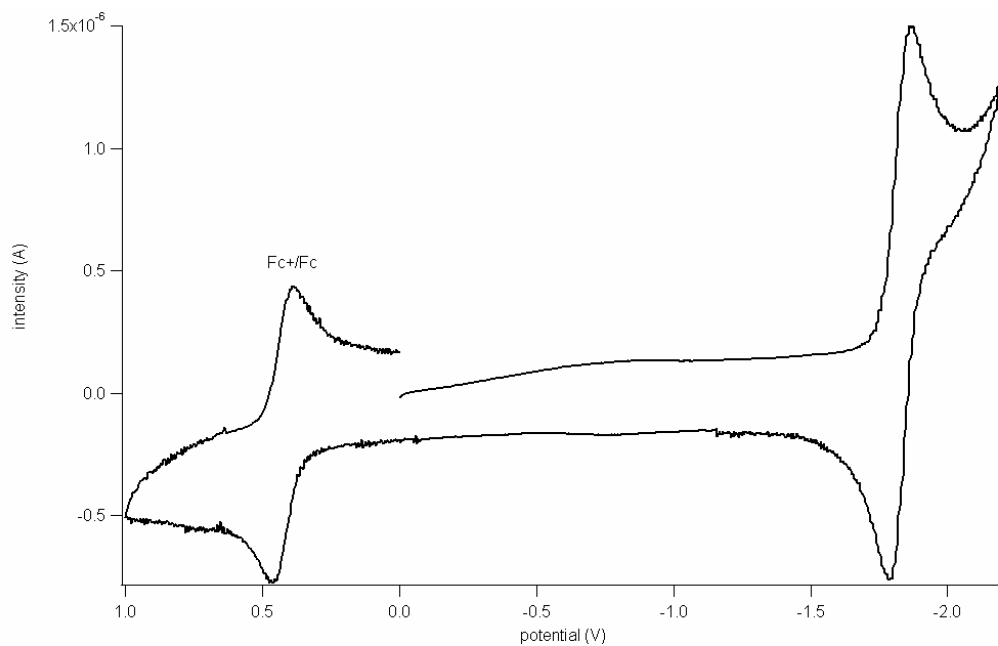


^1H - ^1H COSY spectrum (500 MHz) of **3d** in CDCl_3 at 223 K

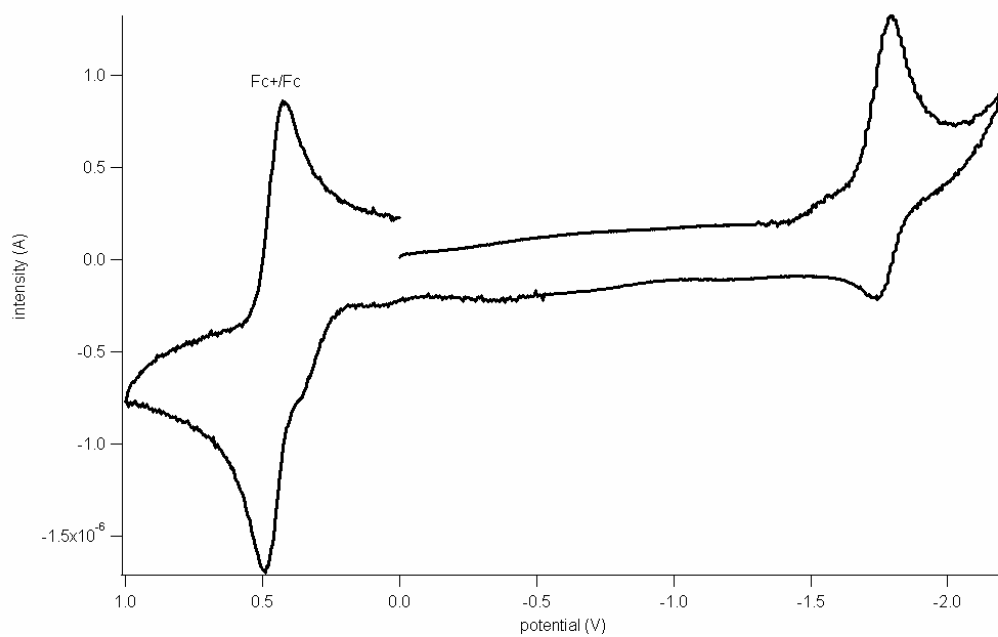
ROESY, 500 MHz, 223 K, CDCl_3 (in green are the negative peaks and correlations related to exchange, in black are pure NOE correlations)



