SUPPORTING INFORMATION

Synthesis and structure of 1,6-dipivaloyl-3,4,7,8-tetramethyl-2,5-dithioglycoluril

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Supporting information:

Experimental protocol for preparation of compounds **4-7** with full spectral data;

crystal structure tables for compounds **6** and **7**

(20 pages)

Experimental:

Preparation of **4**, **5**, **6** and **7**: To 3,4,7,8-tetramethyl-2,5-dithioglycoluril (**3**) (400 mg, 1.72 mmol) in anhydrous THF (25 mL) was added potassium *tert*-butoxide (232 mg, 2.06 mmol) and the mixture was stirred for 30 min at 0 °C. Trimethylacetyl chloride (0.26 mL, 2.06 mmol) was added, and stirring was continued for 2 h. Solvent was removed, the residue was triturated with $CHCl_3$, and the mixture filtered through a short silica column. After concentration, the filtrate was purifed by planar chromatography in CH_2Cl_2 to afford: (1) 76.4 mg (0.192 mmol, 11%) of **6**; mp 155-158 °C; MS (NH_3-CI) *m/z* 399 (MH^+), 226, 142 (base); FT-IR (KBr disk) 2932, 1730, 1708, 1503 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500MHz) δ 3.22 (s, 6H), 1.61 (s, 3H), 1.54 (s, 3H), 1.36 (s, 18H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 185.38, 179.13, 89.02, 86.79, 44.93, 30.09, 28.83, 16.96, 15.81; (2) 112.5 mg (0.270 mmol, 16%) of **7**; mp 209-211 °C; MS (NH_3-CI) *m/z* 399 (MH^+), 226, 142 (base); FT-IR (KBr disk) 2970, 1705, 1639, 1532, 945 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500MHz) δ 3.25 (s, 3H), 3.16 (s, 3H), 1.60 (s, 3H), 1.58 (s, 3H), 1.36 (s, 9H), 1.17 (s, 9H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 190.89, 186.98, 177.93, 168.41, 86.61, 79.68, 44.43, 41.24, 31.43, 30.06, 28.11, 27.40, 20.90,15.78; (3) 119 mg (0.363 mmol, 22%) of **4**; mp 184-187 °C; MS (EI) *m/z* 314 (M^+, weak), 142, 57 (base); FT-IR (KBr disk) 3192, 2968, 1717, 1484, 1317 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.00 (br s, 1H), 3.21 (s, 3H), 3.16 (s, 3H), 1.56 (s, 3H), 1.50 (s, 3H), 1.40 (s, 9H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 187.49, 181.35, 178.06, 86.74, 83.32, 44.66, 30.31, 30.24, 28.23, 19.03, 15.68; and (4) 20.0 mg (0.064 mmol, 4%) of **5**; mp 227-230 °C; MS (NH_3-CI) *m/z* 315 (MH^+), 257, 175, 141 (base); FT-IR (KBr disk) 3162, 2959, 1632, 1527 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ 6.80 (br s, 1H), 3.23 (s, 3H), 3.21 (s, 3H), 1.63 (s, 3H), 1.57 (s, 3H), 1.17 (s, 9H); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 191.03, 180.85, 167.36, 88.04, 75.15, 41.23, 31.83, 30.70, 27.43, 22.82, 15.48.

Table 1. Crystal data and structure refinement for **6**.

