Diastereoselective cyclisation of a dithienylethene switch through single crystal confinement

Kingo Uchida,[a,b] Martin Walko,[b] Jaap J. D. de Jong,[b] Shin-ichiro Sukata,[a] Seiya Kobatake,[c] Auke Meetsma, [b] Jan van Esch, [b] and Ben L. Feringa [b]

[a] *Department of Materials Chemistry, Faculty of Science and Technology, Ryukoku University, CREST-JST, Seta, Otsu, Shiga 520-2194, Japan, Fax: +81-77-543-7483; Tel: +81-77-543-7462; E-mail: uchida@chem.ryukoku.ac.jp*

[b] *Organic and Molecular Inorganic Chemistry, Stratingh Institute, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, Fax: +31-50-363-4296; E-mail: b.l.feringa@rug.nl*

[c] *Department of Applied and Bioapplied Chemistry, Graduate School of Engineering, Osaka City University, Sugimoto3-3-138, Sumiyoshi-ku, Osaka 558-8585, Japan*

Supporting information

X-ray diffraction: Crystal and Molecular Structure.

Suitable colourless block-shaped crystals were obtained by recrystallisation from ethanol. A crystal with the dimensions of 0.49 x 0.21 x 0.18 mm was mounted on top of a glass fibre, and aligned on a *Bruker SMART APEX CCD* diffractometer (Platform with full three-circle goniometer). The diffractometer was equipped with a 4K *CCD* detector set 60.0 mm from the crystal. The crystal was cooled to 170(1) K using the *Bruker KRYOFLEX* low-temperature device. Intensity measurements were performed using graphite monochromated Mo-K$\overline{\alpha}$ radiation from a sealed ceramic diffraction tube (*SIEMENS*). Generator settings were 50 KV/ 40 mA. *SMART* was used for preliminary determination of the unit cell constants and data collection control. The intensities of reflections of a hemisphere were collected by a combination of 3 sets of exposures (frames). Each set had a different ϕ angle for the crystal and each exposure covered a range of 0.3° in ω. A total of 1800 frames were collected with an exposure time of 10.0 seconds per frame. The overall data collection time was 8.0 h. Data integration and global cell refinement was performed with the program *SAINT*. The final unit cell was obtained from the *xyz* centroids of 4487 reflections after integration. Intensity data were corrected for Lorentz and polarization effects, scale variation, for decay and absorption: a multi-scan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular settings (*SADABS*), and reduced to F_o^2. The program suite *SHELXTL* was used for space group determination (*XPREP*).

The unit cell was identified as monoclinic. Reduced cell calculations did not indicate any higher metric lattice symmetry. Space group, $P2_1$, was determined from considerations of the unit cell parameters, statistical analyses of intensity distributions: the *E*-statistics were indicative of a non-centrosymmetric space group. Examination of the final atomic coordinates of the structure did not yield extra crystallographic or metric symmetry elements.

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*. The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined.

Some atoms showed unrealistic displacement parameters when allowed to vary anisotropically, suggesting dynamic disorder (dynamic means that the smeared electron density is due to fluctuations of the atomic positions within each unit cell).

Hydrogen atoms were constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms.

Final refinement on F^2 carried out by full-matrix least-squares techniques converged at $wR(F^2)$ = 0.1700 for 11628 reflections and $R(F)$ = 0.0667 for 8556 reflections with $F_o \geq 4.0\ \sigma(F_o)$ and 819 parameters and 1 restraints. The final difference Fourier map was essentially featureless: no significant peaks (0.90(6) e/Å^3) having chemical meaning above the general background were observed.

The X-ray data allowed determination of the absolute stereochemistry: the absolute structure actually chosen was determined by Flack's **x**-refinement (**x** = 0.07(9)).

The positional and anisotropic displacement parameters for the non-hydrogen atoms and isotropic displacement parameters for hydrogen atoms were refined on F^2 with full-matrix least-squares procedures minimizing the function $Q = \sum_h[w(\,|\,(F_o^2) - k(F_c^2)\,|\,)^2]$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = [\max(F_o^2,0) + 2F_c^2] / 3$, F_0 and F_c are the observed and calculated structure factor amplitudes, respectively; ultimately the suggested *a* (=0.0747) and *b* (= 2.6498) were used in the final refinement.

Crystal data and numerical details on data collection and refinement are given in Table 1. Final fractional atomic coordinates, equivalent displacement parameters and anisotropic displacement parameters for the non-hydrogen atoms are given in Table 2. Molecular geometry data are collected in Table 3. Tables of atom positions, displacement parameters, comprehensive distances and angles and tables of (F_o^2), (F_c^2) and $\sigma(F_o^2)$ are given as supplementary material[*1] for this paper. Neutral atom scattering factors and anomalous dispersion corrections were taken from *International Tables for Crystallography.*

Table 1.

a. Crystal data and details of the structure determination.

Moiety_Formula	$C_{33}H_{28}F_6N_2O_2S_2$
Formula_Weight, g.mol^{-1}	662.72
Crystal system	monoclinic
Space group, no.	$P2_1$, 4
a, Å	12.358(1)
b, Å	14.623(1)
c, Å	19.349(2)
β, deg	106.678(1)
V, Å^3	3349.5(5)
Θ range unit cell: min.-max., deg; reflections	2.60 - 19.91 ; 4487
Formula_*Z*	4
SpaceGroup_*Z*	2
Z' (= Formula_Z / SpaceGroup_*Z)*	2
ρ_{calc}, g.cm^{-3}	1.314
F(000), electrons	1368
μ(Mo K$\bar{\alpha}$), cm^{-1}	2.24
Color, habit	colorless, block
Approx. crystal dimension, mm	0.49 x 0.21 x 0.18

b. Data collection.

Radiation type; λ, Å	Mo K$\bar{\alpha}$, 0.71073
Monochromator	Graphite
Measurement device type	Bruker SMART APEX *CCD* area-detector diffractometer
Detector Area resolution (pixels / mm)	4096 x 4096 / 62 x 62 (binned 512)
Temperature, K	170(1)
Measurement method	φ- and ω-scans
θ range; min. max., deg	2.29, 25.03
Index ranges	h: -14→14; k: -16→17; l: -23→23
Min.- Max. absorption transmission factor	0.9011 – 0.9608
X-ray exposure time, h	8.0
Total data	24172
Unique data	11628
Data with criterion: ($F_o \geq 4.0\ \sigma\ (F_o)$)	8556
R_{int} = $\sum [\lvert F_o^2 - F_o^2 (\text{mean})\rvert] / \sum [F_o^2]$	0.0416
R_{sig} = $\sum \sigma(F_o^2) / \sum [F_o^2]$	0.0747

c. Refinement.

Number of reflections	11628
Number of refined parameters	819
Number of restraints	1
Final agreement factors:	
$wR(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$	0.1700
Weighting scheme: *a, b*	0.0747, 2.6498
$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$	
And $P = [\max(F_o^2,0) + 2F_c^2] / 3$	
$R(F) = \sum (\|\|F_o\| - \|F_c\|\|) / \sum \|F_o\|$	0.0667
For $F_o > 4.0\ \sigma\ (F_o)$	
Absolute-Structure parameter Flack's **x**	0.07(9)
GooF = S = $[\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$	1.035
n = number of reflections	
p = number of parameters refined	
Residual electron density in final	
Difference Fourier map, e/Å^3	-0.66, 0.90(6)
Max. (shift/σ) final cycle	<0.001
Average (shift/σ) final cycle	0.000

Table 2. Final fractional atomic coordinates and equivalent isotropic displacement parameters with s.u.'s in parentheses.
Atoms of the Asymmetric Unit.

