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Volume 55, 2002

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10.1071/CH01094_AC

Accessory Publication: *Aust. J. Che*m., 2002, 55(3), 219-223.

$Fe(pz)_2Br_2$ Synchrotron Powder Diffraction Data (λ = 1.4978 Å)

h	k	l	F^2	$\sigma(F^2)$
0	1	1	22491.	54.
0	0	2	1806.	17.
1	1	0	40010.	116.
1	1	2	56575.	133.
0	2	0	139151.	308.
0	1	3	1166.	9.
1	2	1	6083.	30.
0	2	2	11740.	58.
0	0	4	91983.	383.
2	2	0	68143.	262.
1	1	4	76931.	220.
1	2	3	1877.	9.
0	3	1	28943.	123.
2	2	2	31919.	132.
1	3	0	121116.	305.
0	2	4	75240.	236.
0	1	5	51202.	189.
1	3	2	8294.	43.
0	3	3	4511.	28.
2	3	1	10942.	53.
2	2	4	38672.	173.
0	0	6	11160.	74.
1	2	5	22500.	96.
0	4	0	55439.	270.
1	3	4	64454.	192.
2	3	3	242.	1.
1	1	6	1345.	9.
1	4	1	9217.	48.
0	4	2	15321.	83.
3	3	0	92889.	396.
0	2	6	7583.	43.
0	3	5	58410.	232.
3	3	2	4388.	25.
2	4	0	53291.	218.
1	4	3	128.	1.
2	4	2	19267.	85.
0	1	7	2801.	16.
0	4	4	85622.	305.
2	2	6	13352.	66.
2	3	5	35797.	134.
3	3	4	83489.	299.
1	3	6	5338.	26.
0	5	1	10476.	43.
3	4	1	17150.	70.
1	2	7	10157.	46.
1	5	0	80507.	288.
2	4	4	48084.	164.
0	0	8	31388.	152.
1	4	5	27998.	107.
1	5	2	10946.	48.
0	5	3	158.	1.
3	4	3	796.	4.
1	1	8	33892.	141.

2	5	1	2111.	10.
0	3	7	191.	1.
0	2	8	22479.	96.
0	4	6	438.	2.
4	4	0	80149.	320.
1	5	4	30956.	113.
2	5	3	1318.	5.
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4	4	2	5161.	23.
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3	5	0	48376.	184.
2	2	8	16425.	67.
2	4	6	3598.	15.
0	1	9	53830.	197.
0	5	5	26069.	86.
3	4	5	32227.	107.
3	5	2	12692.	48.
0	6	0	51780.	202.
1	3	8	26693.	96.
1	6	1	8343.	33.
0	6	2	8565.	35.
1	4	7	5874.	23.
4	4	4	44710.	163.
1	2	9	38061.	127.
2	5	5	17901.	65.
2	6	0	46610.	166.
3	5	4	45482.	149.
1	6	3	287.	1.
1	5	6	18268.	67.
4	5	1	3808.	15.
2	6	2	11199.	42.
0	0	10	4577.	18.
0	6	4	68440.	232.

$Fe(pz)_2Br_2$ Powder Neutron Diffraction Data (λ = 1.8852 Å)

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1	1	2	208.30	.82
0	2	0	562.01	2.10
0	1	3	32.31	.15
1	2	1	11.38	.05
0	2	2	9.68	.04
0	0	4	665.30	2.93
2	2	0	17.80	.09
1	1	4	28.72	.14
1	2	3	25.65	.12
0	3	1	233.12	.98
2	2	2	104.89	.48
1	3	0	185.01	.86
0	2	4	2.87	.02
0	1	5	115.43	.57
1	3	2	36.63	.18
0	3	3	223.30	1.09
2	3	1	27.88	.15
2	2	4	.16	.00

0	0	6	51.30	.30
1	2	5	2.04	.01
0	4	0	4.44	.03
1	3	4	165.93	.88
2	3	3	2.41	.01
1	1	6	48.86	.28
1	4	1	17.65	.10
0	4	2	5.21	.03
3	3	0	648.37	3.28
0	2	6	1.12	.01
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3	3	2	74.27	.40
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2	4	2	49.77	.32
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0	4	4	287.81	1.72
2	2	6	127.89	.83
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3	4	1	89.09	.62
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1	4	5	6.70	.05
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2	5	1	53.98	.41
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0	4	6	385.86	2.57
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3	5	0	10.81	.10
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3	6	3	81.43	.51
3	5	6	9.43	.06
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4	5	5	.08	.00
1	7	2	3.93	.02
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_publ_requested_category           FM