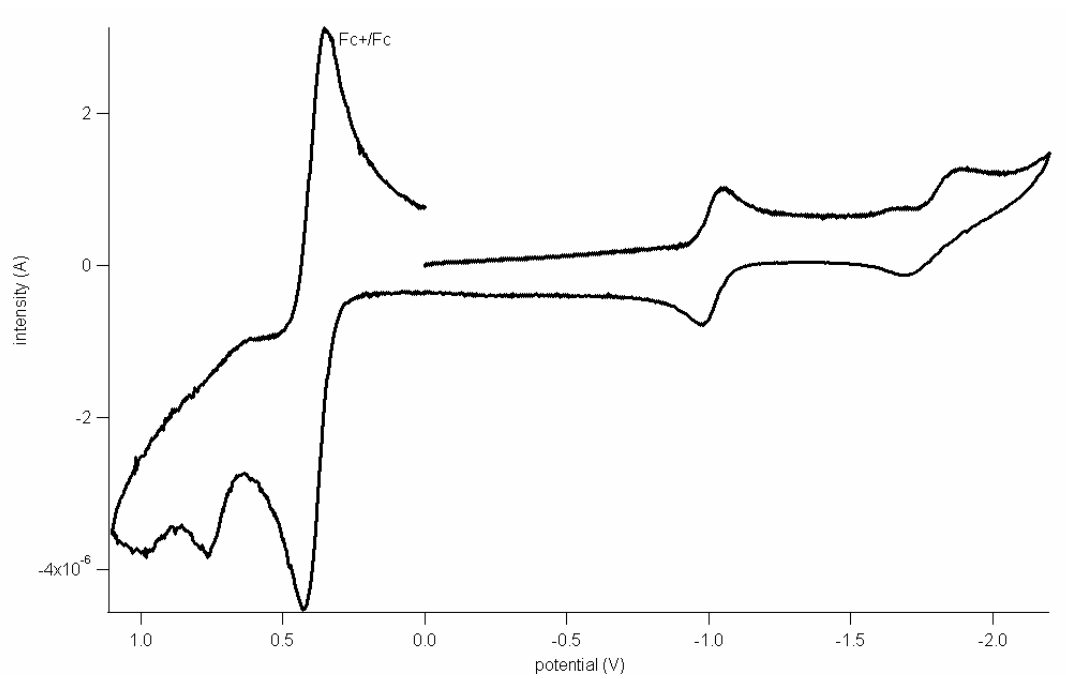
500 MHz ^1H - ^1H ROESY bi-dimensional spectrum of **3d** in CDCl_3 at 223 K.



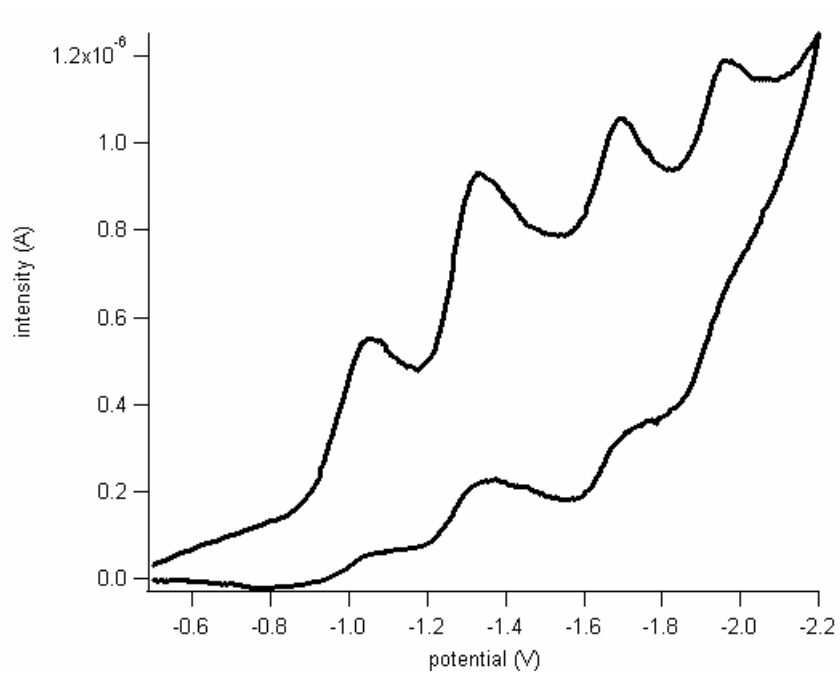
Room temperature cyclic voltammetry of 4,6-diphenylpyrimidine in MeCN (10^{-4} M); scan rate 200 mV/s.