Empirical formula	$C_{18}H_{30}N_4O_2S_2$
Formula weight	398.58
Temperature	299(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
a, α	24.130(3), 90º
b, β	14.2521(17), 126.367(2)º
c, γ	15.4884(17), 90º
Volume	4289.0(8) $Å^3$
Z, Calculated density	8, 1.235 Mg/m^3
Absorption coefficient	0.267 mm^{-1}
F(000)	1712
Crystal size	0.06 × 0.25 × 0.30 mm
Theta range for data collection	1.77 to 24.00º
Limiting indices	$-27\leq h\leq 27$, $-16\leq k\leq 16$, $-17\leq l\leq 17$
Reflections collected / unique	14696 / 3361 [R_{int} = 0.0743]
Completeness to θ = 24.00	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3361 / 0 / 236
Goodness-of-fit on F^2	0.988
Final R indices [$I>2\sigma(I)$]	R1 = 0.0445, wR2 = 0.0856
R indices (all data)	R1 = 0.1101, wR2 = 0.1019
Extinction coefficient	0.00115(16)
Largest diff. peak and hole	0.186 and -0.190 $e.Å^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **6**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
N(1)	-2497(1)	-9728(2)	-3678(2)	35(1)
C(2)	-2546(2)	-9305(2)	-4529(2)	39(1)
N(3)	-3097(1)	-8750(2)	-5031(2)	43(1)
N(4)	-4175(1)	-8959(2)	-5258(2)	49(1)
C(5)	-4296(2)	-9894(2)	-5381(2)	42(1)
N(6)	-3683(1)	-10348(2)	-4648(2)	37(1)
C(7)	-3159(2)	-9664(2)	-3836(2)	35(1)
C(8)	-3452(2)	-8748(2)	-4504(2)	42(1)
C(9)	-3364(2)	-8256(2)	-6029(2)	68(1)
C(10)	-4721(2)	-8257(3)	-5843(3)	76(1)
C(11)	-3292(2)	-7849(2)	-3875(3)	61(1)
C(12)	-3083(2)	-9679(2)	-2790(2)	47(1)
S(13)	-2021(1)	-9509(1)	-4871(1)	56(1)
S(14)	-5050(1)	-10398(1)	-6237(1)	66(1)
C(15)	-1958(2)	-10344(2)	-2911(2)	42(1)
O(16)	-2116(1)	-11120(2)	-2824(2)	69(1)
C(17)	-1220(2)	-9970(2)	-2109(2)	42(1)
C(18)	-3683(1)	-11355(2)	-4454(2)	42(1)
O(19)	-3631(1)	-11599(2)	-3666(2)	59(1)
C(20)	-3703(2)	-12048(2)	-5224(2)	45(1)
C(21)	-1123(2)	-8931(2)	-2195(3)	64(1)
C(22)	-732(2)	-10560(2)	-2213(3)	79(1)
C(23)	-1063(2)	-10152(2)	-1000(2)	69(1)
C(24)	-3674(2)	-11575(2)	-6086(2)	62(1)
C(25)	-3081(2)	-12697(2)	-4536(3)	65(1)
C(26)	-4360(2)	-12658(2)	-5755(3)	75(1)

Table 3. Bond lengths (Å) for **6**.

Bond lengths	
N(1)-C(2)	1.389(3)
N(1)-C(7)	1.468(3)
N(1)-C(15)	1.429(3)
C(2)-N(3)	1.331(3)
C(2)-S(13)	1.664(3)
N(3)-C(8)	1.492(3)
N(3)-C(9)	1.456(3)
N(4)-C(5)	1.354(4)
N(4)-C(8)	1.443(4)
N(4)-C(10)	1.464(4)
C(5)-N(6)	1.380(3)
C(5)-S(14)	1.650(3)
N(6)-C(7)	1.498(3)
N(6)-C(18)	1.467(4)
C(7)-C(8)	1.552(4)
C(7)-C(12)	1.519(3)
C(8)-C(11)	1.515(4)
C(15)-O(16)	1.202(3)
C(15)-C(17)	1.541(4)
C(17)-C(21)	1.518(4)
C(17)-C(22)	1.533(4)
C(17)-C(23)	1.545(4)
C(18)-O(19)	1.201(3)
C(18)-C(20)	1.527(4)
C(20)-C(24)	1.535(4)
C(20)-C(25)	1.532(4)
C(20)-C(26)	1.548(4)

Table 4. Bond angles (°) for **6**.

Angles	
N(1)-C(2)-S(13)	125.0(2)
N(1)-C(7)-N(6)	113.1(2)
N(1)-C(7)-C(8)	100.5(2)
N(1)-C(7)-C(12)	113.0(2)
N(1)-C(15)-C(17)	120.3(3)
C(2)-N(1)-C(7)	110.1(2)
C(2)-N(1)-C(15)	125.4(2)
C(2)-N(3)-C(8)	112.3(2)
C(2)-N(3)-C(9)	124.5(2)
N(3)-C(2)-N(1)	107.8(2)
N(3)-C(2)-S(13)	127.2(2)
N(3)-C(8)-C(7)	100.5(2)
N(3)-C(8)-C(11)	110.2(2)
N(4)-C(5)-N(6)	108.0(3)
N(4)-C(5)-S(14)	125.8(3)
N(4)-C(8)-N(3)	111.5(2)
N(4)-C(8)-C(7)	102.6(2)
N(4)-C(8)-C(11)	114.9(3)
C(5)-N(4)-C(8)	112.1(3)
C(5)-N(4)-C(10)	123.1(3)
C(5)-N(6)-C(7)	110.3(2)
C(5)-N(6)-C(18)	119.8(2)
N(6)-C(5)-S(14)	126.2(3)
N(6)-C(7)-C(8)	99.4(2)
N(6)-C(7)-C(12)	113.2(2)
N(6)-C(18)-C(20)	118.5(2)
C(8)-N(4)-C(10)	124.8(3)
C(9)-N(3)-C(8)	123.0(2)
C(11)-C(8)-C(7)	116.2(2)
C(12)-C(7)-C(8)	116.2(2)
C(15)-N(1)-C(7)	122.6(2)
C(15)-C(17)-C(23)	104.1(2)
O(16)-C(15)-N(1)	117.8(3)
O(16)-C(15)-C(17)	121.2(3)
C(18)-N(6)-C(7)	124.5(2)
C(18)-C(20)-C(26)	109.1(2)
O(19)-C(18)-N(6)	118.6(3)
O(19)-C(18)-C(20)	122.8(3)
C(21)-C(17)-C(15)	115.6(3)
C(21)-C(17)-C(22)	110.9(3)
C(21)-C(17)-C(23)	108.2(2)
C(22)-C(17)-C(15)	108.6(3)
C(22)-C(17)-C(23)	109.1(3)
C(24)-C(20)-C(18)	113.5(3)
C(24)-C(20)-C(25)	109.7(3)
C(24)-C(20)-C(26)	110.2(3)
C(25)-C(20)-C(18)	106.5(2)
C(25)-C(20)-C(26)	107.6(3)