Non-Hydrogen parameters

Residue: 1.

Atom	*x*	*y*	*z*	U_{eq} (Å^2)*
S11	0.13694(14)	0.35621(12)	0.16329(8)	0.0631(5)
S12	0.30679(13)	0.31045(10)	-0.08046(8)	0.0522(4)
F11	0.1244(5)	0.6910(3)	0.0801(3)	0.110(2)
F12	0.2944(5)	0.6848(3)	0.14565(19)	0.110(2)
F13	0.3707(4)	0.7397(3)	0.0463(2)	0.1009(19)
F14	0.2033(5)	0.7893(3)	0.00003(19)	0.0980(19)
F15	0.3355(6)	0.6509(3)	-0.0694(3)	0.126(3)
F16	0.1555(5)	0.6609(3)	-0.0921(2)	0.128(2)
O11	0.2465(3)	0.3215(3)	0.31771(19)	0.0473(12)
O12	0.2125(3)	0.2653(2)	-0.23269(19)	0.0428(12)
N11	0.3697(3)	0.4390(3)	0.3398(2)	0.0405(12)
N12	0.0881(3)	0.3816(3)	-0.2643(2)	0.0322(12)
C11	0.6205(5)	0.4208(4)	0.4221(3)	0.052(2)
C12	0.7261(6)	0.3827(6)	0.4401(3)	0.071(3)
C13	0.7437(7)	0.2990(6)	0.4711(3)	0.076(3)
C14	0.6551(8)	0.2525(5)	0.4846(3)	0.077(3)
C15	0.5482(6)	0.2899(4)	0.4653(3)	0.063(2)
C16	0.5291(5)	0.3761(4)	0.4345(3)	0.0407(16)
C17	0.4143(5)	0.4204(4)	0.4170(3)	0.0460(19)
C18	0.4151(5)	0.5082(4)	0.4587(3)	0.060(2)
C19	0.2880(4)	0.3884(3)	0.2959(3)	0.0352(17)
C110	0.2473(4)	0.4172(3)	0.2202(3)	0.0382(17)
C111	0.2754(4)	0.4894(3)	0.1852(3)	0.0392(17)
C112	0.2121(4)	0.4938(4)	0.1110(3)	0.0450(17)
C113	0.1335(5)	0.4264(5)	0.0918(3)	0.060(2)
C114	0.0477(6)	0.4097(6)	0.0203(4)	0.083(3)
C115	-0.0746(5)	0.2312(4)	-0.2964(4)	0.060(2)
C116	-0.1256(5)	0.1462(5)	-0.3024(4)	0.070(3)

C117	-0.1148(6)	0.0859(5)	-0.3522(5)	0.076(3)
C118	-0.0568(6)	0.1086(4)	-0.3999(4)	0.069(3)
C119	-0.0055(5)	0.1941(4)	-0.3946(3)	0.053(2)
C120	-0.0133(4)	0.2548(4)	-0.3422(3)	0.0389(17)
C121	0.0470(4)	0.3473(3)	-0.3396(3)	0.0363(17)
C122	-0.0285(5)	0.4200(4)	-0.3854(3)	0.054(2)
C123	0.1716(4)	0.3372(3)	-0.2186(3)	0.0325(17)
C124	0.2159(4)	0.3768(3)	-0.1454(3)	0.0353(17)
C125	0.1978(4)	0.4592(3)	-0.1186(3)	0.0362(17)
C126	0.2569(4)	0.4691(3)	-0.0445(3)	0.0401(17)
C127	0.3204(5)	0.3933(3)	-0.0159(3)	0.0466(17)
C128	0.3955(6)	0.3763(5)	0.0595(3)	0.077(3)
C129	0.2316(5)	0.5644(4)	0.0614(3)	0.0438(17)
C130	0.2294(6)	0.6638(4)	0.0799(3)	0.061(2)
C131	0.2637(7)	0.7143(4)	0.0205(3)	0.060(2)
C132	0.2515(7)	0.6444(4)	-0.0388(3)	0.067(2)
C133	0.2474(4)	0.5535(3)	-0.0040(3)	0.0415(17)

Residue: 2.

S21	0.42192(11)	0.75395(11)	0.33439(8)	0.0498(5)
S22	0.11756(11)	0.99896(9)	0.17473(7)	0.0398(4)
F21	0.7062(5)	0.9844(3)	0.2781(7)	0.236(6)
F22	0.6809(4)	1.0372(4)	0.3700(4)	0.156(3)
F23	0.6664(4)	1.1362(5)	0.2136(3)	0.146(3)
F24	0.6895(4)	1.1856(3)	0.3146(3)	0.125(2)
F25	0.4811(4)	1.2137(3)	0.2935(3)	0.119(2)
F26	0.4697(4)	1.1883(3)	0.1814(3)	0.1112(19)
O21	0.4980(3)	0.5805(3)	0.2865(3)	0.0657(14)
O22	-0.0403(3)	1.0739(2)	0.25468(18)	0.0388(11)
N21	0.6223(4)	0.6390(3)	0.2303(3)	0.0604(19)
N22	0.0654(3)	1.1977(3)	0.2998(2)	0.0343(12)
C21	0.6069(9)	0.5741(7)	0.0668(7)	0.121(5)
C22	0.6522(19)	0.5890(7)	0.0053(5)	0.193(10)
C23	0.781(3)	0.5953(11)	0.029(2)	0.32(3)
C24	0.848(4)	0.587(3)	0.071(3)	0.39(3)
C25	0.8055(9)	0.5713(7)	0.1354(8)	0.129(6)

C26	0.6900(8)	0.5654(5)	0.1357(5)	0.085(4)
C27	0.6566(6)	0.5487(5)	0.2053(5)	0.087(3)
C28	0.7607(10)	0.5239(8)	0.2724(6)	0.151(6)
C29	0.5461(4)	0.6470(4)	0.2669(3)	0.0469(19)
C210	0.5159(4)	0.7421(4)	0.2849(3)	0.0405(16)
C211	0.5493(4)	0.8247(3)	0.2661(3)	0.0374(17)
C212	0.4959(4)	0.8993(3)	0.2909(3)	0.0368(17)
C213	0.4255(4)	0.8722(4)	0.3299(3)	0.0397(17)
C214	0.3560(5)	0.9288(5)	0.3658(3)	0.0540(19)
C215	0.1550(5)	1.1906(5)	0.4555(3)	0.056(2)
C216	0.2402(6)	1.2142(6)	0.5191(3)	0.074(3)
C217	0.2458(6)	1.3030(6)	0.5438(3)	0.069(3)
C218	0.1731(5)	1.3674(5)	0.5076(3)	0.061(2)
C219	0.0903(5)	1.3446(4)	0.4447(3)	0.0457(17)
C220	0.0813(4)	1.2562(4)	0.4180(3)	0.0379(17)
C221	-0.0018(4)	1.2300(3)	0.3455(3)	0.0366(17)
C222	-0.0817(4)	1.3054(4)	0.3078(3)	0.0519(19)
C223	0.0465(4)	1.1199(3)	0.2618(2)	0.0317(16)
C224	0.1407(4)	1.0887(3)	0.2357(2)	0.0314(16)
C225	0.2515(4)	1.1120(3)	0.2571(3)	0.0340(17)
C226	0.3205(4)	1.0567(3)	0.2274(2)	0.0329(16)
C227	0.2583(4)	0.9925(3)	0.1804(3)	0.0373(16)
C228	0.2992(5)	0.9216(4)	0.1367(3)	0.0510(19)
C229	0.5184(4)	0.9967(4)	0.2765(3)	0.0381(17)
C230	0.6353(5)	1.0316(4)	0.2941(5)	0.067(3)
C231	0.6278(5)	1.1294(4)	0.2692(3)	0.0478(19)
C232	0.5018(5)	1.1506(4)	0.2472(4)	0.054(2)
C233	0.4426(4)	1.0620(3)	0.2489(3)	0.0346(17)

