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M/S no. OM0006561

Title: Transformations Leading to the Generation of Dithiolene Ligands Initiated by
Reactions of Sulfur-Rich $WS(S_2)(S_2CNR_2)_2$ Complexes with Dimethyl
Acetylenedicarboxylate and Phenylacetylene

Authors: Patrick J. Lim, Vernon C. Cook, Christian J. Doonan, Charles G. Young
and Edward R. T. Tiekink

data_[CGY]

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S(1b) 0.4634(2) -0.0983(3) 0.5736(2) 0.0432(9) Uij ??
S(1a) 0.4839(3) -0.5587(3) 0.0846(2) 0.053(1) Uij ??
S(2a) 0.4740(2) -0.3907(3) 0.1889(2) 0.0380(8) Uij ??
S(2b) 0.4592(2) -0.2586(3) 0.6817(1) 0.0422(9) Uij ??
S(3a) 0.4021(3) -0.1579(4) 0.1692(2) 0.054(1) Uij ??
S(3b) 0.4067(3) -0.4995(3) 0.6593(2) 0.0442(9) Uij ??
S(4b) 0.2538(3) -0.5143(4) 0.5495(2) 0.052(1) Uij ??
S(4a) 0.2778(3) -0.1432(4) 0.0486(2) 0.049(1) Uij ??
S(5a) 0.4828(2) -0.3080(4) 0.0366(1) 0.0465(9) Uij ??
S(5b) 0.4566(2) -0.3483(4) 0.5277(1) 0.0446(9) Uij ??
S(6b) 0.2194(2) -0.3153(4) 0.7031(1) 0.0425(8) Uij ??
S(6a) 0.2311(2) -0.3704(3) 0.2013(1) 0.0357(8) Uij ??
S(7b) 0.1134(2) -0.3137(4) 0.5671(1) 0.0406(8) Uij ??
S(7a) 0.1330(2) -0.3351(5) 0.0649(1) 0.0459(8) Uij ??
O(1a) 0.2371(8) -0.624(1) 0.1005(5) 0.068(4) Uij ??
O(1b) 0.2223(7) -0.0312(9) 0.5973(4) 0.055(3) Uij ??
O(1w) 0.939(1) -0.567(2) 0.7933(9) 0.070(5) Uij ??
O(2b) 0.1757(6) -0.1040(8) 0.5027(4) 0.048(3) Uij ??
O(2a) 0.2036(7) -0.5545(9) 0.0031(4) 0.056(3) Uij ??
O(2w) 0.091(2) -0.620(2) 0.7166(10) 0.076(6) Uij ??
O(3b) 0.2045(7) -0.339(1) 0.4332(4) 0.062(3) Uij ??
O(3a) 0.2420(7) -0.323(1) -0.0669(4) 0.060(3) Uij ??
O(4b) 0.3183(8) -0.1991(8) 0.4097(4) 0.055(3) Uij ??
O(4a) 0.3549(8) -0.464(1) -0.0833(4) 0.067(3) Uij ??
O(5a) -0.0704(8) -0.480(1) 0.2188(5) 0.086(4) Uij ??
O(5b) -0.0910(7) -0.253(1) 0.7390(5) 0.123(5) Uij ??
O(6b) 0.0665(7) -0.277(1) 0.8037(5) 0.082(4) Uij ??
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O(8a) -0.1314(6) -0.307(1) 0.1277(4) 0.074(4) Uij ??
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N(1a) 0.6239(8) -0.5485(9) 0.1842(5) 0.050(3) Uij ??
N(1b) 0.6133(7) -0.1052(10) 0.6726(5) 0.044(3) Uij ??
N(2a) 0.337(1) 0.038(1) 0.1160(7) 0.069(4) Uij ??
N(2b) 0.347(1) -0.693(1) 0.6042(6) 0.062(4) Uij ??
C(1a) 0.5379(9) -0.502(1) 0.1565(6) 0.042(3) Uij ??
C(1b) 0.5215(8) -0.150(1) 0.6477(5) 0.036(3) Uij ??
C(2a) 0.342(1) -0.073(1) 0.1097(7) 0.050(3) Uij ??