Table 5. Torsion angles (º) for **6**.

Torsions	
N(1)-C(2)-N(3)-C(8)	1.8(3)
N(1)-C(2)-N(3)-C(9)	-173.6(3)
N(1)-C(7)-C(8)-N(3)	26.9(3)
N(1)-C(7)-C(8)-N(4)	141.9(2)
N(1)-C(7)-C(8)-C(11)	-91.9(3)
N(1)-C(15)-C(17)-C(21)	0.6(4)
N(1)-C(15)-C(17)-C(22)	-124.8(3)
N(1)-C(15)-C(17)-C(23)	119.1(3)
C(2)-N(1)-C(7)-N(6)	76.3(3)
C(2)-N(1)-C(7)-C(8)	-28.7(3)
C(2)-N(1)-C(7)-C(12)	-153.3(2)
C(2)-N(1)-C(15)-O(16)	-121.8(3)
C(2)-N(1)-C(15)-C(17)	67.5(4)
C(2)-N(3)-C(8)-N(4)	-127.1(3)
C(2)-N(3)-C(8)-C(7)	-19.0(3)
C(2)-N(3)-C(8)-C(11)	104.1(3)
N(4)-C(5)-N(6)-C(7)	13.1(3)
N(4)-C(5)-N(6)-C(18)	168.2(2)
C(5)-N(4)-C(8)-N(3)	85.4(3)
C(5)-N(4)-C(8)-C(7)	-21.4(3)
C(5)-N(4)-C(8)-C(11)	-148.4(2)
C(5)-N(6)-C(7)-N(1)	-130.5(2)
C(5)-N(6)-C(7)-C(8)	-24.7(3)
C(5)-N(6)-C(7)-C(12)	99.3(3)
C(5)-N(6)-C(18)-O(19)	-101.3(3)
C(5)-N(6)-C(18)-C(20)	82.7(3)
N(6)-C(7)-C(8)-N(3)	-88.9(2)
N(6)-C(7)-C(8)-N(4)	26.1(2)
N(6)-C(7)-C(8)-C(11)	152.3(2)
N(6)-C(18)-C(20)-C(24)	3.7(4)
N(6)-C(18)-C(20)-C(25)	124.6(3)
N(6)-C(18)-C(20)-C(26)	-119.5(3)
C(7)-N(1)-C(2)-N(3)	18.1(3)
C(7)-N(1)-C(2)-S(13)	-159.3(2)
C(7)-N(1)-C(15)-O(16)	41.1(4)
C(7)-N(1)-C(15)-C(17)	-129.6(3)
C(7)-N(6)-C(18)-O(19)	50.0(4)
C(7)-N(6)-C(18)-C(20)	-126.0(3)
C(8)-N(4)-C(5)-N(6)	6.0(3)
C(8)-N(4)-C(5)-S(14)	-175.31(19)
C(9)-N(3)-C(8)-N(4)	48.3(4)
C(9)-N(3)-C(8)-C(7)	156.4(3)
C(9)-N(3)-C(8)-C(11)	-80.5(3)
C(10)-N(4)-C(5)-N(6)	-174.7(2)
C(10)-N(4)-C(5)-S(14)	4.0(4)
C(10)-N(4)-C(8)-N(3)	-93.9(3)