Hydrogen parameters:

Residue: 1.

H11	0.60963(-)	0.47973(-)	0.40051(-)	0.06194(-)
H12	0.78708(-)	0.41499(-)	0.43077(-)	0.08545(-)
H13	0.81694(-)	0.27247(-)	0.48359(-)	0.09088(-)
H14	0.66767(-)	0.19428(-)	0.50731(-)	0.09164(-)
H15	0.48704(-)	0.25619(-)	0.47324(-)	0.07551(-)
H17	0.36174(-)	0.37665(-)	0.43066(-)	0.05514(-)
H18	0.46671(-)	0.55212(-)	0.44661(-)	0.09057(-)
H18'	0.44042(-)	0.49519(-)	0.51058(-)	0.09057(-)
H18"	0.33873(-)	0.53395(-)	0.44598(-)	0.09057(-)
H111	0.33176(-)	0.53271(-)	0.20769(-)	0.04716(-)
H114	0.03738(-)	0.46576(-)	-0.00869(-)	0.12421(-)
H114'	-0.02439(-)	0.39203(-)	0.02802(-)	0.12421(-)
H114"	0.07423(-)	0.36055(-)	-0.00522(-)	0.12421(-)
H115	-0.08223(-)	0.27301(-)	-0.26053(-)	0.07201(-)
H116	-0.16897(-)	0.13033(-)	-0.27077(-)	0.08364(-)
H117	-0.14773(-)	0.02689(-)	-0.35418(-)	0.09063(-)
H118	-0.05143(-)	0.06668(-)	-0.43624(-)	0.08251(-)
H119	0.03531(-)	0.21047(-)	-0.42753(-)	0.06319(-)
H121	0.11375(-)	0.33820(-)	-0.35824(-)	0.04346(-)
H122	-0.09338(-)	0.43107(-)	-0.36698(-)	0.08150(-)
H122'	-0.05514(-)	0.39891(-)	-0.43549(-)	0.08150(-)
H122"	0.01449(-)	0.47675(-)	-0.38316(-)	0.08150(-)
H125	0.15073(-)	0.50519(-)	-0.14650(-)	0.04387(-)
H128	0.42687(-)	0.43450(-)	0.08139(-)	0.11520(-)
H128'	0.45718(-)	0.33523(-)	0.05748(-)	0.11520(-)
H128"	0.35121(-)	0.34815(-)	0.08847(-)	0.11520(-)
H161	0.39753(-)	0.48531(-)	0.32142(-)	0.04881(-)
H162	0.05774(-)	0.43024(-)	-0.25061(-)	0.03854(-)

Residue: 2.

H21	0.52810(-)	0.57054(-)	0.06133(-)	0.14528(-)
H22	0.60694(-)	0.59411(-)	-0.04340(-)	0.23249(-)
H23	0.80570(-)	0.61383(-)	-0.01096(-)	0.38406(-)
H24	0.92513(-)	0.58879(-)	0.07080(-)	0.45726(-)
H25	0.86097(-)	0.56454(-)	0.18064(-)	0.15521(-)
H27	0.59491(-)	0.50225(-)	0.19793(-)	0.10429(-)
H28	0.82509(-)	0.56287(-)	0.27225(-)	0.22661(-)
H28'	0.78116(-)	0.45960(-)	0.26939(-)	0.22661(-)
H28"	0.74005(-)	0.53392(-)	0.31711(-)	0.22661(-)
H211	0.60232(-)	0.83195(-)	0.23935(-)	0.04483(-)
H214	0.39382(-)	0.98737(-)	0.38096(-)	0.08100(-)
H214'	0.34730(-)	0.89615(-)	0.40818(-)	0.08100(-)
H214"	0.28136(-)	0.93977(-)	0.33186(-)	0.08100(-)
H215	0.14871(-)	1.12929(-)	0.43846(-)	0.06743(-)
H216	0.29256(-)	1.16962(-)	0.54447(-)	0.08879(-)
H217	0.30175(-)	1.31912(-)	0.58707(-)	0.08253(-)
H218	0.17877(-)	1.42835(-)	0.52514(-)	0.07347(-)
H219	0.03908(-)	1.39016(-)	0.41969(-)	0.05463(-)
H221	-0.04846(-)	1.17761(-)	0.35401(-)	0.04389(-)
H222	-0.03785(-)	1.35852(-)	0.30067(-)	0.07732(-)
H222'	-0.13049(-)	1.32300(-)	0.33761(-)	0.07732(-)
H222"	-0.12841(-)	1.28325(-)	0.26094(-)	0.07732(-)
H225	0.28017(-)	1.16118(-)	0.28921(-)	0.04058(-)
H228	0.37574(-)	0.93709(-)	0.13547(-)	0.07646(-)
H228'	0.24842(-)	0.92040(-)	0.08735(-)	0.07646(-)
H228"	0.29973(-)	0.86124(-)	0.15885(-)	0.07646(-)
H261	0.65415(-)	0.68905(-)	0.22015(-)	0.07243(-)
H262	0.12262(-)	1.23173(-)	0.29693(-)	0.04123(-)

*) $U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a_i}.\mathbf{a_j}$

Anisotropic (displacement) parameters (Å^2)

