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2-Methoxy-*N*′-(morpholin-4-ylcarbonothioyl)benzohydrazide hemihydrate

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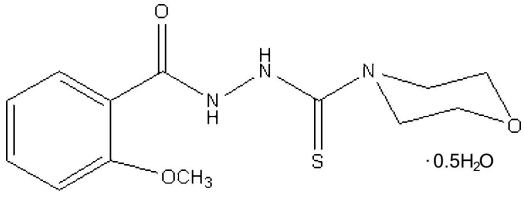
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.118; data-to-parameter ratio = 13.8.

In the title compound, $C_{13}H_{17}N_3O_3S\cdot0.5H_2O$, the morpholine ring adopts a chair conformation. The conformation of the molecule is stabilized by intramolecular N—H···O and N—H···S hydrogen bonds. Intermolecular N—H···O and O—H···O hydrogen bonds link the organic molecules through the water molecules to build up a channel running parallel to the *c* axis and containing the water molecules.

Related literature

For related literature, see: Fisher & Wyvratt (1990); Yoshioka (1995); Ramnathan *et al.* (1996); Badioli *et al.* (2001). Wu *et al.* (2000).



Experimental

Crystal data

$C_{13}H_{17}N_3O_3S\cdot0.5H_2O$
M_r = 304.37
Orthorhombic, *Pccn*
a = 13.4864 (2) Å
b = 24.6003 (6) Å
c = 8.8726 (2) Å
V = 2943.66 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 173 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.880, T_{max} = 0.954
35059 measured reflections
2697 independent reflections
2080 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.118
S = 1.05
2697 reflections
196 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.88 (2)	1.91 (2)	2.593 (2)	134 (2)
N1—H1···S1	0.88 (2)	2.44 (2)	2.8714 (18)	110.8 (19)
N2—H2···O4	0.858 (10)	2.071 (11)	2.921 (2)	171 (2)
O4—H4*A*···O2^{i}	0.846 (10)	1.921 (11)	2.7590 (19)	170 (2)

Symmetry code: (i) $-x+\frac{3}{2}, y, z-\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2277).

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supplementary materials

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2-Methoxy-*N*'-(morpholin-4-ylcarbonothioyl)benzohydrazide hemihydrate

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Comment

Morpholine derivatives are an important type of fungicide (Badioli *et al.*, 2001) and pharmaceutical drugs due to which they have attracted much attention in recent years in pharmaceuticals. The morpholine drugs are used in the reduction of blood sugar and control of lipid levels (Yoshioka, 1995) and insulin resistance (Fisher & Wyvratt,1990). Owing to their important pharmalogical activities and bioactivity, these compounds have received a great attention with respect to their syntheses and in the elucidation of their crystal structures.

The structure of (I) is shown in Fig 1. The morpholine ring exhibits a normal chair conformation. In the morpholine ring, the average Csp^3—Nsp^3, Csp^3—Csp^3 and Csp^3—Osp^3 bond distances [1.472 (2), 1.490 (2) and 1.4309 (2) Å], respectively, are in good agreement with earlier reports (Ramnathan *et al.*,1996). In the chair conformation, the four carbon atoms deviate only slightly from coplanarity. The dihedral angle between the carbonothioyl carbohydrazide unit and morpholine ring is 35.16 (2)°. Hydrazinic atoms H1 and H2 are *trans* to each other, as are the C(8)—S(1) and C(7)—O(2) groups [torsional angles, N2—N1—C7—O2 and N1—N2—C8—S1 = −6.31 (3)° and 5.8 (3)°, respectively]. In addition, the C—S and C—N bond distances are 1.683 (2) Å and 1.375 (2) Å respectively, which are intermediate between C—S (1.82 Å) and C=S (1.56 Å) (Wu *et al.*, 2000) and C—N (1.450 Å) and C=N (1.250 Å) distances. The intermediate bond distances in compound (I) show extensive electron delocalization which provides stability to the molecule.

The conformation of the molecule is stabilized by an N—H···O and N—H···S intramolecular hydrogen bondings. Iintermolecular hydrogen bondings N—H···O [2.920 (2) Å] and O—H···O [2.759 (2) Å] links the molecules through the water to build up a channel running parallel to the *c* axis and containing the water molecules (Table 1, Fig. 2).