C(10)-N(4)-C(8)-C(7)	159.4(2)
C(10)-N(4)-C(8)-C(11)	32.3(4)
C(12)-C(7)-C(8)-N(3)	149.3(2)
C(12)-C(7)-C(8)-N(4)	-95.7(3)
C(12)-C(7)-C(8)-C(11)	30.5(4)
S(13)-C(2)-N(3)-C(8)	179.1(2)
S(13)-C(2)-N(3)-C(9)	3.8(5)
S(14)-C(5)-N(6)-C(7)	-165.53(19)
S(14)-C(5)-N(6)-C(18)	-10.5(3)
C(15)-N(1)-C(2)-N(3)	-177.1(3)
C(15)-N(1)-C(2)-S(13)	5.4(4)
C(15)-N(1)-C(7)-N(6)	-88.9(3)
C(15)-N(1)-C(7)-C(8)	166.0(2)
C(15)-N(1)-C(7)-C(12)	41.4(3)
O(16)-C(15)-C(17)-C(21)	-169.8(3)
O(16)-C(15)-C(17)-C(22)	64.8(4)
O(16)-C(15)-C(17)-C(23)	-51.3(4)
C(18)-N(6)-C(7)-N(1)	75.9(3)
C(18)-N(6)-C(7)-C(8)	-178.3(2)
C(18)-N(6)-C(7)-C(12)	-54.4(3)
O(19)-C(18)-C(20)-C(24)	-172.2(3)
O(19)-C(18)-C(20)-C(25)	-51.3(4)
O(19)-C(18)-C(20)-C(26)	64.6(4)

Table 6. Anisotropic displacement parameters ($Å^2 x \times 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	30(2)	38(2)	35(1)	6(1)	19(1)	1(1)
C(2)	40(2)	37(2)	38(2)	-2(2)	21(2)	-5(2)
N(3)	46(2)	42(2)	41(2)	12(1)	26(2)	8(1)
N(4)	40(2)	54(2)	45(2)	7(2)	21(2)	12(2)
C(5)	32(2)	59(2)	32(2)	-2(2)	18(2)	3(2)
N(6)	31(2)	40(2)	32(1)	-1(1)	15(1)	-2(1)
C(7)	30(2)	38(2)	32(2)	0(2)	16(2)	0(2)
C(8)	41(2)	43(2)	41(2)	-1(2)	24(2)	5(2)
C(9)	75(3)	74(3)	56(2)	28(2)	40(2)	17(2)
C(10)	55(3)	83(3)	77(3)	22(2)	32(2)	33(2)
C(11)	73(3)	44(2)	68(2)	-6(2)	43(2)	6(2)
C(12)	42(2)	62(2)	37(2)	-3(2)	23(2)	-5(2)
S(13)	57(1)	70(1)	53(1)	-3(1)	40(1)	1(1)
S(14)	32(1)	100(1)	50(1)	-20(1)	15(1)	-4(1)
C(15)	41(2)	39(2)	41(2)	2(2)	22(2)	2(2)
O(16)	50(2)	42(2)	77(2)	15(1)	16(1)	-7(1)
C(17)	32(2)	43(2)	45(2)	-1(2)	19(2)	-1(2)
C(18)	29(2)	50(2)	41(2)	-2(2)	17(2)	-7(2)
O(19)	74(2)	59(2)	51(1)	1(1)	42(1)	-14(1)
C(20)	45(2)	44(2)	44(2)	-6(2)	26(2)	-6(2)
C(21)	54(3)	61(3)	64(2)	-11(2)	28(2)	-20(2)
C(22)	45(3)	94(3)	82(3)	-5(2)	29(2)	19(2)
C(23)	51(2)	87(3)	50(2)	5(2)	19(2)	-9(2)
C(24)	77(3)	64(3)	58(2)	-9(2)	46(2)	2(2)
C(25)	63(3)	51(3)	77(3)	0(2)	39(2)	6(2)
C(26)	68(3)	68(3)	84(3)	-30(2)	43(2)	-26(2)

Table 7. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **6**.

	x	*Y*	*z*	U_{eq}
H(9A)	-3058	-8348	-6227	102
H(9B)	-3397	-7598	-5933	102
H(9C)	-3811	-8496	-6584	102
H(10A)	-5158	-8567	-6298	114
H(10B)	-4640	-7880	-6272	114
H(10C)	-4723	-7864	-5341	114
H(11A)	-3495	-7328	-4361	92
H(11B)	-2803	-7765	-3391	92
H(11C)	-3479	-7885	-3474	92
H(12A)	-2901	-10275	-2443	71
H(12B)	-3525	-9584	-2935	71
H(12C)	-2776	-9188	-2329	71
H(21A)	-1217	-8803	-2879	96
H(21B)	-657	-8756	-1634	96
H(21C)	-1432	-8576	-2124	96
H(22A)	-828	-10451	-2902	118
H(22B)	-797	-11213	-2144	118
H(22C)	-265	-10386	-1659	118
H(23A)	-607	-9936	-448	103
H(23B)	-1095	-10812	-913	103
H(23C)	-1390	-9820	-951	103
H(24A)	-3263	-11203	-5748	93
H(24B)	-4070	-11179	-6524	93
H(24C)	-3671	-12047	-6526	93
H(25A)	-2665	-12337	-4203	98
H(25B)	-3089	-13173	-4982	98
H(25C)	-3099	-12986	-3994	98
H(26A)	-4375	-13095	-6241	112
H(26B)	-4759	-12262	-6142	112
H(26C)	-4352	-12996	-5211	112