Residue: 1.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S11	0.0627(10)	0.0661(10)	0.0491(8)	0.0003(8)	-0.0023(7)	-0.0361(8)
S12	0.0569(8)	0.0307(7)	0.0549(8)	-0.0039(7)	-0.0064(7)	0.0161(7)
F11	0.153(5)	0.067(3)	0.131(4)	0.000(3)	0.075(4)	0.037(3)
F12	0.219(6)	0.040(2)	0.048(2)	-0.0066(18)	0.002(3)	-0.024(3)
F13	0.132(4)	0.097(3)	0.074(3)	-0.033(3)	0.030(3)	-0.039(3)
F14	0.189(5)	0.047(2)	0.049(2)	0.0042(18)	0.020(2)	0.039(3)
F15	0.272(7)	0.046(3)	0.109(4)	-0.001(2)	0.131(5)	-0.011(3)
F16	0.223(6)	0.039(2)	0.060(2)	-0.0013(19)	-0.056(3)	0.034(3)
O11	0.061(2)	0.039(2)	0.046(2)	-0.0036(17)	0.0217(18)	-0.0195(19)
O12	0.042(2)	0.033(2)	0.053(2)	-0.0086(17)	0.0130(16)	0.0065(17)
N11	0.041(2)	0.037(2)	0.039(2)	0.0067(19)	0.0041(19)	-0.016(2)
N12	0.034(2)	0.031(2)	0.033(2)	-0.0053(18)	0.0119(17)	0.0044(18)
C11	0.053(4)	0.052(4)	0.051(3)	0.011(3)	0.015(3)	0.004(3)
C12	0.058(4)	0.096(6)	0.055(4)	0.006(4)	0.008(3)	0.020(4)
C13	0.089(5)	0.079(6)	0.048(4)	-0.007(4)	0.003(4)	0.036(5)
C14	0.117(6)	0.042(4)	0.054(4)	0.003(3)	-0.002(4)	0.031(4)
C15	0.104(5)	0.043(4)	0.038(3)	-0.004(3)	0.014(3)	-0.008(4)
C16	0.059(3)	0.033(3)	0.028(2)	0.000(2)	0.009(2)	-0.008(3)
C17	0.048(3)	0.051(4)	0.034(3)	0.003(2)	0.004(2)	-0.016(3)
C18	0.062(4)	0.067(4)	0.043(3)	-0.014(3)	0.001(3)	0.018(3)
C19	0.036(3)	0.025(3)	0.043(3)	-0.005(2)	0.009(2)	-0.010(2)
C110	0.040(3)	0.035(3)	0.037(3)	-0.006(2)	0.007(2)	-0.007(2)
C111	0.048(3)	0.024(3)	0.042(3)	-0.005(2)	0.007(2)	-0.007(2)
C112	0.050(3)	0.043(3)	0.035(3)	0.000(3)	0.001(2)	0.000(3)
C113	0.059(4)	0.064(4)	0.045(3)	0.001(3)	-0.005(3)	-0.021(3)
C114	0.066(4)	0.112(7)	0.054(4)	0.001(4)	-0.008(3)	-0.037(4)
C115	0.054(4)	0.052(4)	0.079(4)	-0.001(3)	0.027(3)	-0.006(3)
C116	0.055(4)	0.063(5)	0.093(5)	0.003(4)	0.025(4)	-0.012(3)
C117	0.051(4)	0.047(4)	0.110(6)	-0.005(4)	-0.008(4)	-0.014(3)
C118	0.070(4)	0.040(4)	0.083(5)	-0.018(3)	0.000(4)	-0.012(3)
C119	0.055(4)	0.045(4)	0.054(3)	-0.009(3)	0.009(3)	-0.003(3)
C120	0.035(3)	0.031(3)	0.043(3)	0.004(2)	-0.001(2)	0.001(2)

C121	0.040(3)	0.034(3)	0.035(3)	-0.008(2)	0.011(2)	-0.002(2)
C122	0.070(4)	0.046(4)	0.041(3)	0.005(3)	0.006(3)	0.001(3)
C123	0.037(3)	0.018(3)	0.045(3)	-0.001(2)	0.016(2)	0.000(2)
C124	0.041(3)	0.026(3)	0.037(3)	-0.003(2)	0.008(2)	0.006(2)
C125	0.037(3)	0.032(3)	0.038(3)	0.002(2)	0.008(2)	0.004(2)
C126	0.048(3)	0.024(3)	0.042(3)	-0.005(2)	0.003(2)	0.004(2)
C127	0.052(3)	0.030(3)	0.047(3)	-0.006(2)	-0.003(3)	0.009(2)
C128	0.084(5)	0.057(4)	0.060(4)	-0.009(3)	-0.026(3)	0.020(4)
C129	0.055(3)	0.029(3)	0.040(3)	0.001(2)	0.002(2)	-0.003(2)
C130	0.092(5)	0.036(3)	0.041(3)	-0.007(3)	-0.001(3)	0.007(3)
C131	0.100(5)	0.029(3)	0.043(3)	0.000(3)	0.008(3)	0.005(3)
C132	0.124(6)	0.028(3)	0.039(3)	-0.001(3)	0.008(4)	0.014(4)
C133	0.052(3)	0.029(3)	0.034(3)	-0.001(2)	-0.003(2)	0.005(2)

Residue: 2.

S21	0.0404(7)	0.0555(9)	0.0510(8)	0.0193(7)	0.0090(6)	-0.0089(7)
S22	0.0422(7)	0.0321(7)	0.0385(7)	-0.0119(6)	0.0009(5)	-0.0017(6)
F21	0.100(4)	0.047(3)	0.634(18)	-0.069(6)	0.220(8)	-0.028(3)
F22	0.077(3)	0.137(5)	0.193(6)	0.096(5)	-0.057(4)	-0.048(3)
F23	0.109(4)	0.235(7)	0.130(4)	0.102(5)	0.094(4)	0.078(4)
F24	0.116(4)	0.068(3)	0.145(4)	-0.037(3)	-0.034(3)	0.015(3)
F25	0.084(3)	0.058(3)	0.248(6)	-0.077(3)	0.099(4)	-0.025(2)
F26	0.078(3)	0.094(3)	0.140(4)	0.076(3)	-0.003(3)	-0.021(3)
O21	0.048(2)	0.038(2)	0.099(3)	0.023(2)	0.002(2)	-0.0204(19)
O22	0.0333(18)	0.0297(19)	0.049(2)	-0.0032(16)	0.0046(15)	-0.0073(16)
N21	0.034(3)	0.028(3)	0.114(4)	-0.001(3)	0.013(3)	-0.001(2)
N22	0.033(2)	0.027(2)	0.045(2)	-0.0031(19)	0.0148(18)	-0.0040(17)
C21	0.116(8)	0.077(7)	0.143(10)	-0.008(6)	-0.006(7)	-0.020(6)
C22	0.43(3)	0.072(7)	0.062(6)	-0.033(5)	0.045(11)	-0.050(12)
C23	0.39(4)	0.087(10)	0.70(7)	-0.10(2)	0.49(5)	-0.061(17)
C24	0.46(7)	0.31(4)	0.47(5)	0.13(4)	0.27(5)	0.15(4)
C25	0.110(8)	0.099(8)	0.205(13)	0.013(8)	0.087(8)	0.030(6)
C26	0.114(7)	0.035(4)	0.126(7)	0.000(4)	0.065(6)	0.004(4)
C27	0.051(4)	0.051(4)	0.167(8)	0.033(5)	0.045(5)	0.017(3)
C28	0.171(10)	0.144(10)	0.168(10)	0.094(8)	0.096(9)	0.113(9)
C29	0.031(3)	0.032(3)	0.067(4)	0.005(3)	-0.003(3)	-0.007(2)