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C(2b)	0.3375(10)	-0.581(1)	0.6047(6)	0.043(3)	Uij ??
C(3b)	0.3348(9)	-0.179(1)	0.5571(5)	0.037(2)	Uij ??
C(3a)	0.3572(10)	-0.483(1)	0.0615(6)	0.041(3)	Uij ??
C(4b)	0.3373(8)	-0.266(1)	0.5148(5)	0.035(2)	Uij ??
C(4a)	0.3657(9)	-0.390(1)	0.0179(5)	0.037(3)	Uij ??
C(5a)	0.0897(8)	-0.397(1)	0.1824(6)	0.037(3)	Uij ??
C(5b)	0.0785(8)	-0.290(1)	0.6908(5)	0.039(2)	Uij ??
C(6b)	0.0318(7)	-0.2977(9)	0.6303(5)	0.030(2)	Uij ??
C(6a)	0.0474(9)	-0.381(1)	0.1208(5)	0.044(3)	Uij ??
C(7a)	0.672(1)	-0.511(1)	0.2463(7)	0.064(5)	Uij ??
C(7b)	0.668(1)	-0.145(1)	0.7304(6)	0.050(4)	Uij ??
C(8a)	0.686(1)	-0.635(1)	0.1594(8)	0.062(5)	Uij ??
C(8b)	0.670(1)	-0.013(1)	0.6418(7)	0.052(4)	Uij ??
C(9b)	0.283(1)	-0.753(2)	0.5555(8)	0.068(4)	Uij ??
C(9a)	0.285(1)	0.112(1)	0.0654(9)	0.076(6)	Uij ??
C(10a)	0.395(2)	0.093(2)	0.1759(10)	0.110(7)	Uij ??
C(10b)	0.421(2)	-0.744(2)	0.6551(9)	0.131(8)	Uij ??
C(11b)	0.237(1)	-0.100(1)	0.5579(7)	0.039(3)	Uij ??
C(11a)	0.261(1)	-0.566(1)	0.0576(7)	0.044(3)	Uij ??
C(12b)	0.068(1)	-0.043(1)	0.4985(7)	0.067(5)	Uij ??
C(12a)	0.094(1)	-0.615(2)	-0.0015(7)	0.090(6)	Uij ??
C(13b)	0.2782(10)	-0.272(1)	0.4506(6)	0.042(3)	Uij ??
C(13a)	0.313(1)	-0.380(1)	-0.0491(6)	0.051(4)	Uij ??
C(14b)	0.263(2)	-0.193(2)	0.3430(7)	0.136(9)	Uij ??
C(14a)	0.302(2)	-0.474(2)	-0.1475(6)	0.083(6)	Uij ??
C(15b)	0.0089(10)	-0.268(1)	0.7460(6)	0.066(4)	Uij ??
C(15a)	0.0193(10)	-0.444(1)	0.2300(6)	0.052(3)	Uij ??
C(16b)	0.005(1)	-0.251(2)	0.8587(7)	0.125(8)	Uij ??
C(16a)	0.000(1)	-0.456(2)	0.3449(7)	0.086(6)	Uij ??
C(17b)	-0.0923(10)	-0.285(1)	0.6121(7)	0.050(3)	Uij ??
C(17a)	-0.072(1)	-0.387(2)	0.1021(7)	0.063(4)	Uij ??
C(18b)	-0.268(1)	-0.379(1)	0.6162(8)	0.068(5)	Uij ??
C(18a)	-0.2516(10)	-0.293(2)	0.1091(8)	0.094(6)	Uij ??
H(7d)	0.7330	-0.1003	0.7423	0.0595	Uij ??
H(7e)	0.6927	-0.2203	0.7239	0.0595	Uij ??
H(7f)	0.6159	-0.1440	0.7641	0.0595	Uij ??
H(7a)	0.6148	-0.5151	0.2775	0.0775	Uij ??
H(7b)	0.6967	-0.4357	0.2428	0.0775	Uij ??
H(7c)	0.7354	-0.5566	0.2602	0.0775	Uij ??
H(8d)	0.6181	0.0490	0.6378	0.0643	Uij ??
H(8e)	0.6915	-0.0342	0.6000	0.0643	Uij ??
H(8f)	0.7363	0.0087	0.6684	0.0643	Uij ??
H(8a)	0.7425	-0.6600	0.1909	0.0751	Uij ??
H(8b)	0.7213	-0.6104	0.1212	0.0751	Uij ??
H(8c)	0.6347	-0.6954	0.1473	0.0751	Uij ??
H(9a)	0.2049	0.1047	0.0596	0.1020	Uij ??
H(9b)	0.3194	0.1040	0.0248	0.1020	Uij ??
H(9c)	0.2999	0.1919	0.0786	0.1020	Uij ??
H(9d)	0.2983	-0.8294	0.5619	0.0763	Uij ??
H(9e)	0.3056	-0.7293	0.5143	0.0763	Uij ??
H(9f)	0.2038	-0.7379	0.5594	0.0763	Uij ??
H(10d)	0.4968	-0.7148	0.6531	0.1470	Uij ??
H(10e)	0.4219	-0.8220	0.6484	0.1470	Uij ??
H(10f)	0.3929	-0.7274	0.6964	0.1470	Uij ??
H(10a)	0.3566	0.0717	0.2141	0.1396	Uij ??
H(10b)	0.3919	0.1723	0.1721	0.1396	Uij ??
H(10c)	0.4734	0.0703	0.1815	0.1396	Uij ??
H(12a)	0.1079	-0.6918	0.0070	0.1058	Uij ??

H(12b)	0.0590	-0.6063	-0.0444	0.1058	Uij ??
H(12c)	0.0451	-0.5855	0.0294	0.1058	Uij ??
H(12d)	0.0199	-0.0710	0.5307	0.0828	Uij ??
H(12e)	0.0309	-0.0538	0.4563	0.0828	Uij ??
H(12f)	0.0828	0.0334	0.5058	0.0828	Uij ??
H(14a)	0.2228	-0.4894	-0.1457	0.1012	Uij ??
H(14b)	0.3379	-0.5343	-0.1696	0.1012	Uij ??
H(14c)	0.3128	-0.4071	-0.1711	0.1012	Uij ??
H(14d)	0.2683	-0.2647	0.3226	0.1573	Uij ??
H(14e)	0.2964	-0.1383	0.3188	0.1573	Uij ??
H(14f)	0.1820	-0.1772	0.3465	0.1573	Uij ??
H(16a)	0.0427	-0.4438	0.3853	0.0999	Uij ??
H(16b)	-0.0206	-0.5331	0.3415	0.0999	Uij ??
H(16c)	-0.0669	-0.4117	0.3423	0.0999	Uij ??
H(16d)	-0.0593	-0.2999	0.8602	0.1433	Uij ??
H(16e)	-0.0202	-0.1765	0.8558	0.1433	Uij ??
H(16f)	0.0543	-0.2612	0.8972	0.1433	Uij ??
H(18a)	-0.2932	-0.3566	0.1212	0.1156	Uij ??
H(18b)	-0.2614	-0.2820	0.0631	0.1156	Uij ??
H(18c)	-0.2794	-0.2287	0.1307	0.1156	Uij ??
H(18d)	-0.2940	-0.4509	0.6271	0.0803	Uij ??
H(18e)	-0.2909	-0.3625	0.5719	0.0803	Uij ??
H(18f)	-0.2996	-0.3248	0.6439	0.0803	Uij ??