Experimental

Potassium[morpholine-4-carbodithioate] was synthesized by the reaction of CS_2 (4.4 ml, 57.39 mmol) with morpholine (5 ml, 57.39 mmol) in MeOH (20 ml) in the presence of KOH (3.2 g, 57.39 mmol). The precipitated product (Yield 78%, 3.9 g, 31.15 mmol) was separated by filtration and reacted with choloroacetic acid ($ClCH_2COOH$) (2.9 g, 31.15 mmol) neutralized with Na_2CO_3. The mixture was kept over night at room temperature and then made strongly acidic with conc. HCl to get the precipitate of (morpholine-4-carbothioyl sulfanyl) acetic acid (yield 69%, 2.7 g, 14.24 mmol). This was filtered off, washed with water and dried at room temperature.

The ester was recrystalized from $CHCl_3$: MeOH mixture. ^{1}H NMR (DMSO-d_6, TMS): 10.62 (s, 1H, –COOH), 2.5 (s,2*H*, CH_2), 3.35 (s, 3H, –OCH_3), 7.90–7.18 (m, 4H, aromatic); ^{13}C NMR (DMSO-d_6, TMS): 205.41 (C=S), 121.22 (C1), 157.22 (C2), 112.50 (C3), 133.74 (C4), 120.54 (C5), 131.44 (C6), 169.65 (C7), 56.68 (C8), 36.53(C9).

The compound (I) was synthesized by reaction of the morpholine ester (2.7 g, 14.24 mmol) and *o*-methoxy benzoic acid hydrazide (2.4 g, 14.24 mmol). Both were dissolved separately in aqueous solution of NaOH, mixed together, kept for 2

h at room temperature and then acidified with dil. AcOH (20% *v*/*v*), whereupon a white precipitate formed. It was suction filtered, washed with water, dried at room temperature and crystalized from $CHCl_3$: MeOH mixture (50: 50 *v*/*v*).

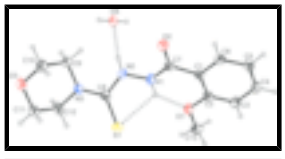
White color single crystals of (I) (m.p.413 K) suitable for X-ray analysis were obtained by slow evaporation of chloroform: methanolic solution over a period of 10 d. (yield 2.64 g, 66%). Analysis found (%) for $C_{15}H_{17}N_3O_4S$ (608.208): C, 51.30; H, 5.97; N, 13.81; S, 10.51. Calculated (%): C, 51.35; H, 5.90; N, 13.99; S, 10.57.

^{1}H NMR (DMSO-d_6, TMS): 12.79, 11.63 (2H, –NH), 3.38 (3*H*, –OCH_3), 2.50, 3.08 (8H, methylene, morpholine), 7.89–7.19 (m, 4H, aromatic). ^{13}C NMR (DMSO-d_6, TMS): 203.08 (C=S), 120.78 (C1), 157.06 (C2), 112.69 (C3), 133.88 (C4), 121.22 (C5), 130.01 (C6), 169.13 (C7), 56.05 (C13), 63.15 (C10,C11), 42.59 (C9,C12).

Refinement

All H atoms were initially located in difference Fourier map. The were then placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–0.99 Å and with U_{iso} = 1.2 U_{eq}(C).

Figures



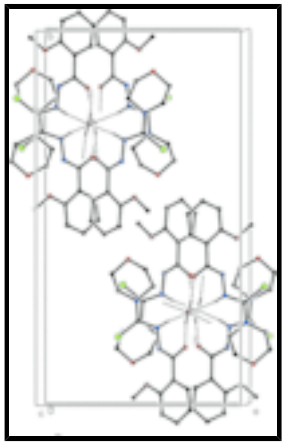
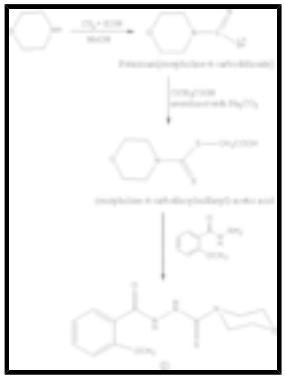


Figure 1.The molecular structure of (I), showing the atom numbering scheme with displacement ellipsoid drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.
Figure 2. Partial packing viewof (I), along *c* axis, showing hydrogen bonding interactions and the formation of channels.



