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Bis(5,8-diazoniadispiro[4.2.4.2]tetradecane) hexakis(thiocyanato-κN)-manganate(II)

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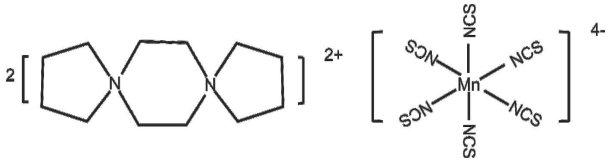
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.141; data-to-parameter ratio = 16.8.

The asymmetric unit of the title compound, $(C_{12}H_{24}N_2)_2[Mn(NCS)_6]$, comprises one cation and one half of the anion. The central Mn atom of the anion is situated on an inversion centre and shows the expected octahedral coordination with only minor deviations from the ideal geometry. Intermolecular C—H···S hydrogen-bonding interactions link all components into a three-dimensional network.

Related literature

For structures containing the complex $[Ni(NCS)_6]^{4-}$ anion, see, for example, Böhland *et al.* (1997); Bose *et al.* (2006); Burla *et al.* (1995); Shen *et al.* (2002); Shi *et al.* (2005).



Experimental

Crystal data

$(C_{12}H_{24}N_2)_2[Mn(NCS)_6]$
M_r = 796.08
Monoclinic, $P2_1/n$
a = 9.8816 (15) Å
b = 13.382 (2) Å
c = 15.173 (2) Å
β = 102.431 (3)°
V = 1959.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 273 (2) K
0.53 × 0.15 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.710, T_{max} = 0.922
10582 measured reflections
3589 independent reflections
2679 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 1.00
3589 reflections
214 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—N1	2.223 (3)	Mn1—N3	2.248 (3)
Mn1—N2	2.239 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···S3^{i}	0.97	2.81	3.629 (3)	143
C10—H10B···S3^{ii}	0.97	2.84	3.750 (3)	157

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2137).

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supplementary materials

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Bis(5,8-diazoniadispiro[4.2.4.2]tetradecane) hexakis(thiocyanato-*κN*)manganate(II)

Y.-X. Li, X.-L. Guo, Z. Wang and Y. Niu

Comment

Organic-inorganic compounds containing the [hexakis(isothiocyanato)manganese(II)] anion, $[Mn(NCS)_6]^{4-}$, have been the subject of several investigations, but reported crystal structures containing this building unit are relatively scarce (Böhland *et al.* (1997); Bose *et al.* (2006); Burla *et al.* (1995); Shen *et al.* (2002); Shi *et al.* (2005). In this communication we report the crystal structure of a new [hexakis(isothiocyanato)manganese(II)] salt containing the 5,8-diazoniadispiro[4.2.4.2]tetradecane counter cation.

The structure of the title compound (Fig. 1) comprises discrete $(C_{12}H_{24}N_2)^{2+}$ cations and $[Mn(NCS)_6]^{4-}$ anions. The anion, which lies on an inversion center, displays the expected homoleptic N_6-octahedral coordination with only minor deviations from the ideal geometry. In the cation, the six-membered ring displays a chair conformation, while the five-membered rings adopt a twist conformation. In the crystal structure, all building units are linked into a three-dimensional extended network *via* intermolecular C—H···S hydrogen bonding interactions (Table, Fig. 2).

Experimental

All chemicals were used as purchased from Jinan Henghua Sci. & Tec. Co., Ltd. The title salt was synthesized from the reaction of 5,8-diazoniadispiro[4.2.4.2]tetradecane dibromide (0.034 g, 0.1 mmol) in methanol (5 ml) and a mixture of $MnCl_2$ (0.012 g, 0.1 mmol) and K(NCS) (0.074 g, 0.4 mmol) in DMF (10 ml). The resulting mixture was set aside for the formation of colourless crystals in approximately 34% yield after several d. Anal. Calc. for $C_{30}H_{48}MnN_{10}S_6$: C 45.26, H 6.07, N 17.59%; Found: C 45.21, H 6.08, N 17.52%.