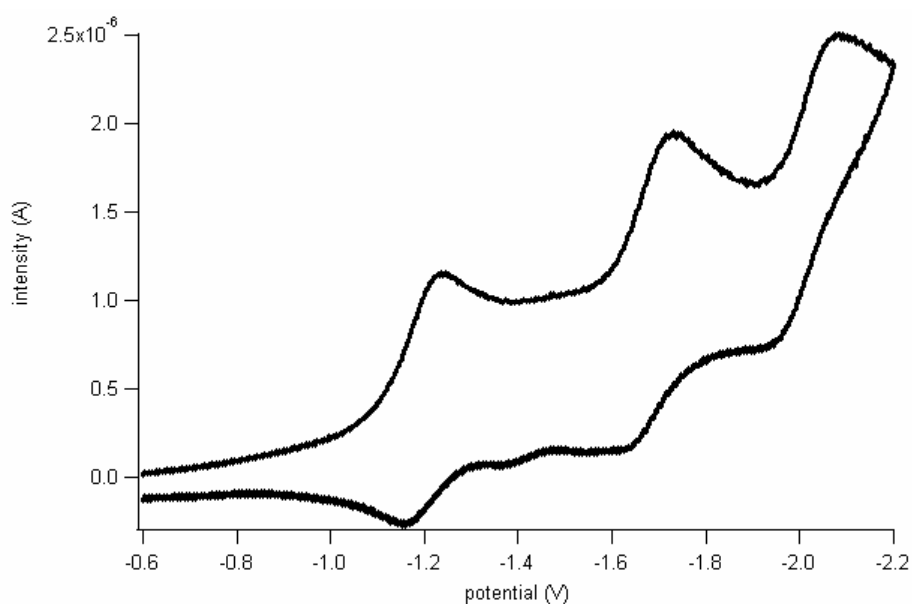
Room temperature cyclic voltammetry of 2,5-diphenylpyrazine in MeCN (10^{-4} M); scan rate 200 mV/s.



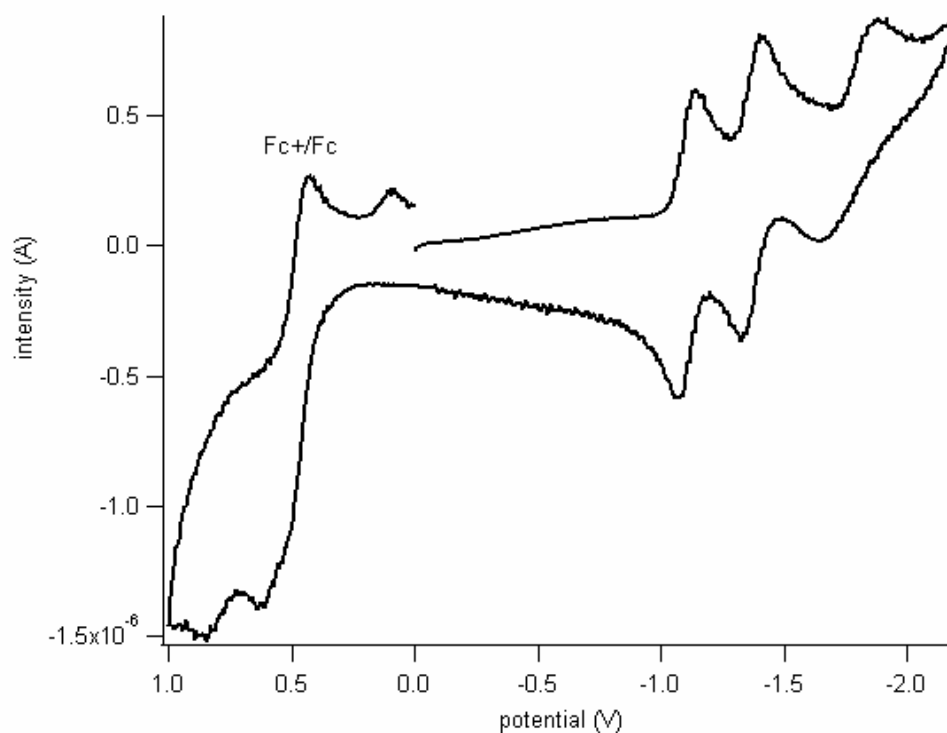
Room temperature cyclic voltammetry of **1c** in MeCN (10^{-4} M); scan rate 400 mV/s.