C210	0.025(2)	0.038(3)	0.051(3)	0.008(3)	-0.001(2)	-0.007(2)
C211	0.035(3)	0.034(3)	0.039(3)	0.009(2)	0.004(2)	0.000(2)
C212	0.037(3)	0.036(3)	0.037(3)	0.000(2)	0.010(2)	-0.004(2)
C213	0.033(3)	0.048(3)	0.035(3)	0.003(2)	0.005(2)	0.001(2)
C214	0.047(3)	0.078(4)	0.041(3)	0.016(3)	0.019(3)	0.006(3)
C215	0.063(4)	0.054(4)	0.052(3)	0.010(3)	0.017(3)	0.022(3)
C216	0.061(4)	0.106(7)	0.049(4)	0.011(4)	0.007(3)	0.020(4)
C217	0.065(4)	0.096(6)	0.040(3)	-0.009(4)	0.007(3)	-0.003(4)
C218	0.067(4)	0.068(4)	0.054(4)	-0.015(3)	0.025(3)	-0.020(4)
C219	0.055(3)	0.043(3)	0.041(3)	-0.005(2)	0.017(3)	-0.004(3)
C220	0.037(3)	0.038(3)	0.044(3)	0.000(2)	0.020(2)	-0.003(2)
C221	0.037(3)	0.033(3)	0.042(3)	-0.005(2)	0.015(2)	-0.006(2)
C222	0.044(3)	0.045(3)	0.064(4)	-0.011(3)	0.011(3)	0.009(3)
C223	0.035(3)	0.022(3)	0.031(2)	0.002(2)	-0.002(2)	-0.005(2)
C224	0.037(3)	0.023(3)	0.033(2)	-0.0041(19)	0.008(2)	0.003(2)
C225	0.042(3)	0.026(3)	0.033(3)	-0.004(2)	0.009(2)	-0.002(2)
C226	0.042(3)	0.025(3)	0.029(2)	0.001(2)	0.006(2)	0.001(2)
C227	0.050(3)	0.030(3)	0.031(2)	-0.001(2)	0.010(2)	0.002(2)
C228	0.067(4)	0.036(3)	0.045(3)	-0.015(2)	0.008(3)	0.001(3)
C229	0.035(3)	0.035(3)	0.048(3)	-0.003(3)	0.018(2)	0.001(2)
C230	0.040(3)	0.048(4)	0.119(6)	-0.001(4)	0.031(4)	-0.002(3)
C231	0.051(3)	0.040(3)	0.056(4)	-0.010(3)	0.021(3)	-0.009(3)
C232	0.059(4)	0.031(3)	0.078(4)	-0.009(3)	0.030(3)	-0.001(3)
C233	0.039(3)	0.034(3)	0.036(3)	-0.011(2)	0.019(2)	-0.002(2)

Thermal vibration amplitudes (Å^2)

$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-2\pi^2 \sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j a_i^* a_j^* U_{ij}\right)$

or

$F(\mathbf{h}) = F_o(\mathbf{h}) \exp\left(-8\pi^2 U_{iso} (\sin(\theta)/\lambda)^2\right)$

Table 3. Selected data on the geometry.
Standard deviations in the last decimal place are given in parentheses.

Residue: 1.

Interatomic Distances (Å)

S11	-C110	1.734(5)	C110	-C111	1.352(7)
S11	-C113	1.713(6)	C111	-C112	1.426(8)
S12	-C124	1.724(5)	C112	-C113	1.359(9)
S12	-C127	1.713(5)	C112	-C129	1.476(8)
F11	-C130	1.358(10)	C113	-C114	1.502(9)
F12	-C130	1.331(7)	C115	-C116	1.383(9)
F13	-C131	1.325(10)	C115	-C120	1.365(9)
F14	-C131	1.322(8)	C116	-C117	1.341(11)
F15	-C132	1.338(11)	C117	-C118	1.362(11)
F16	-C132	1.352(9)	C118	-C119	1.392(9)
O11	-C19	1.234(6)	C119	-C120	1.372(8)
O12	-C123	1.231(6)	C120	-C121	1.538(7)
N11	-C17	1.462(7)	C121	-C122	1.520(8)
N11	-C19	1.340(6)	C123	-C124	1.482(8)
N12	-C121	1.486(7)	C124	-C125	1.356(7)
N12	-C123	1.321(7)	C125	-C126	1.417(8)
C11	-C12	1.369(10)	C126	-C127	1.379(7)
C11	-C16	1.384(9)	C126	-C133	1.485(7)
C12	-C13	1.353(12)	C127	-C128	1.508(8)
C13	-C14	1.376(13)	C129	-C130	1.499(8)
C14	-C15	1.379(12)	C129	-C133	1.344(8)
C15	-C16	1.385(8)	C130	-C131	1.525(9)
C16	-C17	1.507(9)	C131	-C132	1.512(8)
C17	-C18	1.515(8)	C132	-C133	1.498(8)
C110	-C19	1.467(8)			

Bond Angles (deg.)

C110	-S11	-C113	92.1(3)	C120	-C121	-C122	112.7(5)
C124	-S12	-C127	92.3(3)	O12	-C123	-N12	124.3(5)
C17	-N11	-C19	122.7(4)	O12	-C123	-C124	118.9(5)
C121	-N12	-C123	118.2(4)	N12	-C123	-C124	116.8(4)
C12	-C11	-C16	122.0(6)	S12	-C124	-C123	117.5(3)
C11	-C12	-C13	120.1(7)	S12	-C124	-C125	111.5(4)
C12	-C13	-C14	119.7(8)	C123	-C124	-C125	131.1(5)
C13	-C14	-C15	120.4(7)	C124	-C125	-C126	112.6(4)
C14	-C15	-C16	120.6(7)	C125	-C126	-C127	113.1(4)
C11	-C16	-C15	117.2(6)	C125	-C126	-C133	121.5(4)
C11	-C16	-C17	121.4(5)	C127	-C126	-C133	125.4(5)
C15	-C16	-C17	121.4(6)	S12	-C127	-C126	110.5(4)
N11	-C17	-C16	111.4(5)	S12	-C127	-C128	119.5(4)
N11	-C17	-C18	109.2(5)	C126	-C127	-C128	130.0(5)
C16	-C17	-C18	112.5(5)	C112	-C129	-C130	120.4(5)
O11	-C19	-N11	122.2(5)	C112	-C129	-C133	128.6(5)
O11	-C19	-C110	120.8(5)	C130	-C129	-C133	110.9(5)
N11	-C19	-C110	117.0(4)	F11	-C130	-F12	104.2(5)
S11	-C110	-C19	117.9(4)	F11	-C130	-C129	111.6(6)
S11	-C110	-C111	110.6(4)	F11	-C130	-C131	109.4(5)
C19	-C110	-C111	131.3(5)	F12	-C130	-C129	113.9(5)
C110	-C111	-C112	113.2(5)	F12	-C130	-C131	112.7(6)
C111	-C112	-C113	112.7(5)	C129	-C130	-C131	105.2(5)
C111	-C112	-C129	122.8(5)	F13	-C131	-F14	107.3(5)
C113	-C112	-C129	124.6(5)	F13	-C131	-C130	108.4(5)
S11	-C113	-C112	111.3(4)	F13	-C131	-C132	110.3(7)
S11	-C113	-C114	119.6(5)	F14	-C131	-C130	111.9(6)
C112	-C113	-C114	129.1(6)	F14	-C131	-C132	114.1(5)
C116	-C115	-C120	119.8(6)	C130	-C131	-C132	104.8(5)
C115	-C116	-C117	121.0(7)	F15	-C132	-F16	105.8(5)
C116	-C117	-C118	120.5(7)	F15	-C132	-C131	111.5(6)
C117	-C118	-C119	119.1(6)	F15	-C132	-C133	113.1(6)
C118	-C119	-C120	120.6(6)	F16	-C132	-C131	109.5(6)
C115	-C120	-C119	119.1(6)	F16	-C132	-C133	111.5(6)
C115	-C120	-C121	123.7(5)	C131	-C132	-C133	105.5(5)

C119	-C120	-C121	117.2(5)	C126	-C133	-C129	130.6(5)
N12	-C121	-C120	110.8(4)	C126	-C133	-C132	118.9(5)
N12	-C121	-C122	108.4(4)	C129	-C133	-C132	110.5(5)

Torsion Angles (deg.)