_publ_contact_author
;
Dr. Michael James
Neutron Scattering Group, ANSTO,
Menai, NSW, 2234,
AUSTRALIA
;
_publ_contact_letter
;
;
_publ_requested_coeditor_name         ?
_publ_contact_author_phone            612-9717-9299
_publ_contact_author_fax              612-9717-3606
_publ_contact_author_email            mja@ansto.gov.au
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# 2. PROCESSING SUMMARY (IUCr Office Use Only)

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_journal_date_from_coeditor       ?
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_journal_date_printers_first      ?
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# 3. TITLE AND AUTHOR LIST

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The structure and magnetic properties of the two-dimensional
di-pyrazine bridged polymers M(pz)2Br2
(M = Fe(II), Co(II), Ni(II))
;
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_publ_author_footnote
_publ_author_address
' James, Michael'  # SURNAME first
;
;
;
  Neutron Scattering Group,
  ANSTO,
  Lucas Heights Research Laboratories,
  PMB 1,
  Menai NSW 2234,
  Australia.
;

#=============================================================================
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# 4. TEXT

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Br 0 0 0.7693(1) 0.024(1) 1.000 Uiso
N 0.3097(4) 0 0 0.015(1) 1.000 Uiso
C 0.4050(4) -0.1073(4) -0.0765(3) 0.022(1) 1.000 Uiso
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$Ni(pz)_2Br_2$ Synchrotron Powder Diffraction Data (λ = 1.4978 Å)

h	k	l	F^2	$\sigma(F^2)$
0	1	1	24418.	39.
0	0	2	2248.	16.
1	1	0	39158.	82.
1	1	2	62066.	96.
0	2	0	134767.	214.
0	1	3	206.	1.
1	2	1	5345.	20.
0	2	2	12505.	43.
0	0	4	81226.	249.
2	2	0	57867.	171.
1	1	4	62915.	137.
1	2	3	3239.	15.
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1	3	2	8140.	34.
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1	2	5	23751.	72.
0	4	0	42900.	165.
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1	3	4	49945.	117.
2	3	3	194.	1.
1	4	1	8287.	35.
0	4	2	16707.	70.
3	3	0	75288.	245.
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1	5	0	62023.	182.
2	4	4	33841.	97.
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4	4	2	6057.	24.
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1	2	9	30409.	87.
1	6	1	3751.	14.
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4	4	4	27594.	93.
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1	5	6	17818.	51.
3	5	4	28633.	85.
1	6	3	426.	2.

$Ni(pz)_2Br_2$ Powder Neutron Diffraction Data (λ = 1.6653 Å)

h	k	l	F^2	$\sigma(F^2)$
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1	1	0	38.65	2.69
1	1	2	193.17	2.24
0	2	0	588.90	4.68
0	1	3	39.74	2.15
1	2	1	3.06	1.18
0	2	2	3.24	1.30
0	0	4	832.20	18.24
2	2	0	41.01	7.39
1	1	4	30.01	2.38
1	2	3	20.92	1.48
0	3	1	246.79	3.75
2	2	2	112.47	2.33
1	3	0	249.35	4.22
0	2	4	1.05	.27
0	1	5	131.01	4.50
1	3	2	51.51	2.60
0	3	3	223.22	6.04
2	3	1	19.06	2.75
0	0	6	152.21	18.29
2	2	4	1.52	.24
1	2	5	9.13	1.75
0	4	0	.00	.00