Table 8. Conformation and puckering parameters for **6**. See ref. 9 for a discussion of parameter definitions.

	η	Ξ	τ	Q	ϕ	Conformation
Ring	30.5	104.3				
A			-125.7	0.289	140.32	Close to pure envelope (144°) with apex at C7.
B			-113.7	0.271	132.98	Closer to twist (126°) with improper C2-axis through C5.

Table 9. Crystal data and structure refinement for **7**.

Empirical formula	$C_{18}H_{30}N_4O_2S_2$
Formula weight	398.58
Temperature	299(2) K
Wavelength	0.71073 Å
Crystal system, space group	P2(1)/n
Unit cell dimensions	a = 11.8072(17) Å α = 90º
	b = 13.6435(17) Å β = 98.089(4)º
	c = 27.751(4) Å γ = 90º
Volume	4426.1(10) $Å^3$
Z, Calculated density	8, 1.196 Mg/m^3
Absorption coefficient	0.259 mm^{-1}
F(000)	1712
Crystal size	0.25 x 0.11 x 0.09 mm
Theta range for data collection	1.48 to 23.31º
Limiting indices	$-12\leq h\leq 13$, $-15\leq k\leq 14$, $-30\leq l\leq 28$
Reflections collected / unique	28016 / 6332 [R(int) = 0.1561]
Completeness to theta = 23.31	99.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6332 / 0 / 510
Goodness-of-fit on F^2	0.968
Final R indices [$I>2\sigma(I)$]	R1 = 0.0919, wR2 = 0.2177
R indices (all data)	R1 = 0.2122, wR2 = 0.2748
Extinction coefficient	0.0002(3)
Largest diff. peak and hole	0.606 and -0.427 $e.A^{-3}$

Table 10. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **7**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor. There are two almost identical molecules per unit cell, referred to as **7** and **7'**.

	x	*y*	*z*	U_{eq}
7				
N(1)	2873(5)	7226(4)	1549(2)	44(2)
C(2)	3498(7)	8115(5)	1603(3)	50(2)
N(3)	3231(6)	8535(4)	2007(3)	54(2)
N(4)	2683(6)	7875(4)	2755(3)	49(2)
C(5)	3369(7)	7104(5)	2906(3)	39(2)
N(6)	3712(6)	6944(6)	3360(4)	62(3)
C(7)	2477(7)	6957(5)	2007(3)	44(2)
C(8)	2381(7)	7986(5)	2244(3)	43(2)
C(9)	3659(8)	9501(5)	2182(3)	67(3)
C(10)	2304(8)	8552(6)	3124(3)	71(3)
C(11)	1193(7)	8439(5)	2111(3)	65(3)
C(12)	1399(7)	6351(5)	1930(3)	53(3)
S(13)	4406(2)	8500(2)	1251(1)	70(1)
S(14)	3632(2)	6353(1)	2421(1)	45(1)
C(15)	3124(8)	6462(7)	1225(3)	53(2)
O(16)	3554(5)	5720(4)	1404(2)	70(2)
C(17)	2685(8)	6544(7)	686(4)	62(3)
C(18)	4445(8)	6167(7)	3497(4)	57(2)
O(19)	4999(6)	5767(5)	3214(2)	82(2)
C(20)	4521(9)	5867(6)	4026(4)	69(3)
C(21)	3685(9)	6391(8)	397(4)	92(4)
C(22)	2028(10)	7495(7)	528(4)	101(4)
C(23)	1872(9)	5640(8)	584(4)	95(4)
C(24)	5417(12)	5063(9)	4153(4)	120(5)
C(25)	3367(11)	5476(10)	4113(5)	148(7)
C(26)	4846(12)	6755(8)	4350(4)	129(6)
7'				
N(1')	7842(6)	5740(4)	1516(2)	50(2)
C(2')	8450(7)	4846(5)	1544(3)	48(2)
N(3')	8195(5)	4400(4)	1946(3)	49(2)
N(4')	7657(6)	4967(4)	2701(3)	53(2)
C(5')	8336(8)	5736(6)	2875(3)	47(2)
N(6')	8680(7)	5844(7)	3331(4)	70(3)
C(7')	7479(6)	5962(5)	1981(3)	41(2)
C(8')	7326(7)	4913(5)	2181(3)	40(2)
C(9')	8603(8)	3397(5)	2093(4)	72(3)
C(10')	7240(8)	4281(5)	3055(3)	70(3)
C(11')	6166(7)	4499(5)	2042(3)	62(3)
C(12')	6417(6)	6602(5)	1926(3)	54(3)
S(13')	9326(2)	4479(2)	1172(1)	74(1)
S(14')	8639(2)	6523(1)	2412(1)	47(1)
C(15')	8172(7)	6564(6)	1215(4)	50(2)
O(16')	8645(6)	7244(4)	1426(2)	76(2)
C(17')	7697(9)	6597(7)	678(4)	68(3)
C(18')	9414(9)	6601(6)	3493(4)	64(3)
O(19')	9981(6)	7024(5)	3226(3)	90(2)
C(20')	9490(10)	6851(8)	4027(4)	77(3)

