# Supplementary Material

# Methylamine-induced ring opening of 1,3-dithiolium cations

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## X-Ray structure determinations

Crystallography data are summarized in Table S1. Crystals were mounted in inert oil on glass fibres and transferred to the cold gas stream of an Oxford Diffraction Xcalibur A diffractometer using monochromated Mo *K*⍰ radiation (**2b**), or a Nova E diffractometer using mirror-focused Cu *K*⍰ radiation (**2a**). Absorption corrections were based on multi-scans. Structures were refined anisotropically on $F^2$ using the program SHELXL-97 [G. M. Sheldrick, *Acta Cryst*. 2008, *A***64**, 112-122]. Hydrogen atoms of OH groups were refined freely. The methyl hydrogens at C10 (for **2a**), C10 and C11 (for **2b**) were disordered over a hexagon of half-occupied positions. Other hydrogens were included using a riding model or rigid methyl groups.

**Table S1.** Crystallographic data for dithiocarbamates **2a** and **2b**

| Compound | **2a** | **2b** |
|---|---|---|
| Formula | $C_{11}H_{13}NO_2S_2$ | $C_{12}H_{15}NO_2S_2$ |
| $M_r$ | 255.34 | 269.37 |
| Temperature (K) | 93 | 100 |
| Crystal habit | colourless needle | pale yellow prism |
| Crystal size (mm) | 0.20 × 0.07 × 0.03 | 0.3 × 0.1 × 0.1 |
| Crystal system | monoclinic | monoclinic |
| Space group | $P2_1/c$ | $P2_1/c$ |
| Cell dimensions: | | |
| *a* (Å) | 7.44336(15) | 8.4765(3) |
| *b* (Å) | 13.2684(3) | 13.1378(4) |
| *c* (Å) | 11.9664(3) | 11.3199(4) |
| β (°) | 95.491(2) | 93.543(3) |
| Cell volume (Å$^3$) | 1176.40 | 1258.20 |
| *Z* | 4 | 4 |
| $D_x$ (g cm$^{-3}$) | 1.442 | 1.422 |
| Radiation, wavelength (Å) | Cu *K*α, 1.54184 Å | Mo *K*α, 0.71073 Å |
| μ (mm$^{-1}$) | 4.0 | 0.4 |
| 2θ (max) (°) | 152.3 | 60 |
| Reflections collected | 23802 | 65208 |
| Independent reflections | 2459 | 3659 |
| R(int) | 0.055 | 0.048 |
| Transmissions | 0.625 – 1.000 | 0.965 – 1.000 |
| No. of parameters | 152 | 161 |
| Goodness-of-fit on $F^2$ | 1.06 | 1.06 |
| *wR*2 (all reflections) | 0.072 | 0.073 |
| *R*1 ($F > 4\sigma(F)$) | 0.027 | 0.031 |
| Max. Δρ (e Å$^{-3}$) | 0.25 | 0.43 |