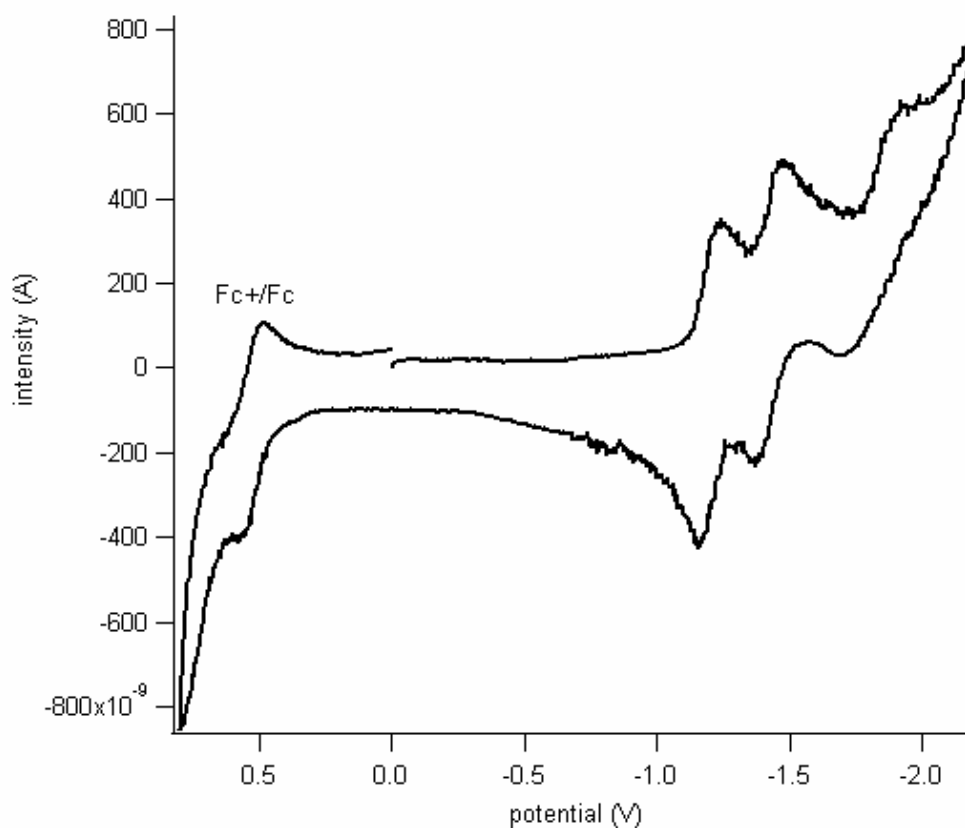
Room temperature cyclic voltammetry of **2b** in THF (10^{-4} M); scan rate 50 mV/s.



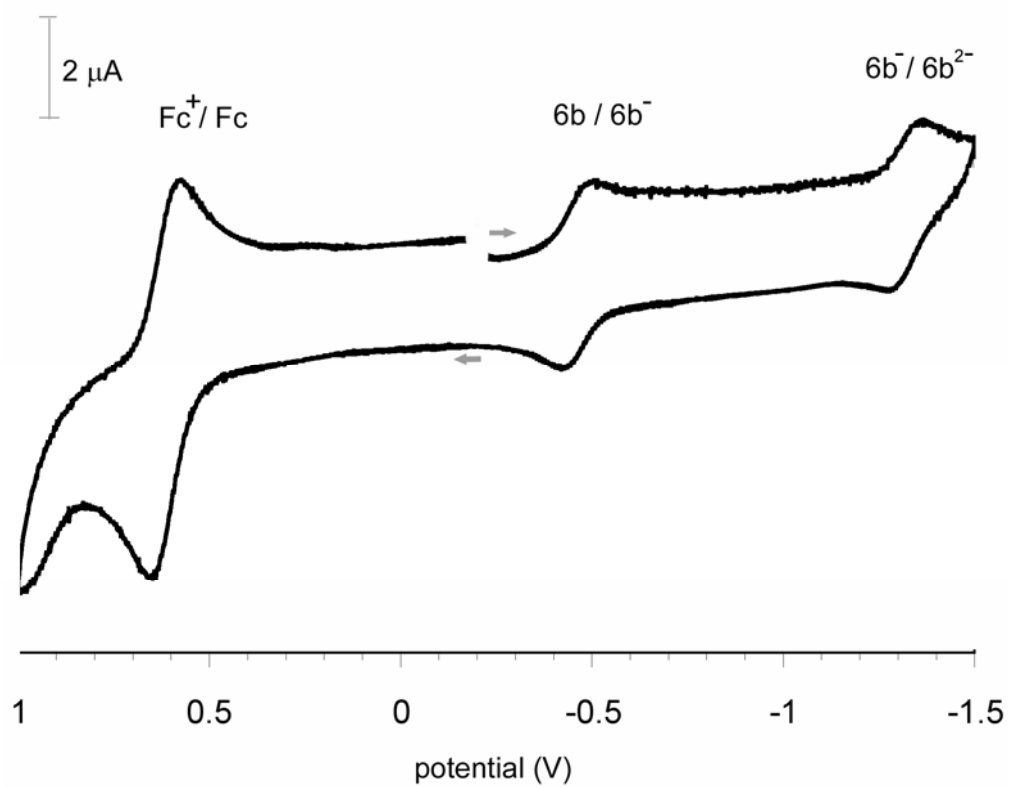
Room temperature cyclic voltammetry of **2c** in MeCN (10^{-4} M); scan rate 400 mV/s.