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W(2)	0.0287(2)	0.0263(3)	0.0301(2)	-0.0009(2)	-0.0001(2)	0.0006(2)
S(1b)	0.044(1)	0.042(2)	0.044(2)	-0.014(1)	0.000(1)	0.008(2)
S(1a)	0.056(2)	0.052(2)	0.052(2)	0.018(2)	0.002(2)	-0.006(2)
S(2a)	0.033(1)	0.042(2)	0.039(2)	0.008(1)	0.003(1)	0.000(1)
S(2b)	0.040(1)	0.047(2)	0.038(2)	-0.014(1)	-0.005(1)	0.004(2)
S(3a)	0.066(2)	0.043(2)	0.052(2)	-0.011(2)	-0.012(2)	0.002(2)
S(3b)	0.049(2)	0.032(2)	0.051(2)	0.008(1)	-0.004(1)	0.004(2)
S(4b)	0.065(2)	0.035(2)	0.052(2)	0.001(2)	-0.013(2)	-0.004(2)
S(4a)	0.067(2)	0.033(2)	0.047(2)	0.005(2)	-0.003(2)	0.006(2)
S(5a)	0.041(1)	0.051(3)	0.049(2)	-0.006(2)	0.013(1)	0.002(2)
S(5b)	0.043(1)	0.049(2)	0.043(2)	0.013(2)	0.013(1)	-0.003(2)
S(6b)	0.028(1)	0.065(2)	0.034(1)	0.002(2)	-0.0009(9)	-0.004(2)
S(6a)	0.027(1)	0.052(2)	0.028(1)	0.002(1)	0.0038(9)	0.001(1)
S(7b)	0.031(1)	0.053(2)	0.037(1)	0.002(2)	-0.0047(9)	0.000(2)
S(7a)	0.036(1)	0.063(2)	0.039(2)	0.006(2)	-0.0015(10)	0.002(2)
O(1a)	0.080(7)	0.061(9)	0.061(7)	-0.018(6)	-0.008(5)	0.008(6)
O(1b)	0.064(5)	0.051(7)	0.049(6)	0.012(5)	0.006(4)	-0.026(5)
O(2b)	0.046(4)	0.053(6)	0.044(5)	0.022(4)	0.000(3)	-0.001(5)
O(2a)	0.069(5)	0.069(8)	0.029(5)	-0.017(5)	-0.002(4)	-0.003(5)
O(3b)	0.072(5)	0.063(7)	0.050(5)	-0.022(5)	0.000(4)	-0.012(6)
O(3a)	0.082(5)	0.064(7)	0.033(4)	0.022(6)	0.002(4)	0.008(6)
O(4b)	0.081(6)	0.053(6)	0.031(5)	0.006(5)	0.009(4)	0.003(4)
O(4a)	0.075(6)	0.099(9)	0.026(5)	0.024(6)	0.003(4)	-0.007(5)
O(5a)	0.053(5)	0.13(1)	0.075(7)	-0.039(6)	0.000(5)	0.038(7)
O(5b)	0.041(4)	0.24(2)	0.088(8)	0.039(8)	-0.001(5)	-0.06(1)

O(6b)	0.041(4)	0.14(1)	0.062(5)	0.013(6)	0.005(4)	-0.025(7)
O(6a)	0.059(5)	0.099(9)	0.042(4)	-0.017(5)	0.015(4)	0.023(6)
O(7b)	0.038(5)	0.074(8)	0.17(1)	0.013(5)	-0.026(6)	0.036(8)
O(7a)	0.046(6)	0.11(1)	0.15(1)	0.003(6)	-0.035(7)	-0.060(9)
O(8a)	0.032(4)	0.12(1)	0.067(7)	-0.014(6)	0.000(4)	-0.008(8)
O(8b)	0.034(4)	0.060(6)	0.058(6)	0.010(4)	0.002(4)	0.007(5)
N(1a)	0.055(6)	0.038(7)	0.057(6)	0.012(5)	0.001(5)	0.013(5)
N(1b)	0.033(4)	0.056(8)	0.043(5)	-0.017(4)	0.004(4)	0.002(5)
N(2a)	0.092(9)	0.034(6)	0.082(9)	0.000(6)	0.006(7)	0.019(6)
N(2b)	0.078(8)	0.026(5)	0.083(9)	0.005(6)	0.017(6)	0.012(6)
C(1a)	0.033(5)	0.043(7)	0.051(6)	0.001(4)	0.016(4)	-0.006(5)
C(1b)	0.031(4)	0.035(6)	0.041(5)	-0.001(4)	0.007(3)	-0.014(4)
C(2a)	0.057(7)	0.034(6)	0.058(7)	-0.018(6)	0.002(6)	0.009(4)
C(2b)	0.043(6)	0.026(5)	0.061(8)	-0.006(5)	0.005(5)	0.007(4)
C(3b)	0.041(4)	0.032(4)	0.037(6)	-0.006(3)	-0.006(5)	0.009(3)
C(3a)	0.050(5)	0.031(5)	0.043(7)	0.004(3)	0.015(5)	0.001(3)
C(4b)	0.038(5)	0.030(6)	0.036(4)	-0.001(4)	0.011(4)	0.011(4)
C(4a)	0.041(5)	0.039(7)	0.031(4)	0.006(4)	0.007(4)	0.003(4)
C(5a)	0.025(3)	0.045(8)	0.042(5)	0.001(4)	0.002(4)	-0.002(5)
C(5b)	0.031(3)	0.041(8)	0.044(5)	-0.004(4)	-0.006(3)	-0.016(6)
C(6b)	0.034(4)	0.019(5)	0.039(4)	0.001(4)	0.002(2)	0.000(5)
C(6a)	0.037(4)	0.061(9)	0.035(5)	0.006(5)	0.004(3)	-0.010(5)
C(7a)	0.064(8)	0.08(1)	0.046(7)	0.025(8)	-0.001(6)	0.018(7)
C(7b)	0.060(7)	0.040(8)	0.049(7)	0.012(6)	-0.009(6)	-0.002(6)
C(8a)	0.063(9)	0.053(10)	0.07(1)	0.021(7)	0.005(7)	-0.012(8)
C(8b)	0.066(9)	0.041(8)	0.049(8)	-0.018(6)	0.008(6)	0.004(6)
C(9a)	0.13(1)	0.015(9)	0.08(1)	0.010(9)	-0.002(10)	0.015(7)
C(10a)	0.17(2)	0.04(1)	0.11(2)	0.00(1)	-0.04(1)	-0.04(1)
C(10b)	0.20(2)	0.05(1)	0.13(2)	0.04(1)	-0.09(1)	0.03(1)
C(11b)	0.039(6)	0.034(7)	0.046(6)	-0.009(4)	0.006(4)	-0.009(5)
C(11a)	0.036(6)	0.044(9)	0.049(6)	0.010(5)	-0.015(5)	-0.012(5)
C(12b)	0.049(7)	0.08(1)	0.08(1)	0.039(7)	0.007(7)	0.022(9)
C(12a)	0.082(10)	0.13(2)	0.07(1)	-0.06(1)	0.015(8)	-0.01(1)
C(13b)	0.048(6)	0.039(6)	0.038(5)	0.020(4)	0.012(4)	-0.008(4)
C(13a)	0.052(7)	0.067(9)	0.035(5)	-0.012(5)	-0.001(5)	0.012(5)
C(14b)	0.27(3)	0.10(2)	0.029(8)	0.03(2)	-0.06(1)	0.01(1)
C(14a)	0.14(2)	0.09(1)	0.014(6)	-0.02(1)	0.001(7)	0.002(8)
C(15b)	0.044(5)	0.10(1)	0.059(5)	0.037(7)	0.012(4)	-0.024(9)
C(15a)	0.045(5)	0.07(1)	0.042(5)	0.004(5)	0.013(4)	0.021(6)
C(16b)	0.046(8)	0.28(3)	0.053(9)	0.04(1)	0.003(6)	-0.03(1)
C(16a)	0.10(1)	0.13(2)	0.037(8)	-0.01(1)	0.036(7)	0.032(10)
C(17b)	0.033(4)	0.063(7)	0.054(8)	0.001(4)	0.006(5)	-0.002(7)
C(17a)	0.044(5)	0.10(1)	0.043(8)	-0.010(6)	-0.015(6)	0.018(7)
C(18b)	0.035(4)	0.08(1)	0.09(1)	0.005(7)	-0.009(7)	-0.009(9)
C(18a)	0.030(4)	0.14(2)	0.12(1)	0.020(9)	0.033(6)	0.01(1)
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_refine_ls_abs_structure_Flack	?					
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_refine_ls_number_restraints	0					