C(21')	6914(8)	5713(7)	512(4)	84(3)
C(22')	8639(9)	6655(8)	372(4)	98(4)
C(23')	6972(9)	7540(7)	612(4)	92(4)
C(24')	10315(13)	7700(11)	4165(4)	156(8)
C(25')	8313(12)	7256(11)	4083(5)	153(7)
C(26')	9709(17)	5977(10)	4340(4)	186(11)

Table 11. Selected bond lengths (Å) for **7** and **7'**.

Bond	
7	
N(1)-C(2)	1.417(9)
N(1)-C(7)	1.462(9)
N(1)-C(15)	1.434(9)
C(2)-N(3)	1.335(10)
C(2)-S(13)	1.635(8)
N(3)-C(8)	1.479(9)
N(3)-C(9)	1.470(9)
N(4)-C(5)	1.357(9)
N(4)-C(8)	1.422(10)
N(4)-C(10)	1.492(9)
C(5)-N(6)	1.286(10)
C(5)-S(14)	1.753(8)
N(6)-C(18)	1.387(12)
C(7)-C(8)	1.560(10)
C(7)-C(12)	1.508(10)
C(7)-S(14)	1.848(8)
C(8)-C(11)	1.531(10)
C(15)-O(16)	1.208(10)
C(15)-C(17)	1.517(12)
C(17)-C(21)	1.531(12)
C(17)-C(22)	1.544(12)
C(17)-C(23)	1.564(12)
C(18)-O(19)	1.219(10)
C(18)-C(20)	1.515(12)
C(20)-C(24)	1.530(13)
C(20)-C(25)	1.513(14)
C(20)-C(26)	1.524(12)
7'	
N(1')-C(2')	1.412(9)
N(1')-C(7')	1.450(9)
N(1')-C(15')	1.484(10)
C(2')-N(3')	1.341(9)
C(2')-S(13')	1.640(8)
N(3')-C(8')	1.469(8)
N(3')-C(9')	1.488(9)
N(4')-C(5')	1.367(10)
N(4')-C(8')	1.443(9)
N(4')-C(10')	1.490(9)
C(5')-N(6')	1.282(11)
C(5')-S(14')	1.749(8)
N(6')-C(18')	1.381(13)
C(7')-C(8')	1.553(9)
C(7')-C(12')	1.518(10)
C(7')-S(14')	1.852(8)
C(8')-C(11')	1.482(10)
C(15')-O(16')	1.193(9)
C(15')-C(17')	1.518(12)
C(17')-C(21')	1.550(12)
C(17')-C(22')	1.492(12)
C(17')-C(23')	1.542(12)

C(18')-O(19')	1.214(10)
C(18')-C(20')	1.510(13)
C(20')-C(24')	1.527(15)
C(20')-C(25')	1.524(14)
C(20')-C(26')	1.477(14)

Table 12. Selected valence angles (°) for **7** and **7'**.