1	1	6	73.43	4.15
1	3	4	136.22	3.68
2	3	3	.00	.05
1	4	1	15.57	2.66
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0	2	6	.75	.02
0	3	5	381.07	7.06
3	3	2	37.54	5.98
2	4	0	.00	.00
0	1	7	3.96	5.91
1	4	3	.00	.41
2	4	2	46.81	3.14
2	2	6	157.36	3.98
0	4	4	375.46	6.52
2	3	5	49.64	2.85
1	3	6	3.41	.12
1	2	7	110.02	2.88
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0	0	8	53.13	5.42
0	5	1	18.21	.48
3	4	1	134.08	3.50
1	5	0	226.80	6.54
2	4	4	20.82	1.39
1	4	5	30.38	1.79
1	1	8	137.58	6.94
1	5	2	2.97	.30
0	3	7	236.19	7.07
0	5	3	8.72	.19
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0	2	8	69.68	3.68
2	5	1	100.45	3.54
0	4	6	656.17	10.90
4	4	0	700.98	11.50
3	3	6	328.77	5.00
2	3	7	5.20	.07
1	5	4	67.17	.96
2	5	3	133.49	1.87
0	1	9	191.29	2.85
2	2	8	105.43	4.97
4	4	2	195.18	7.78
3	5	0	59.26	4.30
2	4	6	5.49	.41
0	5	5	51.70	1.24
3	4	5	225.18	5.40
1	3	8	1.92	.13
3	5	2	24.94	3.94
0	6	0	3.36	.59
1	4	7	7.88	1.27
1	2	9	3.89	.73
1	6	1	6.32	4.24
0	6	2	2.27	2.50
4	4	4	.00	7.11
2	5	5	4.93	2.14
0	0	10	162.66	28.27
2	6	0	19.50	.28
1	5	6	372.02	4.84
3	5	4	130.42	1.36
1	6	3	5.49	.07
0	3	9	385.83	4.79

0	4	8	565.38	9.13
1	1	10	.25	.00
4	5	1	.88	.07
2	6	2	18.85	2.11
0	6	4	425.96	10.67
3	3	8	299.38	11.05
0	2	10	2.92	.12
0	5	7	.00	.11
3	4	7	.00	3.17
4	5	3	13.80	1.15
2	3	9	42.47	3.25
2	4	8	13.20	1.03
3	6	1	218.37	5.29
4	4	6	88.70	5.81
2	6	4	10.89	.76
1	6	5	112.38	4.75
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3	5	6	27.60	1.07
2	5	7	109.08	3.60
0	1	11	15.49	.47
3	6	3	75.52	2.51
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1	3	10	42.28	2.14
0	7	1	356.41	8.63
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5	5	0	329.30	5.25
0	6	6	377.97	6.14
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1	5	8	174.27	4.74
1	7	2	14.67	.23
5	5	2	522.08	8.21
4	6	0	455.07	6.57
1	2	11	42.76	.74
0	7	3	172.62	6.52
2	7	1	18.24	.76
4	6	2	212.84	5.46
2	6	6	24.58	.93
3	6	5	199.05	4.18
0	4	10	153.94	6.32
1	6	7	3.36	.10
0	0	12	709.50	20.25
0	3	11	117.74	2.89
1	7	4	70.11	1.31
5	5	4	24.68	.46
2	7	3	8.29	.13
0	5	9	46.16	.74
3	4	9	186.54	3.01
4	4	8	17.32	.46
3	3	10	247.51	6.90
3	7	0	296.02	9.24
1	1	12	97.49	2.81
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# 1. SUBMISSION DETAILS

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_publ_requested_category           FM

_publ_contact_author
;
Dr. Michael James
Neutron Scattering Group, ANSTO,
Menai, NSW, 2234,
AUSTRALIA
;
_publ_contact_letter
;
;
_publ_requested_coeditor_name        ?
_publ_contact_author_phone           612-9717-9299
_publ_contact_author_fax             612-9717-3606
_publ_contact_author_email           mja@ansto.gov.au
#=====================================================================
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# 2. PROCESSING SUMMARY (IUCr Office Use Only)

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_journal_date_proofs_in           ?
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; ?
;
_journal_techeditor_code          ?
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; ?
;
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_journal_volume                   ?
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_journal_page_first               ?
_journal_page_last                ?
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# 3. TITLE AND AUTHOR LIST

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;
The structure and magnetic properties of the two-dimensional
di-pyrazine bridged polymers M(pz)2Br2
(M = Fe(II), Co(II), Ni(II))
;
loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
' James, Michael'  # SURNAME first
;
;
;
  Neutron Scattering Group,
  ANSTO,
  Lucas Heights Research Laboratories,
  PMB 1,
  Menai NSW 2234,
  Australia.
;

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# 4. TEXT

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_publ_section_exptl_prep
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;
_publ_section_exptl_refinement
;
;

_publ_section_comment
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_publ_section_acknowledgements
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_publ_section_figure_captions
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_computing_cell_refinement            ''
_computing_data_reduction             ''
_computing_structure_solution
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;
_computing_structure_refinement       ''
_computing_publication_material       ''
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_cell_length_c                         11.3131(2)
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_cell_angle_beta                       90
_cell_angle_gamma                      90
_cell_volume                           563.73(1)
_cell_formula_units_Z                  4
_cell_measurement_temperature          293