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_refine_ls_R_factor_obs           0.0421
_refine_ls_wR_factor_all          ?
_refine_ls_wR_factor_obs          0.0559
_refine_ls_goodness_of_fit_all    ?
_refine_ls_goodness_of_fit_obs    1.919
_refine_ls_shift/esd_max          2.4022
_refine_ls_shift/esd_mean         ?
_refine_diff_density_min          -0.85
_refine_diff_density_max          1.30

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  _geom_bond_atom_site_label_2
  _geom_bond_distance
  _geom_bond_site_symmetry_1
  _geom_bond_site_symmetry_2
  _geom_bond_publ_flag
W(1)   S(2a)   2.507(4)  ?? yes
W(1)   S(3a)   2.510(6)  ?? yes
W(1)   S(4a)   2.564(6)  ?? yes
W(1)   S(5a)   2.495(4)  ?? yes
W(1)   S(6a)   2.364(4)  ?? yes
W(1)   S(7a)   2.401(3)  ?? yes
W(1)   C(3a)   2.25(2)   ?? yes
W(1)   C(4a)   2.16(2)   ?? yes
W(2)   S(2b)   2.536(4)  ?? yes
W(2)   S(3b)   2.489(5)  ?? yes
W(2)   S(4b)   2.480(6)  ?? yes
W(2)   S(5b)   2.486(4)  ?? yes
W(2)   S(6b)   2.369(4)  ?? yes
W(2)   S(7b)   2.417(3)  ?? yes
W(2)   C(3b)   2.27(2)   ?? yes
W(2)   C(4b)   2.17(2)   ?? yes
S(1b)  C(1b)   1.77(2)   ?? yes
S(1b)  C(3b)   1.83(2)   ?? yes
S(1a)  C(1a)   1.74(2)   ?? yes
S(1a)  C(3a)   1.81(2)   ?? yes
S(2a)  C(1a)   1.72(2)   ?? yes
S(2b)  C(1b)   1.69(2)   ?? yes
S(3a)  C(2a)   1.74(2)   ?? yes
S(3b)  C(2b)   1.69(2)   ?? yes
S(4b)  C(2b)   1.68(2)   ?? yes
S(4a)  C(2a)   1.68(2)   ?? yes
S(5a)  C(4a)   1.74(2)   ?? yes
S(5b)  C(4b)   1.75(2)   ?? yes
S(6b)  C(5b)   1.70(1)   ?? yes
S(6a)  C(5a)   1.73(1)   ?? yes
S(7b)  C(6b)   1.70(1)   ?? yes
S(7a)  C(6a)   1.69(2)   ?? yes
O(1a)  C(11a)  1.20(2)   ?? yes
O(1b)  C(11b)  1.20(2)   ?? yes
O(2b)  C(11b)  1.32(2)   ?? yes
O(2b)  C(12b)  1.47(2)   ?? yes
O(2a)  C(11a)  1.30(2)   ?? yes
O(2a)  C(12a)  1.49(2)   ?? yes

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O(3b)	C(13b)	1.24(2)	??	yes
O(3a)	C(13a)	1.14(2)	??	yes
O(4b)	C(13b)	1.34(2)	??	yes
O(4b)	C(14b)	1.51(2)	??	yes
O(4a)	C(13a)	1.36(2)	??	yes
O(4a)	C(14a)	1.45(2)	??	yes
O(5a)	C(15a)	1.17(2)	??	yes
O(5b)	C(15b)	1.20(2)	??	yes
O(6b)	C(15b)	1.35(2)	??	yes
O(6b)	C(16b)	1.44(2)	??	yes
O(6a)	C(15a)	1.41(2)	??	yes
O(6a)	C(16a)	1.46(2)	??	yes
O(7b)	C(17b)	1.13(2)	??	yes
O(7a)	C(17a)	1.13(3)	??	yes
O(8a)	C(17a)	1.34(3)	??	yes
O(8a)	C(18a)	1.46(2)	??	yes
O(8b)	C(17b)	1.28(2)	??	yes
O(8b)	C(18b)	1.48(2)	??	yes
N(1a)	C(1a)	1.27(2)	??	yes
N(1a)	C(7a)	1.46(2)	??	yes
N(1a)	C(8a)	1.41(2)	??	yes
N(1b)	C(1b)	1.30(2)	??	yes
N(1b)	C(7b)	1.42(2)	??	yes
N(1b)	C(8b)	1.48(2)	??	yes
N(2a)	C(2a)	1.37(3)	??	yes
N(2a)	C(9a)	1.49(3)	??	yes
N(2a)	C(10a)	1.54(3)	??	yes
N(2b)	C(2b)	1.38(3)	??	yes
N(2b)	C(9b)	1.43(3)	??	yes
N(2b)	C(10b)	1.47(2)	??	yes
C(3b)	C(4b)	1.39(2)	??	yes
C(3b)	C(11b)	1.51(2)	??	yes
C(3a)	C(4a)	1.47(2)	??	yes
C(3a)	C(11a)	1.52(3)	??	yes
C(4b)	C(13b)	1.48(2)	??	yes
C(4a)	C(13a)	1.50(2)	??	yes
C(5a)	C(6a)	1.37(2)	??	yes
C(5a)	C(15a)	1.45(2)	??	yes
C(5b)	C(6b)	1.35(2)	??	yes
C(5b)	C(15b)	1.49(2)	??	yes
C(6b)	C(17b)	1.51(2)	??	yes
C(6a)	C(17a)	1.45(2)	??	yes