Angle	
7	
N(1)-C(2)-S(13)	125.9(7)
N(1)-C(7)-C(8)	101.0(6)
N(1)-C(7)-C(12)	112.4(7)
N(1)-C(7)-S(14)	110.8(5)
N(1)-C(15)-C(17)	119.5(8)
C(2)-N(1)-C(7)	110.3(6)
C(2)-N(1)-C(15)	122.6(7)
C(2)-N(3)-C(8)	114.2(6)
C(2)-N(3)-C(9)	123.5(7)
N(3)-C(2)-N(1)	106.0(7)
N(3)-C(2)-S(13)	128.0(6)
N(3)-C(8)-C(7)	100.1(6)
N(3)-C(8)-C(11)	110.2(6)
N(4)-C(5)-S(14)	112.3(7)
N(4)-C(8)-N(3)	114.0(7)
N(4)-C(8)-C(7)	107.6(6)
N(4)-C(8)-C(11)	112.1(7)
C(5)-N(4)-C(8)	116.4(6)
C(5)-N(4)-C(10)	119.5(8)
C(5)-N(6)-C(18)	119.9(9)
C(5)-S(14)-C(7)	91.2(4)
N(6)-C(5)-N(4)	121.7(8)
N(6)-C(5)-S(14)	125.9(6)
N(6)-C(18)-C(20)	115.0(9)
C(8)-N(4)-C(10)	124.1(6)
C(8)-C(7)-S(14)	103.3(6)
C(9)-N(3)-C(8)	122.0(7)
C(11)-C(8)-C(7)	112.4(7)
C(12)-C(7)-C(8)	116.3(6)
C(12)-C(7)-S(14)	112.2(5)
C(15)-N(1)-C(7)	118.8(6)
C(15)-C(17)-C(21)	109.0(8)
C(15)-C(17)-C(22)	115.4(8)
C(15)-C(17)-C(23)	103.6(7)
O(16)-C(15)-N(1)	117.6(8)
O(16)-C(15)-C(17)	122.2(8)
C(18)-C(20)-C(24)	111.2(9)
C(18)-C(20)-C(26)	109.4(8)
O(19)-C(18)-N(6)	122.4(9)
O(19)-C(18)-C(20)	122.6(9)
C(21)-C(17)-C(22)	111.1(9)
C(21)-C(17)-C(23)	107.3(8)

C(22)-C(17)-C(23)	109.9(8)
C(25)-C(20)-C(18)	108.5(9)
C(25)-C(20)-C(24)	108.6(10)
C(25)-C(20)-C(26)	110.2(10)
C(26)-C(20)-C(24)	109.0(10)
7'	
N(1')-C(2')-S(13')	126.1(7)
N(1')-C(7')-C(8')	101.0(5)
N(1')-C(7')-C(12')	111.9(7)
N(1')-C(7')-S(14')	112.1(5)
N(1')-C(15')-C(17')	119.0(8)
C(2')-N(1')-C(7')	109.9(6)
C(2')-N(1')-C(15')	121.0(6)
C(2')-N(3')-C(8')	113.9(6)
C(2')-N(3')-C(9')	123.0(6)
N(3')-C(2')-N(1')	105.5(7)
N(3')-C(2')-S(13')	128.3(6)
N(3')-C(8')-C(7')	99.0(5)
N(3')-C(8')-C(11')	112.4(7)
N(4')-C(5')-S(14')	112.5(7)
N(4')-C(8')-N(3')	111.2(6)
N(4')-C(8')-C(7')	106.3(6)
N(4')-C(8')-C(11')	112.9(7)
C(5')-N(4')-C(8')	117.0(6)
C(5')-N(4')-C(10')	118.7(8)
C(5')-N(6')-C(18')	120.2(11)
C(5')-S(14')-C(7')	90.6(4)
N(6')-C(5')-N(4')	121.7(9)
N(6')-C(5')-S(14')	125.9(8)
N(6')-C(18')-C(20')	115.9(10)
C(7')-N(1')-C(15')	118.5(6)
C(8')-N(3')-C(9')	122.4(6)
C(8')-N(4')-C(10')	124.1(7)
C(8')-C(7')-S(14')	105.3(6)
C(11')-C(8')-C(7')	114.1(7)
C(12')-C(7')-C(8')	115.5(6)
C(12')-C(7')-S(14')	110.6(5)
C(15')-C(17')-C(21')	113.0(8)
C(15')-C(17')-C(23')	105.3(8)
O(16')-C(15')-N(1')	117.0(8)
O(16')-C(15')-C(17')	122.9(8)
C(18')-C(20')-C(24')	111.5(9)
C(18')-C(20')-C(25')	104.6(9)
O(19')-C(18')-N(6')	122.2(10)
O(19')-C(18')-C(20')	122.0(9)
C(22')-C(17')-C(15')	111.0(8)
C(22')-C(17')-C(21')	109.5(9)
C(22')-C(17')-C(23')	109.5(9)
C(23')-C(17')-C(21')	108.4(8)
C(24')-C(20')-C(25')	104.9(10)
C(26')-C(20')-C(18')	112.1(9)
C(26')-C(20')-C(24')	114.3(12)
C(26')-C(20')-C(25')	108.6(12)

Table 13. Torsion angles (º) for **7** and **7'**.