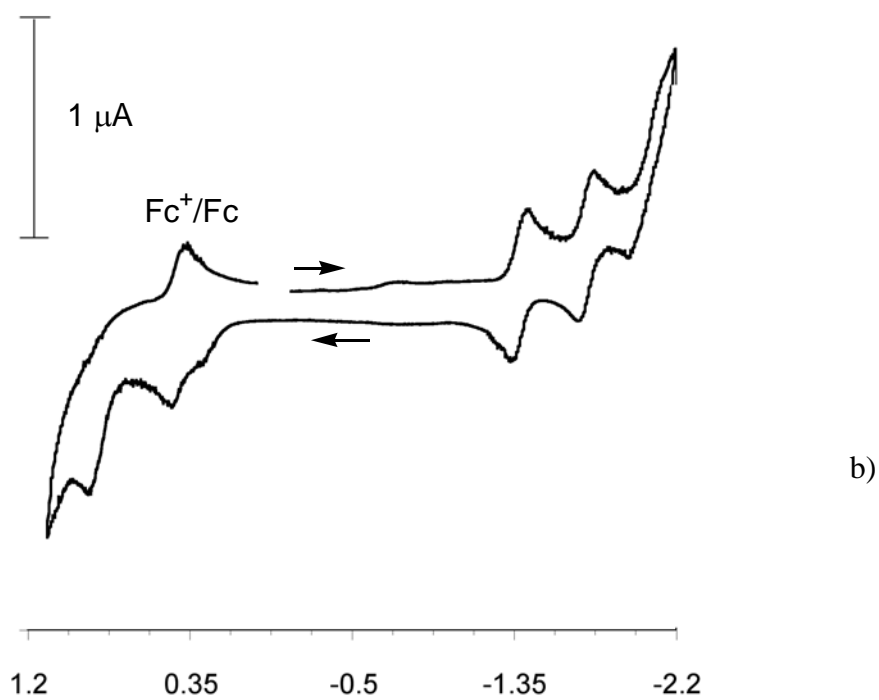
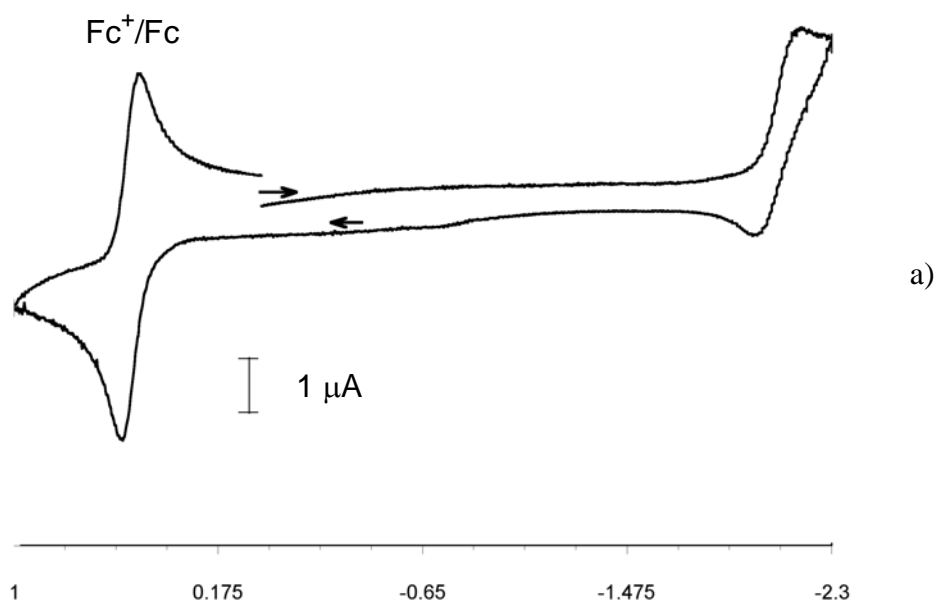
Room temperature cyclic voltammetry of **3b** in MeCN (10^{-4} M); scan rate 200 mV/s.