2-Methoxy-*N*'-(morpholin-4-ylcarbothioyl)benzohydrazide hemihydrate

Crystal data

$C_{13}H_{17}N_3O_3S·0.5H_2O$	$D_x = 1.374$ Mg m^{-3}
$M_r = 304.37$	Melting point: 413 K
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 1473 reflections
a = 13.4864 (2) Å	θ = 1.0–27.5º
b = 24.6003 (6) Å	μ = 0.24 mm^{-1}
c = 8.8726 (2) Å	*T* = 173 (2) K
V = 2943.66 (11) Å^3	Chip, colourless
Z = 8	0.20 × 0.20 × 0.20 mm
F_{000} = 1288	

Data collection

Nonius KappaCCD diffractometer	2697 independent reflections
Radiation source: fine-focus sealed tube	2080 reflections with $I > 2\sigma(I)$
Monochromator: horizonally mounted graphite crystal	$R_{int} = 0.093$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 25.4$º
T = 173(2) K	$\theta_{min} = 2.9$º
φ scans and ω scans with κ offsets	*h* = −16→16
Absorption correction: ψ scan (North *et al.*, 1968)	*k* = −29→29
$T_{min} = 0.880$, $T_{max} = 0.954$	*l* = −10→10
35059 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 1.2085P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2697 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
196 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.39345 (4)	0.18214 (2)	0.81529 (7)	0.0347 (2)
O1	0.53195 (10)	0.05419 (6)	0.78451 (17)	0.0300 (4)
O2	0.72871 (10)	0.15538 (6)	1.00899 (18)	0.0331 (4)
O3	0.44448 (10)	0.38946 (6)	0.8740 (2)	0.0369 (4)
N1	0.59668 (13)	0.15023 (7)	0.8537 (2)	0.0295 (4)
H1	0.5474 (17)	0.1302 (10)	0.820 (3)	0.035*
N2	0.58506 (13)	0.20662 (7)	0.8490 (2)	0.0287 (4)
H2	0.6318 (13)	0.2228 (9)	0.801 (2)	0.034*
N3	0.48296 (12)	0.27922 (7)	0.8073 (2)	0.0324 (5)
C1	0.66929 (13)	0.06691 (8)	0.9476 (2)	0.0216 (5)
C2	0.60297 (14)	0.03135 (8)	0.8743 (2)	0.0219 (4)
C3	0.61164 (14)	−0.02433 (8)	0.8933 (2)	0.0252 (5)
H3	0.5662	−0.0475	0.8477	0.030*
C4	0.68761 (15)	−0.04559 (9)	0.9798 (2)	0.0286 (5)
H4	0.6937	−0.0831	0.9903	0.034*
C5	0.75466 (15)	−0.01163 (9)	1.0509 (2)	0.0281 (5)
H5	0.8061	−0.0260	1.1080	0.034*
C6	0.74412 (14)	0.04413 (8)	1.0358 (2)	0.0246 (5)
H6	0.7881	0.0670	1.0858	0.029*
C7	0.66677 (14)	0.12779 (8)	0.9407 (2)	0.0229 (5)
C8	0.49040 (14)	0.22514 (8)	0.8232 (2)	0.0251 (5)
C9	0.56444 (16)	0.31790 (9)	0.8275 (3)	0.0336 (6)
H9A	0.5843	0.3325	0.7304	0.040*
H9B	0.6211	0.2996	0.8717	0.040*
C10	0.53137 (16)	0.36312 (9)	0.9283 (3)	0.0381 (6)
H10A	0.5184	0.3487	1.0281	0.046*
H10B	0.5843	0.3896	0.9370	0.046*
C11	0.36544 (16)	0.35094 (9)	0.8625 (3)	0.0363 (6)
H11A	0.3062	0.3692	0.8266	0.044*
H11B	0.3512	0.3362	0.9616	0.044*
C12	0.39068 (16)	0.30563 (9)	0.7580 (3)	0.0383 (6)
H12A	0.3372	0.2793	0.7568	0.046*
H12B	0.3989	0.3197	0.6566	0.046*