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loop_

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_geom_angle

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S(2a)	W(1)	S(3a)	73.2(2)	???	yes
S(2a)	W(1)	S(4a)	137.4(2)	???	yes
S(2a)	W(1)	S(5a)	84.0(1)	???	yes
S(2a)	W(1)	S(6a)	73.7(1)	???	yes
S(2a)	W(1)	S(7a)	147.7(2)	???	yes
S(2a)	W(1)	C(3a)	82.2(4)	???	yes

S(2a)	W(1)	C(4a)	105.4(4)	???	yes
S(3a)	W(1)	S(4a)	68.2(2)	???	yes
S(3a)	W(1)	S(5a)	89.0(2)	???	yes
S(3a)	W(1)	S(6a)	88.2(2)	???	yes
S(3a)	W(1)	S(7a)	123.8(2)	???	yes
S(3a)	W(1)	C(3a)	148.3(4)	???	yes
S(3a)	W(1)	C(4a)	130.6(5)	???	yes
S(4a)	W(1)	S(5a)	78.0(2)	???	yes
S(4a)	W(1)	S(6a)	121.3(2)	???	yes
S(4a)	W(1)	S(7a)	72.6(2)	???	yes
S(4a)	W(1)	C(3a)	124.5(5)	???	yes
S(4a)	W(1)	C(4a)	87.0(5)	???	yes
S(5a)	W(1)	S(6a)	157.4(1)	???	yes
S(5a)	W(1)	S(7a)	120.3(1)	???	yes
S(5a)	W(1)	C(3a)	68.4(4)	???	yes
S(5a)	W(1)	C(4a)	43.0(4)	???	yes
S(6a)	W(1)	S(7a)	79.4(1)	???	yes
S(6a)	W(1)	C(3a)	104.1(5)	???	yes
S(6a)	W(1)	C(4a)	140.1(5)	???	yes
S(7a)	W(1)	C(3a)	87.6(4)	???	yes
S(7a)	W(1)	C(4a)	84.2(4)	???	yes
C(3a)	W(1)	C(4a)	38.7(6)	???	yes
S(2b)	W(2)	S(3b)	74.5(2)	???	yes
S(2b)	W(2)	S(4b)	142.0(2)	???	yes
S(2b)	W(2)	S(5b)	85.3(1)	???	yes
S(2b)	W(2)	S(6b)	75.1(1)	???	yes
S(2b)	W(2)	S(7b)	141.0(2)	???	yes
S(2b)	W(2)	C(3b)	79.2(4)	???	yes
S(2b)	W(2)	C(4b)	103.2(4)	???	yes
S(3b)	W(2)	S(4b)	69.7(2)	???	yes
S(3b)	W(2)	S(5b)	86.2(2)	???	yes
S(3b)	W(2)	S(6b)	86.7(2)	???	yes
S(3b)	W(2)	S(7b)	132.3(2)	???	yes
S(3b)	W(2)	C(3b)	143.6(4)	???	yes
S(3b)	W(2)	C(4b)	128.9(4)	???	yes
S(4b)	W(2)	S(5b)	80.4(2)	???	yes
S(4b)	W(2)	S(6b)	114.1(2)	???	yes
S(4b)	W(2)	S(7b)	75.6(2)	???	yes
S(4b)	W(2)	C(3b)	125.1(4)	???	yes
S(4b)	W(2)	C(4b)	90.0(5)	???	yes
S(5b)	W(2)	S(6b)	160.3(1)	???	yes
S(5b)	W(2)	S(7b)	119.3(1)	???	yes
S(5b)	W(2)	C(3b)	66.8(5)	???	yes
S(5b)	W(2)	C(4b)	43.4(4)	???	yes
S(6b)	W(2)	S(7b)	78.7(1)	???	yes
S(6b)	W(2)	C(3b)	110.4(5)	???	yes
S(6b)	W(2)	C(4b)	143.3(5)	???	yes
S(7b)	W(2)	C(3b)	83.5(4)	???	yes
S(7b)	W(2)	C(4b)	81.5(4)	???	yes
C(3b)	W(2)	C(4b)	36.3(6)	???	yes
C(1b)	S(1b)	C(3b)	104.1(7)	???	yes
C(1a)	S(1a)	C(3a)	106.4(8)	???	yes
W(1)	S(2a)	C(1a)	108.5(6)	???	yes
W(2)	S(2b)	C(1b)	111.2(5)	???	yes
W(1)	S(3a)	C(2a)	89.8(7)	???	yes
W(2)	S(3b)	C(2b)	87.5(7)	???	yes
W(2)	S(4b)	C(2b)	87.9(7)	???	yes
W(1)	S(4a)	C(2a)	89.3(8)	???	yes