Refinement

All H atoms bonded to C atoms were generated geometrically and refined as riding atoms with C—H= 0.97Å and U_{iso}(H)= 1.2U_{eq}(C).

Figures

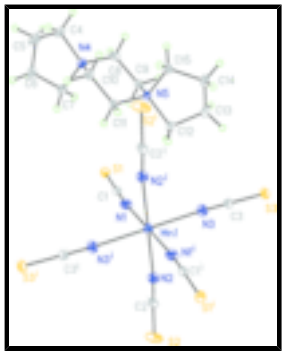

Fig. 1. A view of the structure of the title compound, showing displacement ellipsoids at the 30% probability level. [Symmetry operator: (i) −*x* + 2,-*y* + 2,-*z* + 1.]

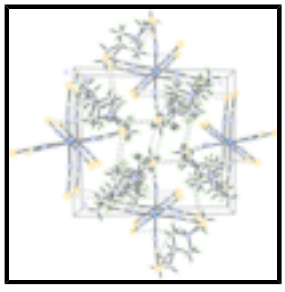

Fig. 2. C—H···π interactions in the title compound.

Bis(5,8-diazoniadispiro[4.2.4.2]tetradecane) hexakis(thiocyanato-κ*N*)- manganate(II)

Crystal data

$(C_{12}H_{24}N_2)_2[Mn(NCS)_6]$	F_{000} = 838
M_r = 796.08	D_x = 1.349 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2869 reflections
a = 9.8816 (15) Å	θ = 2.3–23.4º
b = 13.382 (2) Å	μ = 0.69 mm^{-1}
c = 15.173 (2) Å	*T* = 273 (2) K
β = 102.431 (3)º	Fragment, colorless
V = 1959.4 (5) Å^3	0.53 × 0.15 × 0.12 mm
Z = 2	

Data collection

Bruker APEXII CCD area-detector diffractometer	3589 independent reflections
Radiation source: fine-focus sealed tube	2679 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 273(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −10→11

T_{min} = 0.710, T_{max} = 0.922	k = −16→16
10582 measured reflections	l = −18→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 0.6082P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
3589 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
214 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.5000	0.5000	0.0000	0.0522 (2)
S1	0.39777 (8)	0.43111 (6)	0.30277 (5)	0.0629 (2)
S2	0.96283 (13)	0.64089 (10)	0.14596 (8)	0.1117 (5)
S3	0.69183 (9)	0.15133 (6)	0.01699 (7)	0.0737 (3)
N1	0.4577 (3)	0.4769 (2)	0.1366 (2)	0.0731 (8)
N2	0.7113 (3)	0.5556 (2)	0.06566 (19)	0.0698 (7)
N3	0.5748 (3)	0.3416 (2)	−0.0022 (2)	0.0718 (7)
N4	−0.0605 (2)	0.31563 (18)	0.21676 (15)	0.0522 (6)
N5	0.1560 (2)	0.23697 (15)	0.12676 (15)	0.0454 (5)
C1	0.4340 (3)	0.4584 (2)	0.2058 (2)	0.0535 (7)
C2	0.8136 (4)	0.5917 (2)	0.1000 (2)	0.0588 (7)
C3	0.6225 (3)	0.2633 (2)	0.00443 (18)	0.0518 (7)
C4	−0.2133 (3)	0.3136 (4)	0.2228 (3)	0.0870 (12)
H4A	−0.2701	0.3484	0.1719	0.104*
H4B	−0.2461	0.2454	0.2235	0.104*
C5	−0.2180 (5)	0.3621 (7)	0.3035 (4)	0.0778 (9)