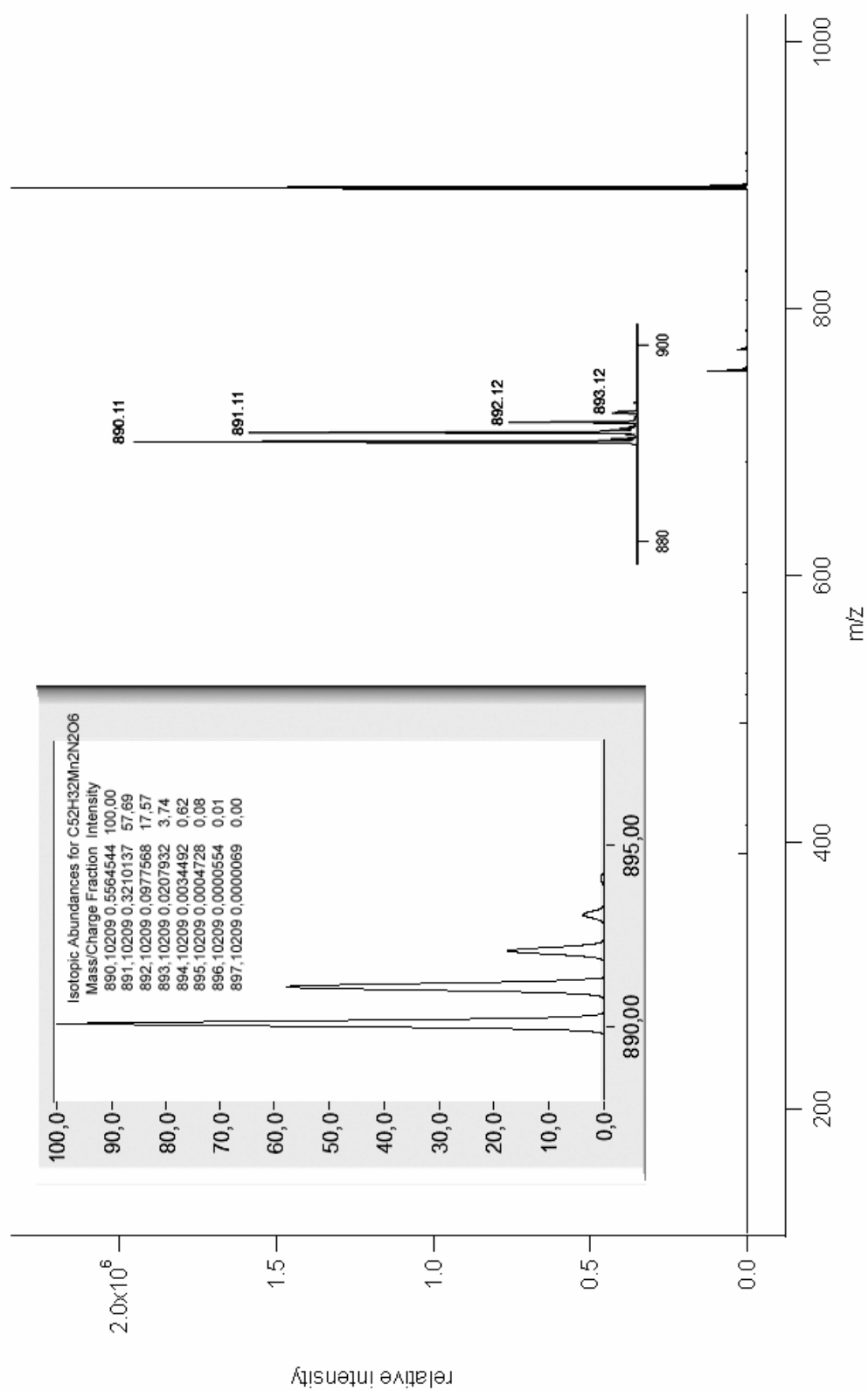
Room temperature cyclic voltammetry of **3d** in MeCN (10^{-4} M); scan rate 200 mV/s.