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#  EXPERIMENTAL DATA

#=============================================================================
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# 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
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Br 0 0 0.7728(1) 0.015(1) 1.000 Uiso
N 0.3051(7) 0 0 0.014(1) 1.000 Uiso
C 0.4018(6) -0.1086(6) -0.0739(4) 0.016(1) 1.000 Uiso
H 0.344(2) -0.204(2) -0.142(1) 0.025(2) 1.000 Uiso

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_refine_ls_extinction_method           ?
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_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?
_refine_ls_number_reflns               226
_refine_ls_number_parameters           ?
_refine_ls_number_restraints           ?
_refine_ls_number_constraints          ?
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  Ni   Br    2.570(1)   ? ?  yes
  Ni   N   2.154(5)   ? ?  yes
  N   C    1.324(5)   ? ?  yes
  C   C   1.387(6)   ? ?  yes
  C   H    1.10(1)   ? ?  yes

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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
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_geom_angle_site_symmetry_2
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  Ni   N   C   121.0(3)    ?  ?  ?  yes
  C   N   C   121.3(4)     ?  ?  ?  yes
  N   C   C    121.0(4)     ?  ?  ?  yes
  N   C   H    127(1)     ?  ?  ?  yes
  C   C   H    112(1)     ?  ?  ?  yes

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#     End of CIF
#=============================================================================
=====
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$Co(pz)_2Br_2$ Synchrotron Powder Diffraction Data (λ = 1.4978 Å)

h	k	l	F^2	$\sigma(F^2)$
0	1	1	23456.	61.
0	0	2	1046.	9.
1	1	0	40172.	128.
1	1	2	50726.	136.
0	2	0	132441.	328.
0	1	3	571.	4.
1	2	1	6251.	29.
0	2	2	11561.	56.
0	0	4	74494.	325.
2	2	0	59853.	244.
1	1	4	67665.	212.
1	2	3	2090.	12.
0	3	1	26210.	110.
2	2	2	29587.	122.
1	3	0	117606.	318.
0	2	4	63086.	214.
0	1	5	47513.	177.
1	3	2	7237.	35.
0	3	3	3177.	17.
2	3	1	9533.	45.
2	2	4	32203.	143.
0	0	6	7178.	40.
1	2	5	21619.	89.
0	4	0	43901.	201.
1	3	4	49893.	164.
1	1	6	935.	5.
2	3	3	139.	1.
1	4	1	8230.	38.
0	4	2	12536.	59.
3	3	0	74644.	307.
0	2	6	5063.	24.
0	3	5	52311.	199.
3	3	2	3809.	18.
2	4	0	43375.	169.
1	4	3	227.	1.
0	1	7	3281.	15.
2	4	2	15660.	62.
0	4	4	67860.	237.
2	2	6	8265.	35.
2	3	5	30558.	108.
3	3	4	65819.	226.
1	3	6	3612.	15.
1	2	7	9711.	38.
0	5	1	7959.	29.
3	4	1	12464.	46.
1	5	0	58050.	198.
0	0	8	22442.	82.
2	4	4	36230.	120.
1	4	5	22545.	78.
1	5	2	9058.	34.
1	1	8	20117.	74.
0	5	3	162.	1.

3	4	3	412.	2.
0	3	7	480.	2.
2	5	1	1889.	7.
0	2	8	14948.	55.
0	4	6	551.	2.
4	4	0	63089.	212.
1	5	4	20858.	68.
3	3	6	158.	1.
2	5	3	1301.	5.
2	3	7	3322.	12.
4	4	2	4070.	14.
0	1	9	41862.	126.
3	5	0	34407.	104.
2	2	8	10175.	32.
2	4	6	2183.	7.
0	5	5	21400.	64.
3	4	5	25805.	77.
3	5	2	9240.	30.
0	6	0	38232.	120.
1	3	8	15604.	49.
1	4	7	5310.	17.
1	6	1	5287.	17.
0	6	2	5325.	17.
1	2	9	27110.	97.