W(1)	S(5a)	C(4a)	58.2(5)	???	yes
W(2)	S(5b)	C(4b)	58.5(5)	???	yes
W(2)	S(6b)	C(5b)	112.3(6)	???	yes
W(1)	S(6a)	C(5a)	111.1(6)	???	yes
W(2)	S(7b)	C(6b)	109.6(4)	???	yes
W(1)	S(7a)	C(6a)	110.6(5)	???	yes
C(11b)	O(2b)	C(12b)	117(1)	???	yes
C(11a)	O(2a)	C(12a)	114(1)	???	yes
C(13b)	O(4b)	C(14b)	118(1)	???	yes
C(13a)	O(4a)	C(14a)	113(1)	???	yes
C(15b)	O(6b)	C(16b)	116(1)	???	yes
C(15a)	O(6a)	C(16a)	115(1)	???	yes
C(17a)	O(8a)	C(18a)	120(1)	???	yes
C(17b)	O(8b)	C(18b)	118(1)	???	yes
C(1a)	N(1a)	C(7a)	121(1)	???	yes
C(1a)	N(1a)	C(8a)	126(1)	???	yes
C(7a)	N(1a)	C(8a)	112(1)	???	yes
C(1b)	N(1b)	C(7b)	121(1)	???	yes
C(1b)	N(1b)	C(8b)	122(1)	???	yes
C(7b)	N(1b)	C(8b)	115(1)	???	yes
C(2a)	N(2a)	C(9a)	123(2)	???	yes
C(2a)	N(2a)	C(10a)	119(1)	???	yes
C(9a)	N(2a)	C(10a)	117(2)	???	yes
C(2b)	N(2b)	C(9b)	118(1)	???	yes
C(2b)	N(2b)	C(10b)	117(1)	???	yes
C(9b)	N(2b)	C(10b)	124(2)	???	yes
S(1a)	C(1a)	S(2a)	120.5(10)	???	yes
S(1a)	C(1a)	N(1a)	117(1)	???	yes
S(2a)	C(1a)	N(1a)	122(1)	???	yes
S(1b)	C(1b)	S(2b)	119.5(8)	???	yes
S(1b)	C(1b)	N(1b)	117(1)	???	yes
S(2b)	C(1b)	N(1b)	122(1)	???	yes
S(3a)	C(2a)	S(4a)	112(1)	???	yes
S(3a)	C(2a)	N(2a)	122(1)	???	yes
S(4a)	C(2a)	N(2a)	124(1)	???	yes
S(3b)	C(2b)	S(4b)	114(1)	???	yes
S(3b)	C(2b)	N(2b)	123(1)	???	yes
S(4b)	C(2b)	N(2b)	121(1)	???	yes
W(2)	C(3b)	S(1b)	121.9(7)	???	yes
W(2)	C(3b)	C(4b)	67.7(10)	???	yes
W(2)	C(3b)	C(11b)	115(1)	???	yes
S(1b)	C(3b)	C(4b)	118(1)	???	yes
S(1b)	C(3b)	C(11b)	106(1)	???	yes
C(4b)	C(3b)	C(11b)	122(1)	???	yes
W(1)	C(3a)	S(1a)	119.7(9)	???	yes
W(1)	C(3a)	C(4a)	67.3(10)	???	yes
W(1)	C(3a)	C(11a)	117(1)	???	yes
S(1a)	C(3a)	C(4a)	118(1)	???	yes
S(1a)	C(3a)	C(11a)	106(1)	???	yes
C(4a)	C(3a)	C(11a)	124(1)	???	yes
W(2)	C(4b)	S(5b)	78.1(6)	???	yes
W(2)	C(4b)	C(3b)	75.9(9)	???	yes
W(2)	C(4b)	C(13b)	133(1)	???	yes
S(5b)	C(4b)	C(3b)	113(1)	???	yes
S(5b)	C(4b)	C(13b)	116(1)	???	yes
C(3b)	C(4b)	C(13b)	126(1)	???	yes
W(1)	C(4a)	S(5a)	78.7(7)	???	yes
W(1)	C(4a)	C(3a)	74.0(9)	???	yes

W(1)	C(4a)	C(13a)	133(1)	???	yes
S(5a)	C(4a)	C(3a)	113(1)	???	yes
S(5a)	C(4a)	C(13a)	116(1)	???	yes
C(3a)	C(4a)	C(13a)	126(1)	???	yes
S(6a)	C(5a)	C(6a)	118(1)	???	yes
S(6a)	C(5a)	C(15a)	120(1)	???	yes
C(6a)	C(5a)	C(15a)	120(1)	???	yes
S(6b)	C(5b)	C(6b)	117(1)	???	yes
S(6b)	C(5b)	C(15b)	120(1)	???	yes
C(6b)	C(5b)	C(15b)	121(1)	???	yes
S(7b)	C(6b)	C(5b)	121(1)	???	yes
S(7b)	C(6b)	C(17b)	114(1)	???	yes
C(5b)	C(6b)	C(17b)	124(1)	???	yes
S(7a)	C(6a)	C(5a)	119(1)	???	yes
S(7a)	C(6a)	C(17a)	116(1)	???	yes
C(5a)	C(6a)	C(17a)	122(1)	???	yes
O(1b)	C(11b)	O(2b)	122(1)	???	yes
O(1b)	C(11b)	C(3b)	126(1)	???	yes
O(2b)	C(11b)	C(3b)	110(1)	???	yes
O(1a)	C(11a)	O(2a)	125(1)	???	yes
O(1a)	C(11a)	C(3a)	125(1)	???	yes
O(2a)	C(11a)	C(3a)	108(1)	???	yes
O(3b)	C(13b)	O(4b)	121(1)	???	yes
O(3b)	C(13b)	C(4b)	125(1)	???	yes
O(4b)	C(13b)	C(4b)	112(1)	???	yes
O(3a)	C(13a)	O(4a)	125(1)	???	yes
O(3a)	C(13a)	C(4a)	127(1)	???	yes
O(4a)	C(13a)	C(4a)	106(1)	???	yes
O(5b)	C(15b)	O(6b)	124(1)	???	yes
O(5b)	C(15b)	C(5b)	121(1)	???	yes
O(6b)	C(15b)	C(5b)	113(1)	???	yes
O(5a)	C(15a)	O(6a)	124(1)	???	yes
O(5a)	C(15a)	C(5a)	124(1)	???	yes
O(6a)	C(15a)	C(5a)	110(1)	???	yes
O(7b)	C(17b)	O(8b)	122(1)	???	yes
O(7b)	C(17b)	C(6b)	128(2)	???	yes
O(8b)	C(17b)	C(6b)	108(1)	???	yes
O(7a)	C(17a)	O(8a)	119(1)	???	yes
O(7a)	C(17a)	C(6a)	127(2)	???	yes
O(8a)	C(17a)	C(6a)	112(1)	???	yes

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'x, y, z'

'-x, -y, -z'

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_refine_special_details

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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.
;