H5A	−0.2162	0.3127	0.3506	0.208*
H5B	−0.3042	0.3990	0.2962	0.208*
C6	−0.1051 (4)	0.4288 (3)	0.3302 (3)	0.0796 (11)
H6A	−0.0737	0.4286	0.3953	0.095*
H6B	−0.1324	0.4962	0.3108	0.095*
C7	0.0067 (3)	0.3931 (3)	0.2866 (2)	0.0624 (8)
H7A	0.0811	0.3631	0.3309	0.075*
H7B	0.0441	0.4481	0.2577	0.075*
C8	0.0024 (3)	0.2135 (2)	0.2360 (2)	0.0582 (7)
H8A	0.0033	0.1959	0.2982	0.070*
H8B	−0.0551	0.1651	0.1975	0.070*
C9	0.1473 (3)	0.2074 (2)	0.22088 (19)	0.0544 (7)
H9A	0.1811	0.1396	0.2322	0.065*
H9B	0.2068	0.2509	0.2636	0.065*
C10	−0.0488 (3)	0.3443 (2)	0.12343 (19)	0.0520 (7)
H10A	−0.0841	0.4116	0.1107	0.062*
H10B	−0.1055	0.2996	0.0804	0.062*
C11	0.0972 (3)	0.33998 (19)	0.11145 (18)	0.0483 (6)
H11A	0.1000	0.3614	0.0508	0.058*
H11B	0.1537	0.3857	0.1535	0.058*
C12	0.3072 (3)	0.2362 (2)	0.1172 (2)	0.0666 (8)
H12A	0.3218	0.2839	0.0720	0.080*
H12B	0.3695	0.2518	0.1742	0.080*
C13	0.3285 (4)	0.1318 (3)	0.0886 (3)	0.0802 (10)
H13A	0.4034	0.1289	0.0565	0.096*
H13B	0.3503	0.0877	0.1404	0.096*
C14	0.1949 (3)	0.1030 (3)	0.0284 (2)	0.0731 (9)
H14A	0.1782	0.0321	0.0339	0.088*
H14B	0.1970	0.1173	−0.0340	0.088*
C15	0.0839 (3)	0.1620 (2)	0.0562 (2)	0.0565 (7)
H15A	0.0237	0.1185	0.0817	0.068*
H15B	0.0284	0.1966	0.0047	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0530 (4)	0.0457 (3)	0.0566 (4)	0.0007 (3)	0.0087 (3)	0.0067 (3)
S1	0.0679 (5)	0.0649 (5)	0.0582 (5)	0.0009 (4)	0.0187 (4)	−0.0070 (3)
S2	0.1121 (9)	0.1153 (9)	0.0864 (7)	−0.0565 (7)	−0.0255 (6)	0.0210 (6)
S3	0.0617 (5)	0.0549 (5)	0.0956 (6)	0.0095 (4)	−0.0032 (4)	−0.0172 (4)
N1	0.083 (2)	0.0689 (18)	0.0693 (19)	−0.0124 (15)	0.0204 (15)	0.0036 (14)
N2	0.0604 (17)	0.0664 (17)	0.0783 (18)	−0.0023 (14)	0.0056 (14)	0.0072 (14)
N3	0.0711 (18)	0.0584 (16)	0.0807 (19)	0.0109 (14)	0.0051 (14)	0.0068 (13)
N4	0.0405 (12)	0.0662 (15)	0.0518 (13)	−0.0041 (10)	0.0139 (10)	−0.0138 (11)
N5	0.0430 (12)	0.0385 (11)	0.0553 (13)	0.0046 (9)	0.0114 (9)	−0.0018 (9)
C1	0.0552 (17)	0.0427 (14)	0.0621 (19)	−0.0016 (12)	0.0113 (13)	−0.0049 (13)
C2	0.074 (2)	0.0470 (16)	0.0533 (17)	−0.0013 (15)	0.0080 (15)	0.0052 (13)
C3	0.0477 (15)	0.0569 (18)	0.0479 (15)	−0.0028 (13)	0.0039 (12)	−0.0076 (12)