$Co(pz)_2Br_2$ Powder Neutron Diffraction Data (λ = 1.6653 Å)

h	k	l	F^2	$\sigma(F^2)$
0	1	1	46.53	.56
0	0	2	538.06	2.87
1	1	0	65.84	1.75
1	1	2	261.42	1.76
0	2	0	390.91	3.27
0	1	3	10.81	1.24
1	2	1	31.48	.93
0	2	2	.00	1.10
0	0	4	503.93	11.46
2	2	0	94.43	4.66
1	1	4	9.74	1.62
1	2	3	54.99	1.18
0	3	1	179.89	2.19
2	2	2	172.90	2.05
1	3	0	248.52	2.86
0	2	4	35.08	2.71
0	1	5	74.77	3.01
1	3	2	14.51	1.55
0	3	3	153.52	4.50
2	3	1	8.65	1.84
2	2	4	.00	2.34
0	0	6	17.02	11.53
1	2	5	.00	1.77
0	4	0	.00	7.11
1	3	4	98.39	2.11
1	1	6	15.85	1.77
2	3	3	1.60	.20
1	4	1	19.06	1.50
0	4	2	26.79	2.13
3	3	0	458.56	9.15

0	2	6	44.57	3.87
0	3	5	307.72	4.35
3	3	2	37.85	3.01
2	4	0	24.65	3.89
1	4	3	4.85	2.18
0	1	7	23.30	3.12
2	4	2	83.18	2.47
0	4	4	250.53	4.37
2	2	6	137.26	2.94
2	3	5	14.68	2.31
3	3	4	92.73	3.96
1	3	6	24.44	.64
1	2	7	107.87	2.22
0	5	1	.94	.04
3	4	1	54.37	2.21
1	5	0	168.07	4.73
0	0	8	12.09	.38
2	4	4	10.55	2.32
1	4	5	7.73	2.07
1	5	2	17.81	2.51
1	1	8	55.85	4.81
0	5	3	1.51	.04
3	4	3	71.99	2.04
0	3	7	139.78	3.07
2	5	1	111.21	2.78
0	2	8	29.73	5.26
0	4	6	368.50	7.09
4	4	0	427.87	12.28
1	5	4	109.74	1.33
3	3	6	192.29	2.17
2	5	3	168.50	1.94
2	3	7	6.85	.57
4	4	2	121.88	5.01
0	1	9	194.94	2.76
3	5	0	82.65	1.20
2	2	8	144.55	2.58
2	4	6	25.51	2.13
0	5	5	21.88	.59
3	4	5	113.91	3.05
3	5	2	65.86	2.92
0	6	0	34.62	7.76
1	3	8	1.91	.52
1	4	7	17.06	3.44
1	6	1	6.80	1.40
0	6	2	3.23	.80
1	2	9	4.11	3.09
4	4	4	2.17	4.91
2	5	5	26.32	3.38
2	6	0	10.69	5.69
3	5	4	90.84	1.51
1	5	6	333.45	3.28
1	6	3	.09	.00
0	0	10	245.00	4.56
4	5	1	12.63	1.34
2	6	2	29.32	1.64
0	3	9	182.67	2.50
0	4	8	299.46	3.59
0	6	4	358.77	6.15
1	1	10	29.13	4.32
3	3	8	190.91	7.05

4	5	3	27.82	2.42
0	2	10	.43	.04
0	5	7	10.38	1.17
3	4	7	.40	.04
3	6	1	111.45	3.61
2	3	9	31.39	2.81
2	4	8	1.15	.11
2	6	4	.96	.11
4	4	6	53.73	5.57
1	6	5	6.73	3.21
3	5	6	4.67	.56
3	6	3	29.01	1.93
2	2	10	37.02	1.50
2	5	7	76.25	1.89
0	7	1	177.94	5.23
1	4	9	12.95	.51
1	7	0	35.50	1.40
5	5	0	192.15	7.60
0	1	11	.02	.00
0	6	6	101.71	5.74
1	3	10	12.34	1.30
4	5	5	.00	.02
1	7	2	1.06	.02
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1	5	8	89.88	1.30
0	7	3	141.36	6.73
2	7	1	3.56	1.15
4	6	2	25.44	3.09
1	2	11	19.18	3.06
2	6	6	.00	.97
3	6	5	35.30	3.80
1	7	4	30.11	2.71
5	5	4	3.57	.32
2	7	3	.24	.04
0	4	10	12.95	3.15
1	6	7	8.15	1.81
0	5	9	13.55	.39
3	4	9	61.57	1.77
3	7	0	94.71	2.66
4	4	8	2.55	.07
0	3	11	26.50	.92
4	6	4	16.01	.50
0	0	12	551.81	16.22
3	3	10	34.82	1.20
0	7	5	48.74	5.09
3	7	2	19.84	2.60
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;  Data typed by hand - Output from Rietica V1.70
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# 1. SUBMISSION DETAILS