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_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
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_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment mixed
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' $F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$ '
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S1 S 0.58789(14) 0.32235(10) 0.70505(10) 0.0387(3) Uani 1 1 d ...
S2 S 0.33923(14) 0.47545(9) 0.66993(10) 0.0383(3) Uani 1 1 d ...
S3 S 0.41188(14) 0.19331(9) 0.91692(9) 0.0362(3) Uani 1 1 d ...
S4 S 0.13614(13) 0.35920(9) 0.87992(9) 0.0345(3) Uani 1 1 d ...
S5 S 0.13157(14) 0.31217(9) 0.67769(9) 0.0368(3) Uani 1 1 d ...
S6 S 0.40047(14) 0.14111(10) 0.71803(10) 0.0397(3) Uani 1 1 d ...
O1 O 0.4407(5) 0.1699(4) 1.1461(3) 0.0750(14) Uani 1 1 d ...
O2 O 0.2150(5) 0.1224(3) 1.1813(3) 0.0537(10) Uani 1 1 d ...
O3 O -0.0776(5) 0.3451(5) 1.0847(4) 0.094(2) Uani 1 1 d ...
O4 O 0.1121(4) 0.3380(3) 1.1572(3) 0.0524(10) Uani 1 1 d ...
O5 O 0.0917(7) 0.2588(5) 0.4664(3) 0.104(2) Uani 1 1 d ...
O6 O -0.0633(4) 0.1788(3) 0.5983(3) 0.0553(10) Uani 1 1 d ...
O7 O 0.2125(7) 0.0274(5) 0.5621(5) 0.108(2) Uani 1 1 d ...
O8 O 0.4126(6) -0.0273(3) 0.6341(4) 0.0671(13) Uani 1 1 d ...
N1 N 0.6223(5) 0.5200(3) 0.6018(3) 0.0407(10) Uani 1 1 d ...
N2 N -0.5000 0.5000 1.0000 0.0401(14) Uani 1 2 d S ..
N3 N 0.0000 0.0000 1.0000 0.0449(15) Uani 1 2 d S ..
C1 C 0.5310(5) 0.4502(4) 0.6508(3) 0.0336(10) Uani 1 1 d ...
C2 C 0.2885(5) 0.2267(4) 1.0188(3) 0.0346(11) Uani 1 1 d ...
C3 C 0.1673(5) 0.2986(4) 1.0029(3) 0.0340(10) Uani 1 1 d ...
C4 C 0.1611(6) 0.2097(4) 0.6265(3) 0.0370(11) Uani 1 1 d ...
C5 C 0.2762(6) 0.1328(4) 0.6453(4) 0.0403(12) Uani 1 1 d ...
C6 C 0.5655(7) 0.6279(4) 0.5590(4) 0.0487(14) Uani 1 1 d ...
H6A H 0.6480 0.6658 0.5269 0.073 Uiso 1 1 calc R ..
H6B H 0.5053 0.6560 0.6118 0.073 Uiso 1 1 calc R ..
H6C H 0.5059 0.6330 0.5101 0.073 Uiso 1 1 calc R ..
C7 C 0.7849(6) 0.4899(5) 0.5863(5) 0.0588(16) Uani 1 1 d ...
H7A H 0.8329 0.5495 0.5499 0.088 Uiso 1 1 calc R ..
H7B H 0.8122 0.4401 0.5484 0.088 Uiso 1 1 calc R ..
H7C H 0.8162 0.4602 0.6506 0.088 Uiso 1 1 calc R ..
C8 C 0.3262(6) 0.1704(4) 1.1207(4) 0.0411(12) Uani 1 1 d ...
C9 C 0.2334(9) 0.0751(6) 1.2849(5) 0.077(2) Uani 1 1 d ...
H9A H 0.1474 0.0426 1.3223 0.115 Uiso 1 1 calc R ..

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H9B H 0.2436 0.1270 1.3141 0.115 Uiso 1 1 calc R..
 H9C H 0.3214 0.0244 1.2873 0.115 Uiso 1 1 calc R..
 C10 C 0.0526(6) 0.3289(4) 1.0844(4) 0.0441(12) Uani 1 1 d...
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 H11A H 0.0585 0.3645 1.2919 0.109 Uiso 1 1 calc R..
 H11B H -0.0539 0.3043 1.2735 0.109 Uiso 1 1 calc R..
 H11C H -0.0584 0.4230 1.2216 0.109 Uiso 1 1 calc R..
 C12 C 0.0612(7) 0.2169(4) 0.5546(4) 0.0459(13) Uani 1 1 d...
 C13 C -0.1623(8) 0.1805(6) 0.5311(5) 0.0692(19) Uani 1 1 d...
 H13A H -0.2500 0.1510 0.5703 0.104 Uiso 1 1 calc R..
 H13B H -0.1110 0.1411 0.4850 0.104 Uiso 1 1 calc R..
 H13C H -0.1912 0.2504 0.4939 0.104 Uiso 1 1 calc R..
 C14 C 0.2940(7) 0.0398(5) 0.6091(5) 0.0546(15) Uani 1 1 d...
 C15 C 0.4333(3) -0.1225(2) 0.6059(2) 0.088(3) Uani 1 1 d...
 H15A H 0.5218 -0.1658 0.6272 0.133 Uiso 1 1 calc R..
 H15B H 0.4439 -0.1070 0.5339 0.133 Uiso 1 1 calc R..
 H15C H 0.3481 -0.1577 0.6379 0.133 Uiso 1 1 calc R..
 C16 C -0.5492(3) 0.5836(2) 1.0515(2) 0.058(3) Uani 0.50 1 d PR..
 C16' C -0.5420(3) 0.4012(2) 1.0792(2) 0.062(3) Uani 0.50 1 d PR..
 C17 C -0.7152(3) 0.5979(2) 1.0994(2) 0.102(3) Uani 1 1 d R..
 C18 C -0.5957(3) 0.5198(2) 0.9180(2) 0.049(3) Uani 0.50 1 d PR..
 C18' C -0.6594(3) 0.5006(2) 1.0459(2) 0.066(4) Uani 0.50 1 d PR..
 C19 C -0.5590(3) 0.6198(2) 0.8315(2) 0.089(3) Uani 1 1 d R..
 C20 C 0.1395(3) 0.0026(2) 0.9191(2) 0.066(4) Uani 0.50 1 d PR..
 C20' C 0.0250(3) -0.0944(2) 0.9649(2) 0.082(5) Uani 0.50 1 d PR..
 C21 C 0.1671(3) -0.0954(2) 0.8774(2) 0.104(3) Uani 1 1 d R..
 C22 C 0.0051(3) -0.0958(2) 1.0844(2) 0.058(3) Uani 0.50 1 d PR..
 C22' C 0.1445(3) -0.0016(2) 1.0483(2) 0.073(4) Uani 0.50 1 d PR..
 C23 C 0.1480(3) -0.1086(2) 1.1370(2) 0.110(3) Uani 1 1 d R..