C4	0.0441 (17)	0.132 (3)	0.090 (3)	−0.0091 (19)	0.0240 (16)	−0.042 (2)
C5	0.0744 (19)	0.0477 (15)	0.088 (2)	0.0017 (14)	0.0370 (16)	−0.0168 (15)
C6	0.070 (2)	0.095 (3)	0.076 (2)	0.0153 (19)	0.0188 (17)	−0.0264 (19)
C7	0.0552 (17)	0.075 (2)	0.0581 (17)	−0.0022 (15)	0.0149 (13)	−0.0236 (15)
C8	0.0688 (19)	0.0582 (17)	0.0488 (16)	−0.0111 (14)	0.0153 (13)	0.0041 (13)
C9	0.0574 (17)	0.0454 (15)	0.0568 (17)	0.0082 (13)	0.0048 (13)	0.0071 (12)
C10	0.0508 (16)	0.0533 (16)	0.0502 (15)	0.0141 (12)	0.0073 (11)	−0.0029 (12)
C11	0.0579 (16)	0.0384 (13)	0.0520 (15)	0.0039 (11)	0.0194 (12)	0.0035 (11)
C12	0.0456 (16)	0.067 (2)	0.092 (2)	0.0008 (14)	0.0249 (15)	−0.0129 (17)
C13	0.068 (2)	0.077 (2)	0.104 (3)	0.0157 (18)	0.034 (2)	−0.014 (2)
C14	0.076 (2)	0.082 (2)	0.067 (2)	0.0044 (18)	0.0292 (17)	−0.0226 (17)
C15	0.0619 (18)	0.0507 (16)	0.0554 (16)	0.0044 (13)	0.0097 (13)	−0.0101 (13)

Geometric parameters (Å, °)

Mn1—N1	2.223 (3)	C6—C7	1.483 (4)
Mn1—N1^{i}	2.223 (3)	C6—H6A	0.9700
Mn1—N2^{i}	2.239 (3)	C6—H6B	0.9700
Mn1—N2	2.239 (3)	C7—H7A	0.9700
Mn1—N3^{i}	2.248 (3)	C7—H7B	0.9700
Mn1—N3	2.248 (3)	C8—C9	1.500 (4)
S1—C1	1.629 (3)	C8—H8A	0.9700
S2—C2	1.628 (3)	C8—H8B	0.9700
S3—C3	1.641 (3)	C9—H9A	0.9700
N1—C1	1.150 (4)	C9—H9B	0.9700
N2—C2	1.140 (4)	C10—C11	1.493 (4)
N3—C3	1.144 (4)	C10—H10A	0.9700
N4—C10	1.496 (4)	C10—H10B	0.9700
N4—C8	1.504 (4)	C11—H11A	0.9700
N4—C7	1.528 (4)	C11—H11B	0.9700
N4—C4	1.532 (4)	C12—C13	1.492 (5)
N5—C11	1.494 (3)	C12—H12A	0.9700
N5—C9	1.502 (4)	C12—H12B	0.9700
N5—C15	1.527 (3)	C13—C14	1.486 (5)
N5—C12	1.532 (3)	C13—H13A	0.9700
C4—C5	1.396 (5)	C13—H13B	0.9700
C4—H4A	0.9700	C14—C15	1.485 (4)
C4—H4B	0.9700	C14—H14A	0.9700
C5—C6	1.417 (6)	C14—H14B	0.9700
C5—H5A	0.9700	C15—H15A	0.9700
C5—H5B	0.9700	C15—H15B	0.9700
N1—Mn1—N1^{i}	180.00 (15)	N4—C7—H7A	110.6
N1—Mn1—N2^{i}	91.38 (11)	C6—C7—H7B	110.6
N1^{i}—Mn1—N2^{i}	88.62 (11)	N4—C7—H7B	110.6
N1—Mn1—N2	88.62 (11)	H7A—C7—H7B	108.7
N1^{i}—Mn1—N2	91.38 (11)	C9—C8—N4	112.8 (2)
N2^{i}—Mn1—N2	180.0	C9—C8—H8A	109.0