_publ_requested_journal               'Australian Journal of Chemistry'

_publ_requested_category           FM

_publ_contact_author
;
Dr. Michael James
Neutron Scattering Group, ANSTO,
Menai, NSW, 2234,
AUSTRALIA
;
_publ_contact_letter
;
;
_publ_requested_coeditor_name         ?
_publ_contact_author_phone            612-9717-9299
_publ_contact_author_fax              612-9717-3606
_publ_contact_author_email            mja@ansto.gov.au
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_journal_date_printers_final      ?
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_journal_date_proofs_in           ?
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_journal_coeditor_notes
; ?
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_journal_techeditor_code          ?
_journal_techeditor_notes
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_journal_volume                   ?
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_journal_page_first               ?
_journal_page_last                ?
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# 3. TITLE AND AUTHOR LIST

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The structure and magnetic properties of the two-dimensional
di-pyrazine bridged polymers M(pz)2Br2
(M = Fe(II), Co(II), Ni(II))
;
loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
' James, Michael'  # SURNAME first
;
;
;
  Neutron Scattering Group,
  ANSTO,
  Lucas Heights Research Laboratories,
  PMB 1,
  Menai NSW 2234,
  Australia.
;

#=============================================================================
=====

# 4. TEXT

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_publ_section_exptl_prep
;
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_publ_section_exptl_refinement
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;

_publ_section_comment
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_publ_section_acknowledgements
; ?
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_publ_section_figure_captions
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;
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_computing_cell_refinement            ''
_computing_data_reduction             ''
_computing_structure_solution
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;
_computing_structure_refinement       ''
_computing_publication_material       ''
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_cell_length_c                         11.2457(1)
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_cell_volume                           579.16(1)
_cell_formula_units_Z                  4
_cell_measurement_temperature          293

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_symmetry_space_group_name_Hall        ?

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;
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#  EXPERIMENTAL DATA

#=============================================================================
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# ATOMIC COORDINATES AND THERMAL PARAMETERS

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_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_thermal_displace_type
Co 0 0 0 0.013(1) 1.000 Uiso
Br 0 0 0.7712(2) 0.012(1) 1.000 Uiso
N 0.3083(4) 0 0 0.016(1) 1.000 Uiso
C 0.4035(5) -0.1113(5) -0.0770(3) 0.020(1) 1.000 Uiso
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# REFINEMENT DATA

_refine_special_details                ?
_refine_ls_structure_factor_coef       ?
_refine_ls_matrix_type                 ?
_refine_ls_weighting_scheme            ?
_refine_ls_hydrogen_treatment          ?
_refine_ls_extinction_method           ?
_refine_ls_extinction_coef             ?
_refine_ls_abs_structure_details       ?
_refine_ls_abs_structure_Flack         ?
_refine_ls_number_reflns               233
_refine_ls_number_parameters           ?
_refine_ls_number_restraints           ?
_refine_ls_number_constraints          ?
_refine_ls_R_factor_all                0.022
_refine_ls_R_factor_obs                0.022
```

```
_refine_ls_wR_factor_all               0.029
_refine_ls_wR_factor_obs               0.029

#=============================================================================
=====

#  MOLECULAR GEOMETRY

_geom_special_details        ?

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
  Co   Co   7.1764(1)   ? ?  yes
  Co   Br    2.573(2)   ? ?  yes
  Co   N   2.212(3)   ? ?  yes
  N   C    1.362(4)   ? ?  yes
  C   C   1.385(5)   ? ?  yes
  C   H    1.01(1)   ? ?  yes

#-----------------------------------------------------------------------------
--------
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
  Co   N   C   121.1(2)    ?  ?  ?  yes
  C   N   C   119.8(3)     ?  ?  ?  yes
  N   C   C    120.1(3)     ?  ?  ?  yes
  N   C   H    121(1)     ?  ?  ?  yes
  C   C   H    119(1)     ?  ?  ?  yes

#=============================================================================
=====
#     End of CIF
#=============================================================================
=====
```