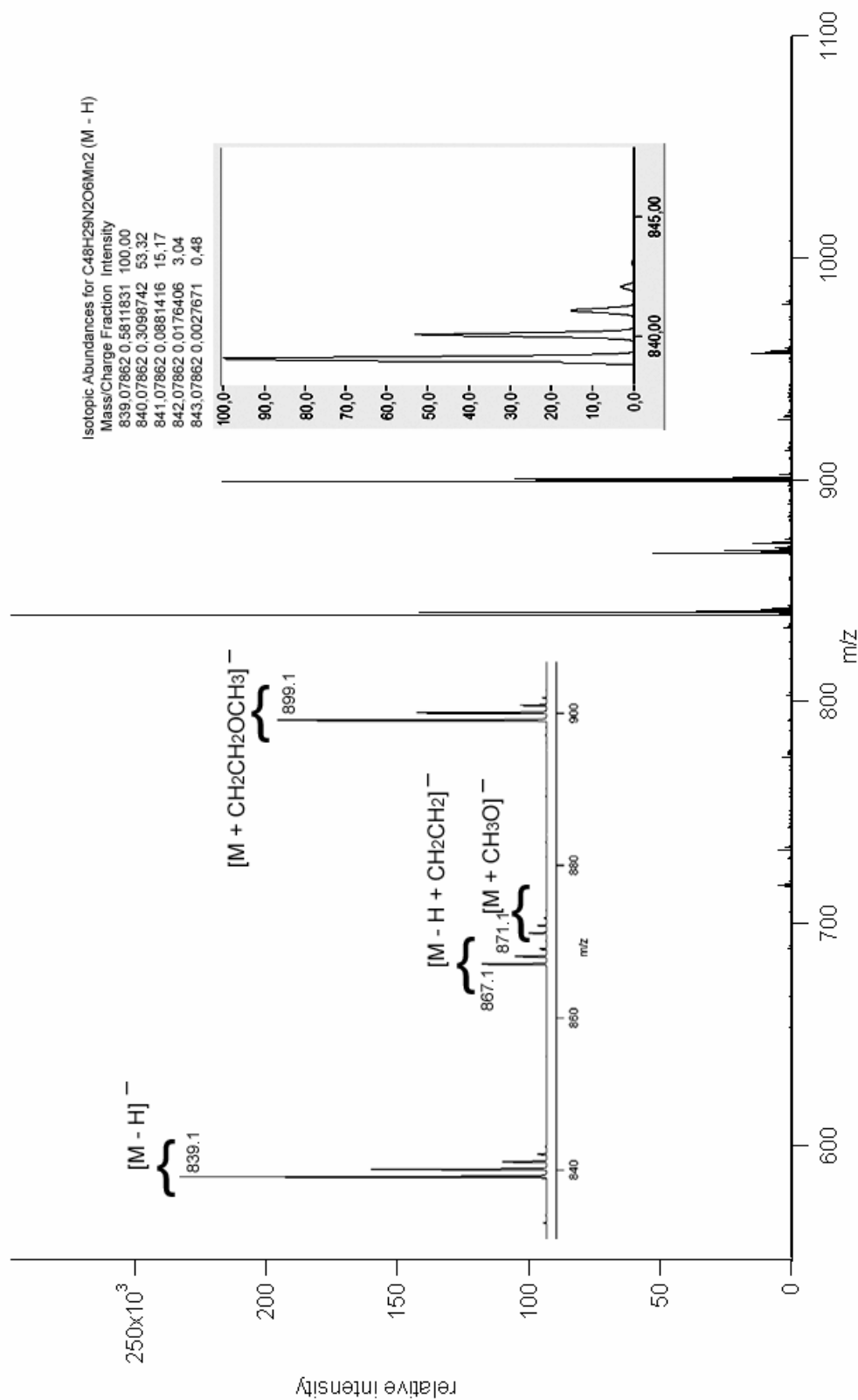


Room temperature cyclic voltammetry of **6b** in MeCN (10^{-4} M); scan rate 80 mV/s.