N1—Mn1—N3^{i}	89.36 (11)	N4—C8—H8A	109.0
N1^{i}—Mn1—N3^{i}	90.64 (11)	C9—C8—H8B	109.0
N2^{i}—Mn1—N3^{i}	92.38 (10)	N4—C8—H8B	109.0
N2—Mn1—N3^{i}	87.62 (10)	H8A—C8—H8B	107.8
N1—Mn1—N3	90.64 (11)	C8—C9—N5	112.5 (2)
N1^{i}—Mn1—N3	89.36 (11)	C8—C9—H9A	109.1
N2^{i}—Mn1—N3	87.62 (10)	N5—C9—H9A	109.1
N2—Mn1—N3	92.38 (10)	C8—C9—H9B	109.1
N3^{i}—Mn1—N3	180.0	N5—C9—H9B	109.1
C1—N1—Mn1	175.4 (3)	H9A—C9—H9B	107.8
C2—N2—Mn1	174.0 (3)	N4—C10—C11	112.3 (2)
C3—N3—Mn1	173.1 (3)	N4—C10—H10A	109.1
C10—N4—C8	107.7 (2)	C11—C10—H10A	109.1
C10—N4—C7	111.8 (2)	N4—C10—H10B	109.1
C8—N4—C7	112.5 (2)	C11—C10—H10B	109.1
C10—N4—C4	109.8 (2)	H10A—C10—H10B	107.9
C8—N4—C4	110.1 (3)	N5—C11—C10	111.7 (2)
C7—N4—C4	104.9 (2)	N5—C11—H11A	109.3
C11—N5—C9	106.9 (2)	C10—C11—H11A	109.3
C11—N5—C15	113.0 (2)	N5—C11—H11B	109.3
C9—N5—C15	112.3 (2)	C10—C11—H11B	109.3
C11—N5—C12	110.2 (2)	H11A—C11—H11B	107.9
C9—N5—C12	110.2 (2)	C13—C12—N5	103.6 (2)
C15—N5—C12	104.3 (2)	C13—C12—H12A	111.0
N1—C1—S1	178.9 (3)	N5—C12—H12A	111.0
N2—C2—S2	177.6 (3)	C13—C12—H12B	111.0
N3—C3—S3	178.4 (3)	N5—C12—H12B	111.0
C5—C4—N4	105.3 (3)	H12A—C12—H12B	109.0
C5—C4—H4A	110.7	C14—C13—C12	105.0 (3)
N4—C4—H4A	110.7	C14—C13—H13A	110.7
C5—C4—H4B	110.7	C12—C13—H13A	110.7
N4—C4—H4B	110.7	C14—C13—H13B	110.7
H4A—C4—H4B	108.8	C12—C13—H13B	110.7
C4—C5—C6	111.7 (4)	H13A—C13—H13B	108.8
C4—C5—H5A	109.3	C13—C14—C15	107.5 (3)
C6—C5—H5A	109.3	C13—C14—H14A	110.2
C4—C5—H5B	109.3	C15—C14—H14A	110.2
C6—C5—H5B	109.3	C13—C14—H14B	110.2
H5A—C5—H5B	107.9	C15—C14—H14B	110.2
C5—C6—C7	106.6 (3)	H14A—C14—H14B	108.5
C5—C6—H6A	110.4	C14—C15—N5	106.7 (2)
C7—C6—H6A	110.4	C14—C15—H15A	110.4
C5—C6—H6B	110.4	N5—C15—H15A	110.4
C7—C6—H6B	110.4	C14—C15—H15B	110.4
H6A—C6—H6B	108.6	N5—C15—H15B	110.4
C6—C7—N4	105.9 (2)	H15A—C15—H15B	108.6
C6—C7—H7A	110.6		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···S3^{ii}	0.97	2.81	3.629 (3)	143
C10—H10B···S3^{iii}	0.97	2.84	3.750 (3)	157

Symmetry codes: (ii) *x*−1/2, −*y*+1/2, *z*+1/2; (iii) *x*−1, *y*, *z*.