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 S4 0.0326(6) 0.0411(6) 0.0277(6) -0.0078(5) -0.0073(5) -0.0015(5)
 S5 0.0370(7) 0.0403(6) 0.0368(6) -0.0108(5) -0.0140(5) -0.0054(5)
 S6 0.0406(7) 0.0379(6) 0.0478(7) -0.0187(6) -0.0140(6) -0.0036(5)
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 O2 0.062(3) 0.057(2) 0.036(2) 0.0077(17) -0.0132(18) -0.024(2)
 O3 0.034(2) 0.188(6) 0.062(3) -0.056(4) -0.006(2) 0.006(3)
 O4 0.050(2) 0.078(3) 0.035(2) -0.0259(19) -0.0075(17) -0.005(2)
 O5 0.125(5) 0.159(6) 0.039(3) 0.014(3) -0.032(3) -0.093(4)
 O6 0.049(2) 0.086(3) 0.040(2) -0.017(2) -0.0125(18) -0.025(2)
 O7 0.098(4) 0.107(4) 0.177(6) -0.106(5) -0.078(4) 0.023(3)
 O8 0.090(3) 0.044(2) 0.084(3) -0.034(2) -0.042(3) 0.007(2)
 N1 0.040(2) 0.044(2) 0.036(2) -0.0073(19) 0.0022(19) -0.0162(19)
 N2 0.033(3) 0.056(4) 0.038(3) -0.014(3) -0.010(3) -0.017(3)
 N3 0.038(3) 0.046(4) 0.049(4) -0.007(3) 0.001(3) -0.021(3)
 C1 0.037(3) 0.039(3) 0.027(2) -0.012(2) -0.003(2) -0.009(2)
 C2 0.033(3) 0.043(3) 0.031(2) -0.006(2) -0.008(2) -0.014(2)

C3 0.030(2) 0.044(3) 0.029(2) -0.009(2) -0.0038(19) -0.012(2)
 C4 0.047(3) 0.042(3) 0.027(2) -0.010(2) -0.006(2) -0.018(2)
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 C6 0.064(4) 0.042(3) 0.040(3) -0.008(2) 0.001(3) -0.023(3)
 C7 0.043(3) 0.065(4) 0.066(4) -0.011(3) -0.005(3) -0.020(3)
 C8 0.046(3) 0.043(3) 0.034(3) -0.005(2) -0.013(2) -0.008(2)
 C9 0.097(6) 0.081(5) 0.037(3) 0.017(3) -0.022(4) -0.020(4)
 C10 0.040(3) 0.055(3) 0.034(3) -0.008(2) -0.008(2) -0.005(2)
 C11 0.085(5) 0.090(5) 0.034(3) -0.023(3) -0.002(3) 0.003(4)
 C12 0.054(3) 0.053(3) 0.034(3) -0.008(2) -0.012(2) -0.019(3)
 C13 0.059(4) 0.098(5) 0.065(4) -0.022(4) -0.031(3) -0.022(4)
 C14 0.064(4) 0.058(4) 0.055(4) -0.029(3) -0.010(3) -0.018(3)
 C15 0.127(7) 0.048(4) 0.110(6) -0.042(4) -0.043(6) 0.000(4)
 C16 0.069(8) 0.060(7) 0.063(8) -0.031(6) -0.028(6) -0.012(6)
 C16' 0.085(10) 0.052(7) 0.052(7) -0.004(6) -0.014(7) -0.033(7)
 C17 0.065(5) 0.160(9) 0.102(6) -0.090(7) -0.025(5) 0.034(5)
 C18 0.048(6) 0.070(8) 0.040(6) -0.018(5) -0.017(5) -0.015(6)
 C18' 0.021(5) 0.126(12) 0.065(8) -0.045(8) -0.003(5) -0.020(6)
 C19 0.124(7) 0.082(5) 0.047(4) 0.001(4) -0.027(4) 0.002(5)
 C20 0.049(7) 0.071(9) 0.062(8) -0.001(7) 0.008(6) -0.023(6)
 C20' 0.092(11) 0.049(7) 0.119(13) -0.029(8) -0.020(10) -0.031(7)
 C21 0.105(7) 0.105(7) 0.097(6) -0.054(6) 0.023(5) -0.005(5)
 C22 0.055(7) 0.053(7) 0.057(7) 0.005(6) -0.006(6) -0.024(6)
 C22' 0.057(8) 0.089(10) 0.078(10) -0.014(8) -0.021(7) -0.029(7)
 C23 0.120(8) 0.110(7) 0.075(6) 0.001(5) -0.043(6) 0.026(6)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 W1 S6 2.3407(14) . ?
 W1 S3 2.3616(14) . ?
 W1 S5 2.3642(13) . ?
 W1 S1 2.4475(15) . ?
 W1 S2 2.4626(15) . ?
 S1 C1 1.714(5) . ?
 S2 C1 1.716(5) . ?
 S3 C2 1.745(5) . ?
 S4 C3 1.745(5) . ?
 S5 C4 1.730(5) . ?
 S6 C5 1.755(5) . ?
 O1 C8 1.196(6) . ?
 O2 C8 1.326(6) . ?
 O2 C9 1.444(6) . ?
 O3 C10 1.181(7) . ?

O4 C10 1.325(6) . ?
O4 C11 1.450(7) . ?
O5 C12 1.196(7) . ?
O6 C12 1.308(7) . ?
O6 C13 1.460(7) . ?
O7 C14 1.185(7) . ?
O8 C14 1.323(8) . ?
O8 C15 1.453(5) . ?
N1 C1 1.331(6) . ?
N1 C6 1.458(7) . ?
N1 C7 1.464(7) . ?
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N2 C18' 1.472(3) 2_467 ?
N2 C16 1.492(3) 2_467 ?
N2 C16 1.492(3) . ?
N2 C16' 1.527(3) 2_467 ?
N2 C16' 1.527(3) . ?
N2 C18 1.547(3) 2_467 ?
N2 C18 1.547(3) . ?
N3 C22 1.481(3) 2_557 ?
N3 C22 1.481(3) . ?
N3 C20' 1.491(3) . ?
N3 C20' 1.491(3) 2_557 ?
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 C4 S5 W1 108.88(18) . . ?
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 C14 O8 C15 115.8(4) . . ?
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C18' N2 C18' C16' 178(34) 2_467 ... ?
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C16' N2 C18' C17 122.28(6) ... ?
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C16 C16' C18' N2 -42.16(13) 2_467 ... ?
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