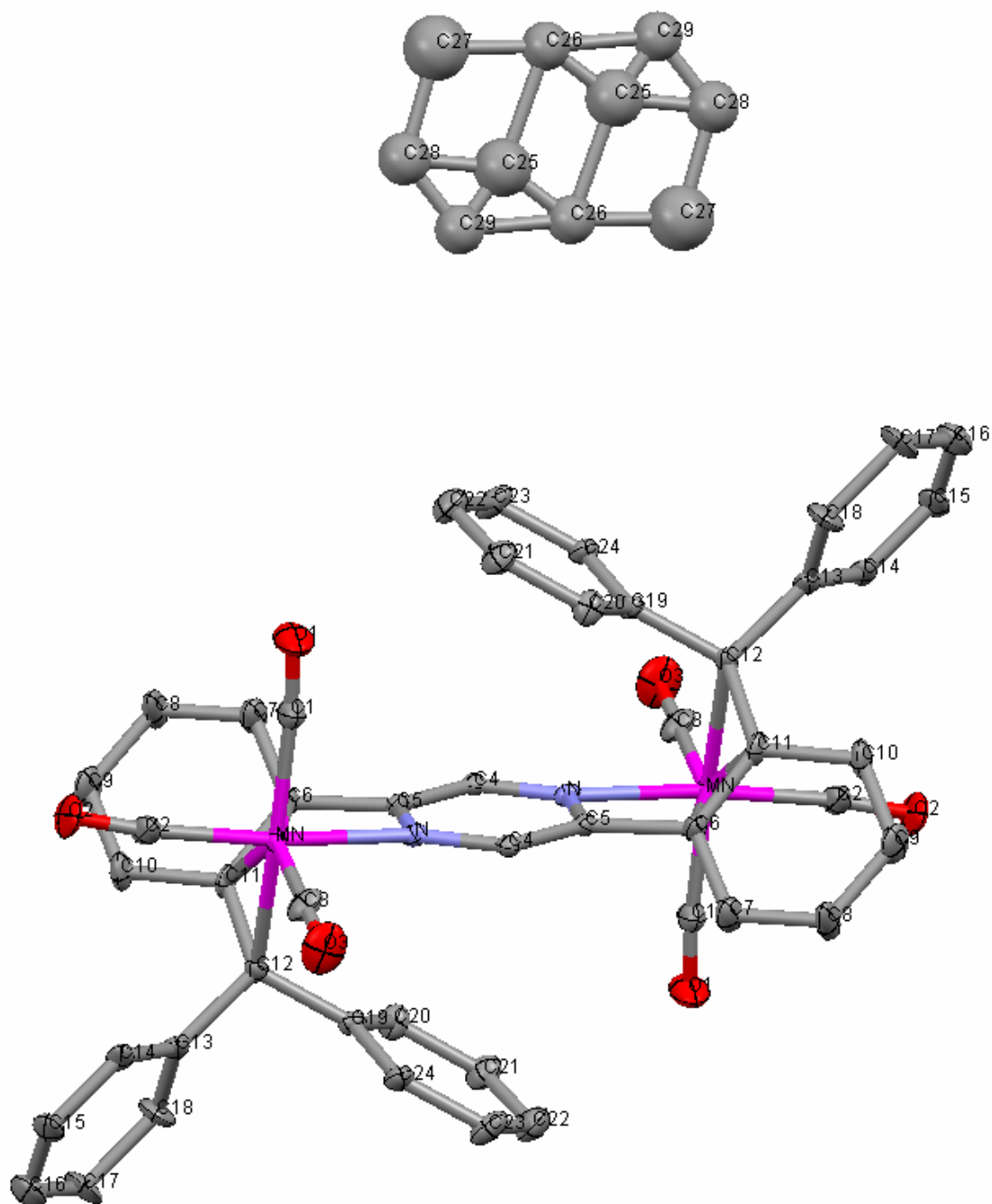


a) Room temperature cyclic voltammetry of **7** in MeCN; scan rate 800 mV/s. b) Room temperature cyclic voltammetry of **8** in MeCN; scan rate 100 mV/s.

Negative mode electrospray mass spectrum of a 1,2-dimethoxyethane solution of [1b]⁻.



Negative mode electrospray mass spectrum of a solution of **[3b]⁻** 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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data_global
#=====
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_audit_creation_date          4-06-02

# 1. SUBMISSION DETAILS

_publ_contact_author_name    # Name of author for correspondence
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;
_publ_contact_author_address # Address of author for correspondence
;
;
_publ_contact_author_phone   'xxxxxxxxxxxx'
_publ_contact_author_fax     'xxxxxxxxxxxx'
_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)

_journal_date_recd_electronic ?

_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        ?
_journal_techeditor_notes
; ?
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_journal_coden_ASTM             ?
_journal_name_full              ?
_journal_year                   ?
_journal_volume                 ?

_journal_issue                  ?
_journal_page_first             ?
_journal_page_last              ?

_journal_suppl_publ_number      ?
_journal_suppl_publ_pages       ?

#=====
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# 3. TITLE AND AUTHOR LIST

_publ_section_title
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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_abstract

; ?

;

_publ_section_comment

; ?

;

_publ_section_exptl_prep

; ?

;

_publ_section_exptl_refinement

; ?

;

_publ_section_references

;

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 Netherlands.

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

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_publ_section_figure_captions

; ?

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_publ_section_acknowledgements

; ?

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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.
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data_4b
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#####
=====
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# 5. CHEMICAL DATA
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;
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_chemical_formula_structural    ?
_chemical_formula_analytical    ?
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_chemical_formula_weight        994.87
_chemical_melting_point         ?
_chemical_compound_source       ?
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loop_
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  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_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
O ? 0.008 0.006 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_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
;

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# 7. EXPERIMENTAL DATA

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_diffrn_ambient_temperature      294
_diffrn_radiation_wavelength     0.71073
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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_time ?
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_diffrn_reflns_number         7762
_diffrn_reflns_av_R_equivalents 0.040
_diffrn_reflns_av_sigmaI/netI 0.333
_diffrn_reflns_limit_h_min    -11
_diffrn_reflns_limit_h_max    12
_diffrn_reflns_limit_k_min    -13
_diffrn_reflns_limit_k_max    8
_diffrn_reflns_limit_l_min    -17
_diffrn_reflns_limit_l_max    19
_diffrn_reflns_theta_min      2.5
_diffrn_reflns_theta_max      27.47

_reflns_number_total          6067
_reflns_number_gt             4434
_reflns_threshold_expression   >3.0\s(I)

_computing_structure_solution  Direct_methods_(SIR,_Burla_et_al.,_1989)
_computing_structure_refinement LSFM_OpenMoleN_(1997)
_computing_molecular_graphics  ?
_computing_publication_material CIFGEN_IN_OpenMoleN_(1997)

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#=====
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8. REFINEMENT DATA

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_refine_ls_abs_structure_Flack    ?
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_refine_ls_number_parameters      282
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_refine_ls_number_constraints     0
_refine_ls_R_factor_all           0.177
_refine_ls_R_factor_gt            0.154
_refine_ls_wR_factor_all          0.591
_refine_ls_wR_factor_ref          0.237
_refine_ls_goodness_of_fit_all    10.444
_refine_ls_goodness_of_fit_ref    4.130
_refine_ls_shift/su_max           *****
_refine_ls_shift/esd_mean         0.453
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9. ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_thermal_displace_type
_atom_site_calc_flag
_atom_site_calc_attached_atom
_atom_site_type_symbol
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
```

Electronic Supporting Information

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
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								
_atom_site_aniso_type_symbol								
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	

Electronic Supporting Information

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)	.	.	.	?

Electronic Supporting Information

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)	.	.	.	?