C113	-S11	-C110	-C19	178.0(4)
C113	-S11	-C110	-C111	2.2(4)
C110	-S11	-C113	-C112	-0.8(5)
C110	-S11	-C113	-C114	-179.0(6)
C127	-S12	-C124	-C123	-179.6(4)
C127	-S12	-C124	-C125	0.5(4)
C124	-S12	-C127	-C126	-0.3(5)
C124	-S12	-C127	-C128	-179.7(5)
C19	-N11	-C17	-C16	104.6(6)
C19	-N11	-C17	-C18	-130.5(5)
C17	-N11	-C19	-O11	-1.4(8)
C17	-N11	-C19	-C110	177.2(5)
C123	-N12	-C121	-C120	68.7(6)
C123	-N12	-C121	-C122	-167.2(5)
C121	-N12	-C123	-O12	-5.5(7)
C121	-N12	-C123	-C124	175.9(4)
C16	-C11	-C12	-C13	-0.1(9)
C12	-C11	-C16	-C15	-0.8(9)
C12	-C11	-C16	-C17	177.6(5)
C11	-C12	-C13	-C14	-0.2(9)
C12	-C13	-C14	-C15	1.4(9)
C13	-C14	-C15	-C16	-2.4(9)
C14	-C15	-C16	-C11	2.0(8)
C14	-C15	-C16	-C17	-176.4(5)
C11	-C16	-C17	-N11	62.5(7)
C11	-C16	-C17	-C18	-60.5(7)
C15	-C16	-C17	-N11	-119.1(6)
C15	-C16	-C17	-C18	117.9(6)
S11	-C110	-C19	-O11	1.7(7)
S11	-C110	-C19	-N11	-176.9(4)

C111	-C110	-C19	-O11	176.5(5)
C111	-C110	-C19	-N11	-2.2(8)
S11	-C110	-C111	-C112	-3.0(6)
C19	-C110	-C111	-C112	-178.1(5)
C110	-C111	-C112	-C113	2.5(7)
C110	-C111	-C112	-C129	-177.3(5)
C111	-C112	-C113	-S11	-0.8(7)
C111	-C112	-C113	-C114	177.3(6)
C129	-C112	-C113	-S11	179.0(5)
C129	-C112	-C113	-C114	-2.9(11)
C111	-C112	-C129	-C130	-53.8(8)
C111	-C112	-C129	-C133	129.6(7)
C113	-C112	-C129	-C130	126.4(7)
C113	-C112	-C129	-C133	-50.2(10)
C120	-C115	-C116	-C117	0.7(11)
C116	-C115	-C120	-C119	1.4(9)
C116	-C115	-C120	-C121	-179.7(6)
C115	-C116	-C117	-C118	-2.6(12)
C116	-C117	-C118	-C119	2.3(12)
C117	-C118	-C119	-C120	-0.1(10)
C118	-C119	-C120	-C115	-1.7(9)
C118	-C119	-C120	-C121	179.3(6)
C115	-C120	-C121	-N12	33.2(7)
C115	-C120	-C121	-C122	-88.5(7)
C119	-C120	-C121	-N12	-147.9(5)
C119	-C120	-C121	-C122	90.5(6)
O12	-C123	-C124	-S12	-9.8(7)
O12	-C123	-C124	-C125	170.1(5)
N12	-C123	-C124	-S12	168.9(4)
N12	-C123	-C124	-C125	-11.2(8)
S12	-C124	-C125	-C126	-0.6(6)
C123	-C124	-C125	-C126	179.5(5)
C124	-C125	-C126	-C127	0.4(7)
C124	-C125	-C126	-C133	-178.9(5)
C125	-C126	-C127	-S12	0.0(6)
C125	-C126	-C127	-C128	179.4(6)

C133	-C126	-C127	-S12	179.2(4)
C133	-C126	-C127	-C128	-1.4(10)
C125	-C126	-C133	-C129	134.3(6)
C125	-C126	-C133	-C132	-43.4(8)
C127	-C126	-C133	-C129	-44.9(9)
C127	-C126	-C133	-C132	137.4(6)
C112	-C129	-C130	-F11	-66.7(7)
C112	-C129	-C130	-F12	50.8(9)
C112	-C129	-C130	-C131	174.7(6)
C133	-C129	-C130	-F11	110.4(6)
C133	-C129	-C130	-F12	-132.0(6)
C133	-C129	-C130	-C131	-8.1(7)
C112	-C129	-C133	-C126	-4.0(11)
C112	-C129	-C133	-C132	173.8(6)
C130	-C129	-C133	-C126	179.1(6)
C130	-C129	-C133	-C132	-3.0(8)
F11	-C130	-C131	-F13	137.8(5)
F11	-C130	-C131	-F14	19.7(7)
F11	-C130	-C131	-C132	-104.5(6)
F12	-C130	-C131	-F13	22.4(8)
F12	-C130	-C131	-F14	-95.7(7)
F12	-C130	-C131	-C132	140.1(6)
C129	-C130	-C131	-F13	-102.3(6)
C129	-C130	-C131	-F14	139.7(6)
C129	-C130	-C131	-C132	15.5(8)
F13	-C131	-C132	-F15	-24.0(7)
F13	-C131	-C132	-F16	-140.7(6)
F13	-C131	-C132	-C133	99.3(6)
F14	-C131	-C132	-F15	96.9(8)
F14	-C131	-C132	-F16	-19.9(9)
F14	-C131	-C132	-C133	-139.9(6)
C130	-C131	-C132	-F15	-140.4(6)
C130	-C131	-C132	-F16	102.9(6)
C130	-C131	-C132	-C133	-17.2(8)
F15	-C132	-C133	-C126	-46.6(8)
F15	-C132	-C133	-C129	135.2(6)

F16	-C132	-C133	-C126	72.4(7)
F16	-C132	-C133	-C129	-105.7(6)
C131	-C132	-C133	-C126	-168.8(6)
C131	-C132	-C133	-C129	13.0(8)

The sign of the torsion angle is positive if when looking from atom-2 to atom-3 a clockwise motion of atom-1 would superimpose it on atom-4.

Residue: 2.