Fig. 1

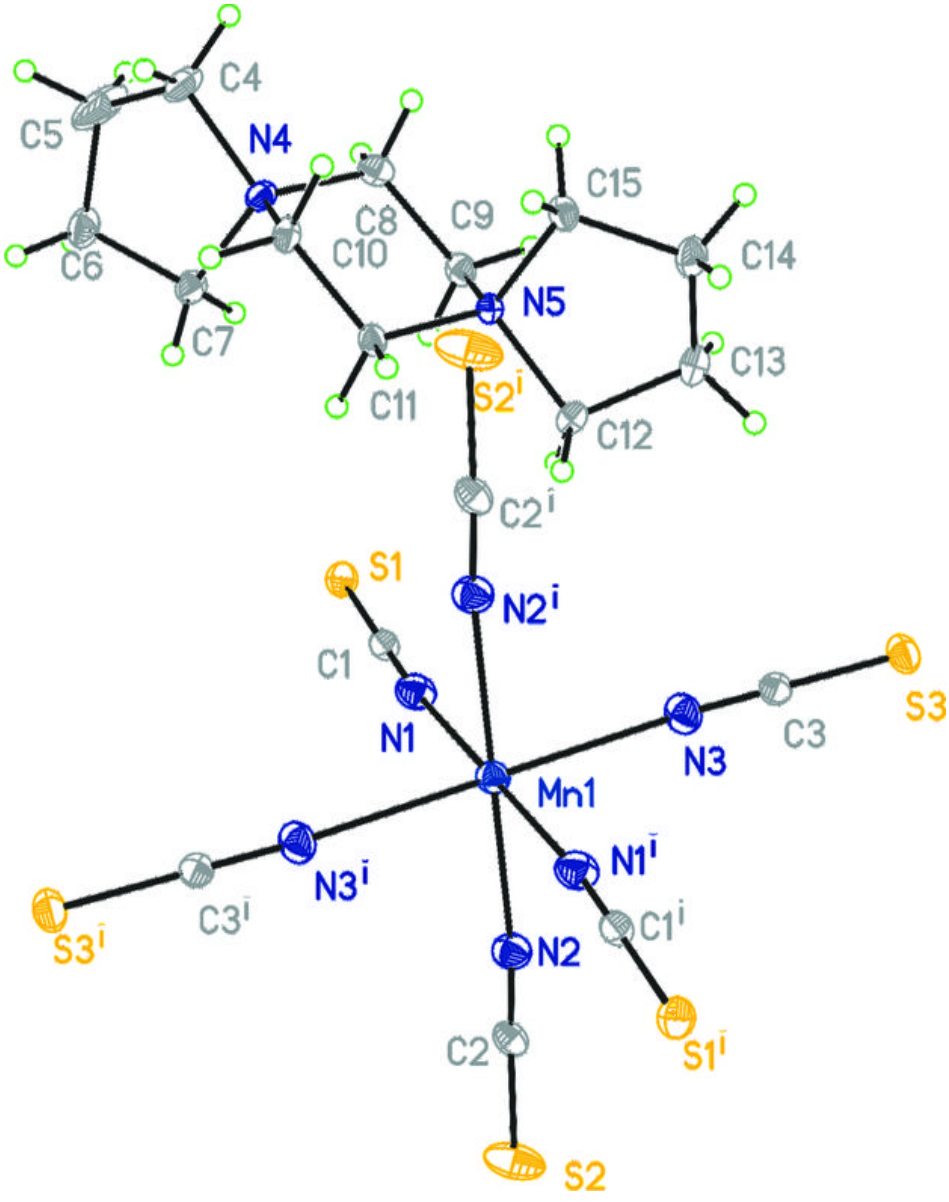
C4
C5
N4
C6
C7
C8
C9
C10
C11
C15
C14
N5
C13
S2i
C12
C2i
S1
N2i
C1
N1
N3
C3
S3
Mn1
N3i
C3i
S3i
N1i
C1i
N2
C2
S1i
S2

Fig. 2