C13	0.46377 (15)	0.01932 (9)	0.7067 (3)	0.0311 (5)
H13A	0.5000	−0.0056	0.6444	0.047*
H13B	0.4206	0.0409	0.6449	0.047*
H13C	0.4251	−0.0006	0.7788	0.047*
O4	0.7500	0.2500	0.6727 (3)	0.0296 (5)
H4A	0.7627 (18)	0.2227 (7)	0.618 (3)	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0235 (3)	0.0308 (3)	0.0499 (4)	−0.0057 (2)	0.0010 (3)	−0.0044 (3)
O1	0.0286 (8)	0.0227 (8)	0.0388 (9)	−0.0015 (6)	−0.0139 (7)	0.0021 (7)
O2	0.0269 (8)	0.0221 (8)	0.0501 (10)	−0.0010 (6)	−0.0079 (7)	−0.0056 (7)
O3	0.0285 (8)	0.0213 (8)	0.0608 (11)	0.0055 (6)	−0.0087 (7)	−0.0028 (8)
N1	0.0287 (10)	0.0161 (9)	0.0435 (12)	−0.0005 (7)	−0.0095 (9)	0.0028 (8)
N2	0.0241 (9)	0.0167 (9)	0.0454 (12)	−0.0009 (7)	0.0011 (8)	0.0041 (8)
N3	0.0221 (10)	0.0201 (10)	0.0549 (13)	0.0023 (7)	−0.0074 (8)	−0.0057 (9)
C1	0.0207 (10)	0.0214 (11)	0.0228 (11)	−0.0008 (8)	0.0037 (8)	−0.0004 (9)
C2	0.0213 (10)	0.0239 (11)	0.0205 (11)	0.0016 (8)	−0.0001 (8)	0.0006 (9)
C3	0.0291 (11)	0.0217 (11)	0.0249 (12)	−0.0031 (8)	−0.0005 (9)	−0.0018 (9)
C4	0.0349 (12)	0.0202 (11)	0.0308 (12)	0.0034 (9)	0.0018 (10)	0.0031 (9)
C5	0.0260 (11)	0.0286 (12)	0.0298 (12)	0.0045 (9)	−0.0028 (9)	0.0059 (10)
C6	0.0201 (10)	0.0264 (12)	0.0272 (11)	−0.0010 (8)	−0.0015 (8)	0.0008 (9)
C7	0.0196 (10)	0.0223 (11)	0.0268 (11)	−0.0004 (8)	0.0039 (8)	−0.0004 (9)
C8	0.0208 (11)	0.0242 (12)	0.0304 (12)	0.0006 (8)	0.0007 (9)	−0.0038 (9)
C9	0.0240 (12)	0.0212 (12)	0.0556 (16)	0.0001 (8)	−0.0008 (10)	0.0001 (11)
C10	0.0317 (12)	0.0250 (12)	0.0576 (17)	0.0011 (9)	−0.0116 (11)	−0.0034 (11)
C11	0.0257 (11)	0.0298 (13)	0.0534 (16)	0.0045 (9)	−0.0014 (11)	−0.0014 (11)
C12	0.0280 (13)	0.0316 (13)	0.0553 (17)	0.0076 (9)	−0.0124 (11)	−0.0063 (12)
C13	0.0276 (11)	0.0329 (12)	0.0328 (13)	−0.0036 (9)	−0.0087 (9)	−0.0039 (10)
O4	0.0285 (11)	0.0201 (11)	0.0403 (14)	0.0043 (9)	0.000	0.000

Geometric parameters (Å, °)

S1—C8	1.683 (2)	C4—C5	1.383 (3)
O1—C2	1.367 (2)	C4—H4	0.9300
O1—C13	1.435 (2)	C5—C6	1.386 (3)
O2—C7	1.235 (2)	C5—H5	0.9300
O3—C10	1.423 (3)	C6—H6	0.9300
O3—C11	1.430 (3)	C9—C10	1.496 (3)
N1—C7	1.339 (3)	C9—H9A	0.9700
N1—N2	1.397 (2)	C9—H9B	0.9700
N1—H1	0.88 (2)	C10—H10A	0.9700
N2—C8	1.375 (3)	C10—H10B	0.9700
N2—H2	0.858 (10)	C11—C12	1.490 (3)
N3—C8	1.342 (3)	C11—H11A	0.9700
N3—C9	1.464 (3)	C11—H11B	0.9700
N3—C12	1.471 (3)	C12—H12A	0.9700
C1—C6	1.395 (3)	C12—H12B	0.9700