Interatomic Distances (Å)

S21	-C210	1.713(6)	C210	-C211	1.359(7)
S21	-C213	1.733(6)	C211	-C212	1.427(7)
S22	-C224	1.733(4)	C212	-C213	1.364(8)
S22	-C227	1.714(5)	C212	-C229	1.493(7)
F21	-C230	1.223(10)	C213	-C214	1.499(9)
F22	-C230	1.416(12)	C215	-C216	1.414(9)
F23	-C231	1.300(8)	C215	-C220	1.377(9)
F24	-C231	1.282(8)	C216	-C217	1.379(12)
F25	-C232	1.361(8)	C217	-C218	1.35(1)
F26	-C232	1.339(9)	C218	-C219	1.387(8)
O21	-C29	1.254(7)	C219	-C220	1.385(8)
O22	-C223	1.240(6)	C220	-C221	1.531(8)
N21	-C27	1.508(9)	C221	-C222	1.520(7)
N21	-C29	1.336(8)	C223	-C224	1.468(7)
N22	-C221	1.455(7)	C224	-C225	1.355(7)
N22	-C223	1.338(6)	C225	-C226	1.412(7)
C21	-C22	1.47(2)	C226	-C227	1.378(7)
C21	-C26	1.436(16)	C226	-C233	1.448(7)
C22	-C23	1.53(4)	C227	-C228	1.514(8)
C23	-C24	0.99(7)	C229	-C230	1.477(9)
C24	-C25	1.50(6)	C229	-C233	1.337(7)
C25	-C26	1.432(16)	C230	-C231	1.503(9)
C26	-C27	1.537(13)	C231	-C232	1.524(9)
C27	-C28	1.585(15)	C232	-C233	1.493(8)
C210	-C29	1.506(8)			

Bond Angles (deg.)

C210	-S21	-C213	92.4(3)	C220	-C221	-C222	115.5(4)
C224	-S22	-C227	91.8(2)	O22	-C223	-N22	122.1(4)
C27	-N21	-C29	123.5(5)	O22	-C223	-C224	122.6(4)
C221	-N22	-C223	124.8(4)	N22	-C223	-C224	115.0(4)
C22	-C21	-C26	115.3(12)	S22	-C224	-C223	118.5(3)
C21	-C22	-C23	111.9(16)	S22	-C224	-C225	110.7(4)
C22	-C23	-C24	143(4)	C223	-C224	-C225	130.4(4)
C23	-C24	-C25	107(5)	C224	-C225	-C226	114.0(4)
C24	-C25	-C26	127(2)	C225	-C226	-C227	111.8(5)
C21	-C26	-C25	116.1(10)	C225	-C226	-C233	123.6(4)
C21	-C26	-C27	121.8(9)	C227	-C226	-C233	124.4(4)
C25	-C26	-C27	122.1(9)	S22	-C227	-C226	111.6(4)
N21	-C27	-C26	108.2(6)	S22	-C227	-C228	119.8(4)
N21	-C27	-C28	100.0(7)	C226	-C227	-C228	128.5(5)
C26	-C27	-C28	113.3(8)	C212	-C229	-C230	120.6(5)
O21	-C29	-N21	124.1(5)	C212	-C229	-C233	127.6(5)
O21	-C29	-C210	118.4(5)	C230	-C229	-C233	111.9(5)
N21	-C29	-C210	117.6(5)	F21	-C230	-F22	101.2(8)
S21	-C210	-C29	118.4(4)	F21	-C230	-C229	118.1(6)
S21	-C210	-C211	111.5(4)	F21	-C230	-C231	116.0(7)
C29	-C210	-C211	130.1(5)	F22	-C230	-C229	109.3(6)
C210	-C211	-C212	112.6(5)	F22	-C230	-C231	104.3(5)
C211	-C212	-C213	113.2(4)	C229	-C230	-C231	106.8(5)
C211	-C212	-C229	122.5(5)	F23	-C231	-F24	103.3(6)
C213	-C212	-C229	124.3(5)	F23	-C231	-C230	109.5(6)
S21	-C213	-C212	110.3(4)	F23	-C231	-C232	110.0(5)
S21	-C213	-C214	120.1(4)	F24	-C231	-C230	114.9(6)
C212	-C213	-C214	129.6(5)	F24	-C231	-C232	114.8(5)
C216	-C215	-C220	120.2(7)	C230	-C231	-C232	104.3(5)
C215	-C216	-C217	118.9(7)	F25	-C232	-F26	106.7(5)
C216	-C217	-C218	121.2(6)	F25	-C232	-C231	108.9(5)
C217	-C218	-C219	120.1(7)	F25	-C232	-C233	112.8(5)
C218	-C219	-C220	120.8(6)	F26	-C232	-C231	110.5(5)
C215	-C220	-C219	118.9(5)	F26	-C232	-C233	111.4(6)
C215	-C220	-C221	118.5(5)	C231	-C232	-C233	106.6(5)

C219	-C220	-C221	122.5(5)	C226	-C233	-C229	129.0(4)
N22	-C221	-C220	106.8(4)	C226	-C233	-C232	121.1(4)
N22	-C221	-C222	110.5(4)	C229	-C233	-C232	109.7(5)

Torsion Angles (deg.)

C213	-S21	-C210	-C29	-177.8(4)
C213	-S21	-C210	-C211	0.4(5)
C210	-S21	-C213	-C212	0.6(4)
C210	-S21	-C213	-C214	-179.8(5)
C227	-S22	-C224	-C223	-172.2(3)
C227	-S22	-C224	-C225	1.2(4)
C224	-S22	-C227	-C226	0.1(4)
C224	-S22	-C227	-C228	179.8(4)
C29	-N21	-C27	-C26	149.9(7)
C29	-N21	-C27	-C28	-91.4(8)
C27	-N21	-C29	-O21	2.6(10)
C27	-N21	-C29	-C210	-176.9(6)
C223	-N22	-C221	-C220	131.1(5)
C223	-N22	-C221	-C222	-102.5(5)
C221	-N22	-C223	-O22	9.9(7)
C221	-N22	-C223	-C224	-164.2(4)
C26	-C21	-C22	-C23	-1.9(13)
C22	-C21	-C26	-C25	-0.7(12)
C22	-C21	-C26	-C27	-179.4(8)
C21	-C22	-C23	-C24	9(5)
C22	-C23	-C24	-C25	-8(7)
C23	-C24	-C25	-C26	3(5)
C24	-C25	-C26	-C21	1(2)
C24	-C25	-C26	-C27	180(2)
C21	-C26	-C27	-N21	-80.3(9)
C21	-C26	-C27	-C28	169.8(8)
C25	-C26	-C27	-N21	101.1(9)
C25	-C26	-C27	-C28	-8.9(11)
S21	-C210	-C29	-O21	2.7(7)
S21	-C210	-C29	-N21	-177.9(4)

C211	-C210	-C29	-O21	-175.1(6)
C211	-C210	-C29	-N21	4.4(9)
S21	-C210	-C211	-C212	-1.3(6)
C29	-C210	-C211	-C212	176.6(5)
C210	-C211	-C212	-C213	1.8(7)
C210	-C211	-C212	-C229	-179.6(5)
C211	-C212	-C213	-S21	-1.5(6)
C211	-C212	-C213	-C214	179.0(5)
C229	-C212	-C213	-S21	180.0(4)
C229	-C212	-C213	-C214	0.5(9)
C211	-C212	-C229	-C230	-51.9(8)
C211	-C212	-C229	-C233	129.2(6)
C213	-C212	-C229	-C230	126.5(7)
C213	-C212	-C229	-C233	-52.4(9)
C220	-C215	-C216	-C217	1.9(10)
C216	-C215	-C220	-C219	-1.7(9)
C216	-C215	-C220	-C221	173.9(5)
C215	-C216	-C217	-C218	-1.3(11)
C216	-C217	-C218	-C219	0.6(10)
C217	-C218	-C219	-C220	-0.4(10)
C218	-C219	-C220	-C215	0.9(9)
C218	-C219	-C220	-C221	-174.5(5)
C215	-C220	-C221	-N22	-57.7(6)
C215	-C220	-C221	-C222	179.1(5)
C219	-C220	-C221	-N22	117.8(5)
C219	-C220	-C221	-C222	-5.5(8)
O22	-C223	-C224	-S22	15.7(5)
O22	-C223	-C224	-C225	-156.2(5)
N22	-C223	-C224	-S22	-170.3(3)
N22	-C223	-C224	-C225	17.8(7)
S22	-C224	-C225	-C226	-2.2(5)
C223	-C224	-C225	-C226	170.2(4)
C224	-C225	-C226	-C227	2.3(6)
C224	-C225	-C226	-C233	-172.6(4)
C225	-C226	-C227	-S22	-1.3(5)
C225	-C226	-C227	-C228	179.0(5)

C233	-C226	-C227	-S22	173.5(4)
C233	-C226	-C227	-C228	-6.2(8)
C225	-C226	-C233	-C229	121.1(6)
C225	-C226	-C233	-C232	-54.1(7)
C227	-C226	-C233	-C229	-53.2(8)
C227	-C226	-C233	-C232	131.6(6)
C212	-C229	-C230	-F21	44.1(12)
C212	-C229	-C230	-F22	-70.8(7)
C212	-C229	-C230	-C231	176.9(5)
C233	-C229	-C230	-F21	-136.9(9)
C233	-C229	-C230	-F22	108.3(6)
C233	-C229	-C230	-C231	-4.0(8)
C212	-C229	-C233	-C226	1.5(10)
C212	-C229	-C233	-C232	177.1(6)
C230	-C229	-C233	-C226	-177.5(6)
C230	-C229	-C233	-C232	-1.9(7)
F21	-C230	-C231	-F23	24.2(11)
F21	-C230	-C231	-F24	-91.6(10)
F21	-C230	-C231	-C232	141.8(9)
F22	-C230	-C231	-F23	134.5(6)
F22	-C230	-C231	-F24	18.8(8)
F22	-C230	-C231	-C232	-107.8(6)
C229	-C230	-C231	-F23	-109.8(6)
C229	-C230	-C231	-F24	134.4(6)
C229	-C230	-C231	-C232	7.9(7)
F23	-C231	-C232	-F25	-129.5(6)
F23	-C231	-C232	-F26	-12.7(7)
F23	-C231	-C232	-C233	108.5(6)
F24	-C231	-C232	-F25	-13.5(8)
F24	-C231	-C232	-F26	103.4(6)
F24	-C231	-C232	-C233	-135.5(6)
C230	-C231	-C232	-F25	113.1(6)
C230	-C231	-C232	-F26	-130.1(6)
C230	-C231	-C232	-C233	-8.9(7)
F25	-C232	-C233	-C226	63.5(8)
F25	-C232	-C233	-C229	-112.6(6)

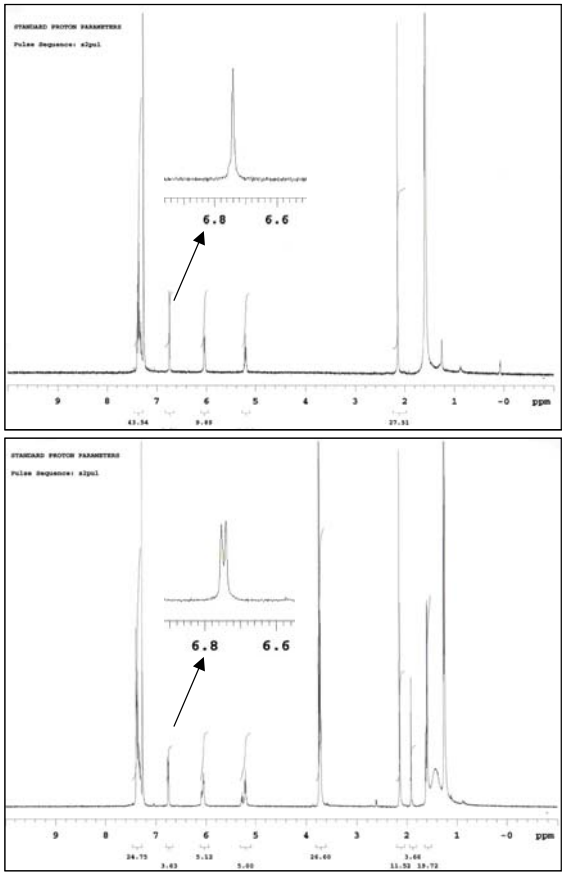
F26	-C232	-C233	-C226	-56.5(7)
F26	-C232	-C233	-C229	127.5(6)
C231	-C232	-C233	-C226	-177.1(5)
C231	-C232	-C233	-C229	6.9(7)

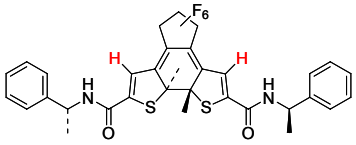
The sign of the torsion angle is positive if when looking from atom-2 to atom-3 a clockwise motion of atom-1 would superimpose it on atom-4.

All refinement calculations and graphics were performed on a HP XW6200 (Intel XEON 3.2 GHz) / Debian-Linux computer at the University of Groningen with the program packages *SHELXL* (least-square refinements), a locally modified version of the program *PLUTO* (preparation of illustrations) and *PLATON* package (checking the final results for missed symmetry with the *MISSYM* option, solvent accessible voids with the *SOLV* option, calculation of geometric data and the *ORTEP* illustrations).

*[1] Supplementary crystallographic data for this paper are available from the IUCr electronic archives (Reference: CCDC 291880, as a CIF file). These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/ retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk).

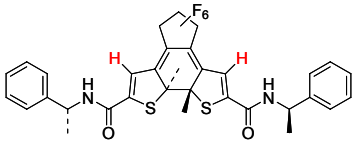
^{1}H NMR spectra of the closed ring isomer 2cR



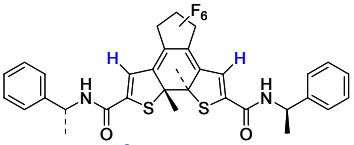


6.74 ppm

H1 NMR($CDCl_3$) spectrum of **2cR** formed in crystalline state



6.74 ppm



6.75 ppm

H1 NMR($CDCl_3$) spectrum of **2cR** formed in acetonitrile solution

Fig. S-1. ^{1}H NMR spectra in $CDCl_3$ solvent of the closed-ring isomer **2cR** formed in crystalline state (upper) and in acetonitrile solution (lower) upon 254 nm light irradiation.