C1—C2	1.410 (3)	C13—H13A	0.9600
C1—C7	1.499 (3)	C13—H13B	0.9600
C2—C3	1.385 (3)	C13—H13C	0.9600
C3—C4	1.383 (3)	O4—H4A	0.846 (10)
C3—H3	0.9300		
C2—O1—C13	118.93 (16)	N3—C8—S1	124.11 (15)
C10—O3—C11	109.65 (16)	N2—C8—S1	121.33 (16)
C7—N1—N2	120.40 (18)	N3—C9—C10	109.42 (18)
C7—N1—H1	119.7 (16)	N3—C9—H9A	109.8
N2—N1—H1	117.6 (16)	C10—C9—H9A	109.8
C8—N2—N1	116.00 (16)	N3—C9—H9B	109.8
C8—N2—H2	116.5 (17)	C10—C9—H9B	109.8
N1—N2—H2	113.1 (16)	H9A—C9—H9B	108.2
C8—N3—C9	125.13 (17)	O3—C10—C9	112.4 (2)
C8—N3—C12	122.18 (17)	O3—C10—H10A	109.1
C9—N3—C12	112.61 (17)	C9—C10—H10A	109.1
C6—C1—C2	117.93 (18)	O3—C10—H10B	109.1
C6—C1—C7	116.15 (18)	C9—C10—H10B	109.1
C2—C1—C7	125.92 (18)	H10A—C10—H10B	107.8
O1—C2—C3	122.46 (18)	O3—C11—C12	111.71 (19)
O1—C2—C1	117.27 (17)	O3—C11—H11A	109.3
C3—C2—C1	120.27 (18)	C12—C11—H11A	109.3
C4—C3—C2	120.26 (19)	O3—C11—H11B	109.3
C4—C3—H3	119.9	C12—C11—H11B	109.3
C2—C3—H3	119.9	H11A—C11—H11B	107.9
C3—C4—C5	120.6 (2)	N3—C12—C11	109.79 (19)
C3—C4—H4	119.7	N3—C12—H12A	109.7
C5—C4—H4	119.7	C11—C12—H12A	109.7
C4—C5—C6	119.14 (19)	N3—C12—H12B	109.7
C4—C5—H5	120.4	C11—C12—H12B	109.7
C6—C5—H5	120.4	H12A—C12—H12B	108.2
C5—C6—C1	121.75 (19)	O1—C13—H13A	109.5
C5—C6—H6	119.1	O1—C13—H13B	109.5
C1—C6—H6	119.1	H13A—C13—H13B	109.5
O2—C7—N1	122.24 (19)	O1—C13—H13C	109.5
O2—C7—C1	120.90 (18)	H13A—C13—H13C	109.5
N1—C7—C1	116.83 (17)	H13B—C13—H13C	109.5
N3—C8—N2	114.55 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.88 (2)	1.91 (2)	2.593 (2)	134 (2)
N1—H1···S1	0.88 (2)	2.44 (2)	2.8714 (18)	110.8 (19)
N2—H2···O4	0.858 (10)	2.071 (11)	2.921 (2)	171 (2)
O4—H4A···O2^{i}	0.846 (10)	1.921 (11)	2.7590 (19)	170 (2)

Symmetry codes: (i) −*x*+3/2, *y*, *z*−1/2.

Fig. 1

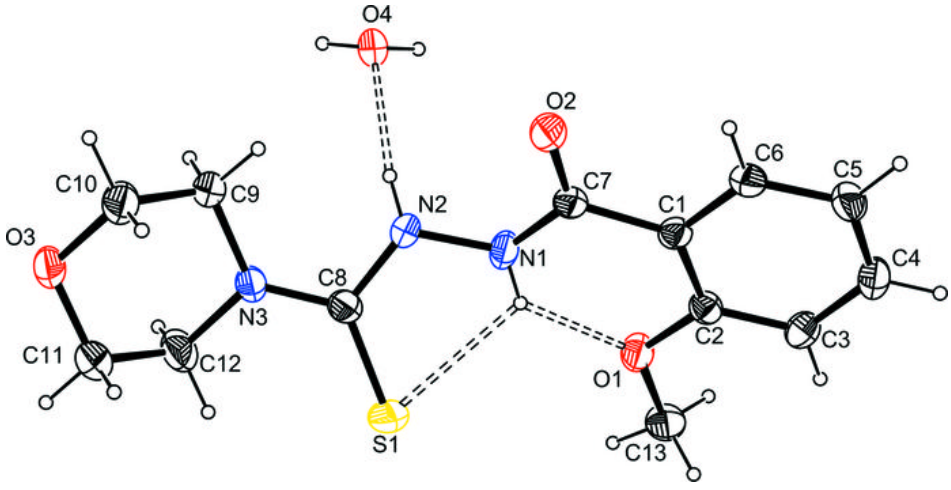


Fig. 2

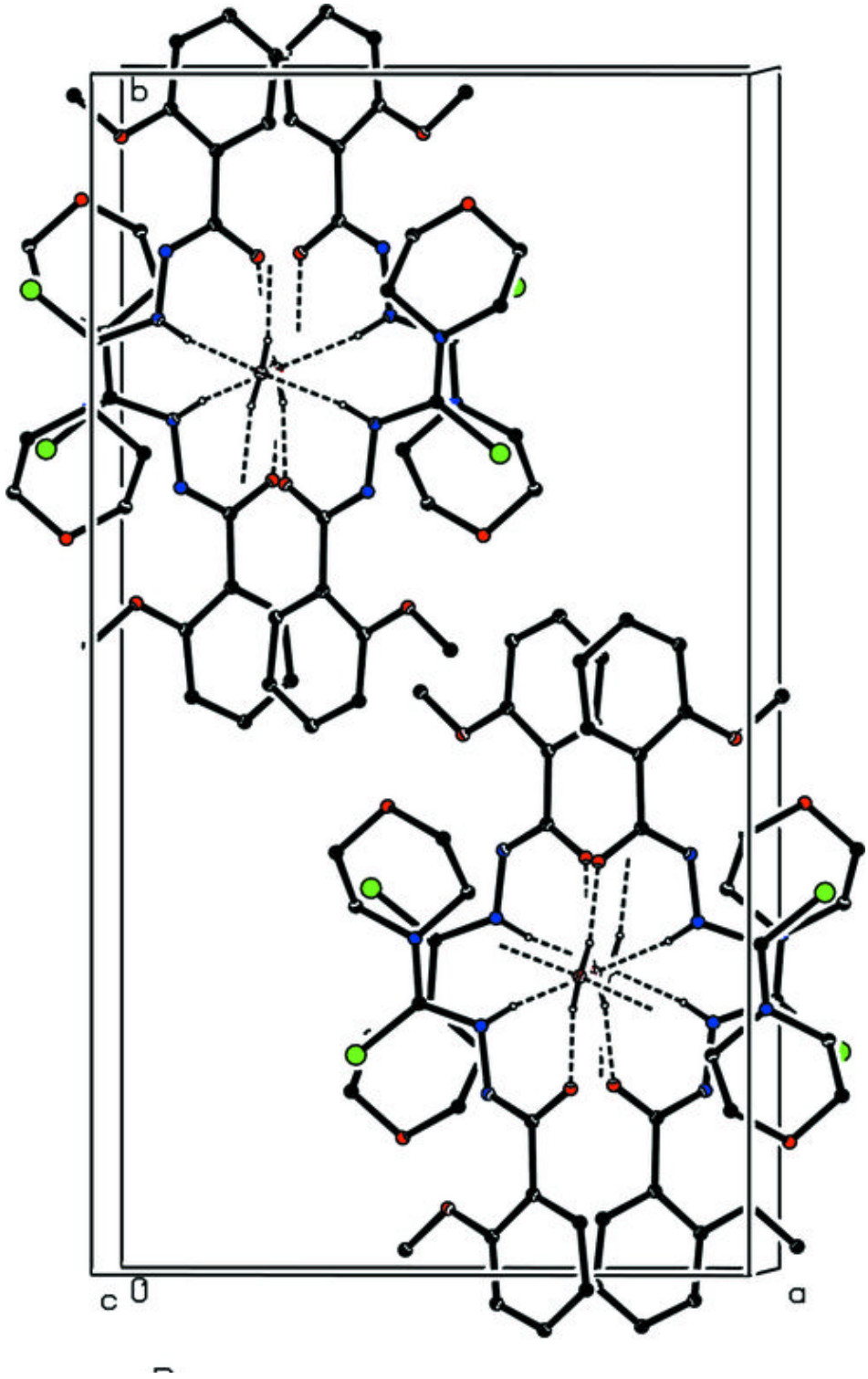
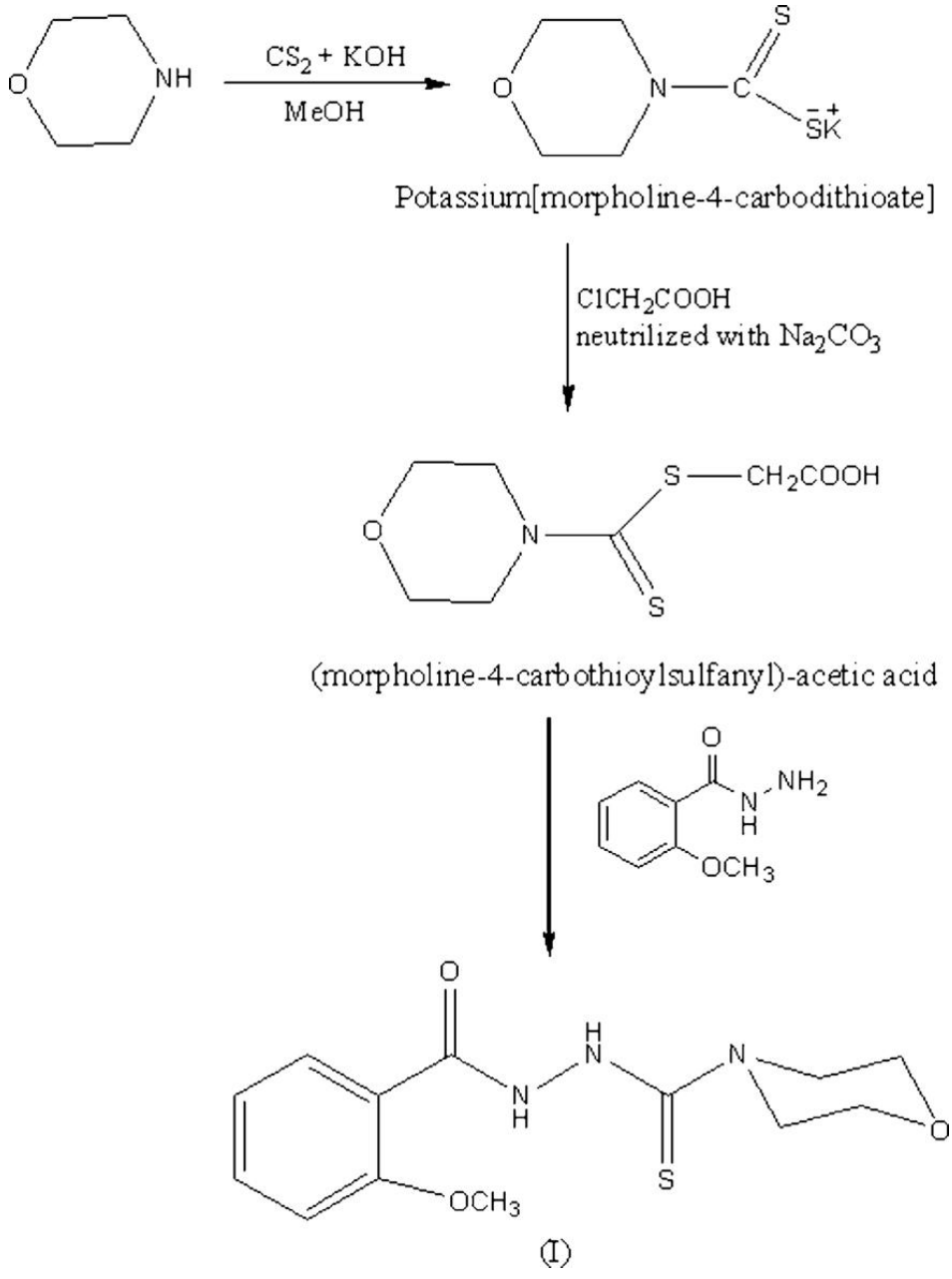


Fig. 3


CS2 + KOH
MeOH
Potassium[morpholine-4-carbodithioate]
ClCH2COOH
neutrilized with Na2CO3
(morpholine-4-carbothioylsulfanyl)-acetic acid
(I)