Torsion Angles	
7	
N(1)-C(2)-N(3)-C(8)	-2.0(9)
N(1)-C(2)-N(3)-C(9)	-176.9(7)
N(1)-C(7)-C(8)-N(3)	-26.2(8)
N(1)-C(7)-C(8)-N(4)	-145.5(6)
N(1)-C(7)-C(8)-C(11)	90.6(8)
N(1)-C(7)-S(14)-C(5)	132.1(5)
N(1)-C(15)-C(17)-C(21)	128.2(8)
N(1)-C(15)-C(17)-C(22)	2.4(12)
N(1)-C(15)-C(17)-C(23)	-117.8(8)
C(2)-N(1)-C(7)-C(8)	27.9(8)
C(2)-N(1)-C(7)-C(12)	152.5(6)
C(2)-N(1)-C(7)-S(14)	-81.0(6)
C(2)-N(1)-C(15)-O(16)	108.8(9)
C(2)-N(1)-C(15)-C(17)	-80.4(10)
C(2)-N(3)-C(8)-N(4)	133.1(7)
C(2)-N(3)-C(8)-C(7)	18.6(9)
C(2)-N(3)-C(8)-C(11)	-99.9(8)
N(4)-C(5)-N(6)-C(18)	-177.7(7)
N(4)-C(5)-S(14)-C(7)	-13.1(6)
C(5)-N(4)-C(8)-N(3)	-85.5(7)
C(5)-N(4)-C(8)-C(7)	24.4(9)
C(5)-N(4)-C(8)-C(11)	148.4(6)
C(5)-N(6)-C(18)-O(19)	18.0(13)
C(5)-N(6)-C(18)-C(20)	-163.1(8)
N(6)-C(5)-S(14)-C(7)	163.2(7)
N(6)-C(18)-C(20)-C(24)	-175.5(8)
N(6)-C(18)-C(20)-C(25)	65.1(11)
N(6)-C(18)-C(20)-C(26)	-55.1(12)
C(7)-N(1)-C(2)-N(3)	-17.4(8)
C(7)-N(1)-C(2)-S(13)	159.9(6)
C(7)-N(1)-C(15)-O(16)	-36.4(11)
C(7)-N(1)-C(15)-C(17)	134.4(8)
C(8)-N(4)-C(5)-N(6)	178.7(7)
C(8)-N(4)-C(5)-S(14)	-4.8(8)
C(8)-C(7)-S(14)-C(5)	24.6(5)
C(9)-N(3)-C(8)-N(4)	-52.0(9)
C(9)-N(3)-C(8)-C(7)	-166.5(7)
C(9)-N(3)-C(8)-C(11)	75.0(10)
C(10)-N(4)-C(5)-N(6)	-0.7(11)
C(10)-N(4)-C(5)-S(14)	175.8(6)
C(10)-N(4)-C(8)-N(3)	93.8(8)
C(10)-N(4)-C(8)-C(7)	-156.2(7)
C(10)-N(4)-C(8)-C(11)	-32.2(10)
C(12)-C(7)-C(8)-N(3)	-148.1(7)
C(12)-C(7)-C(8)-N(4)	92.5(8)
C(12)-C(7)-C(8)-C(11)	-31.3(10)
C(12)-C(7)-S(14)-C(5)	-101.4(6)
S(13)-C(2)-N(3)-C(8)	-179.3(6)
S(13)-C(2)-N(3)-C(9)	5.8(12)

S(14)-C(5)-N(6)-C(18)	6.3(11)
S(14)-C(7)-C(8)-N(3)	88.5(6)
S(14)-C(7)-C(8)-N(4)	-30.9(7)
S(14)-C(7)-C(8)-C(11)	-154.7(6)
C(15)-N(1)-C(2)-N(3)	-165.2(8)
C(15)-N(1)-C(2)-S(13)	12.1(11)
C(15)-N(1)-C(7)-C(8)	177.1(7)
C(15)-N(1)-C(7)-C(12)	-58.3(9)
C(15)-N(1)-C(7)-S(14)	68.1(8)
O(16)-C(15)-C(17)-C(21)	-61.4(11)
O(16)-C(15)-C(17)-C(22)	172.7(9)
O(16)-C(15)-C(17)-C(23)	52.5(11)
O(19)-C(18)-C(20)-C(24)	3.5(13)
O(19)-C(18)-C(20)-C(25)	-115.9(11)
O(19)-C(18)-C(20)-C(26)	123.9(11)
7'	
N(1')-C(2')-N(3')-C(8')	5.6(9)
N(1')-C(2')-N(3')-C(9')	175.8(7)
N(1')-C(7')-C(8')-N(3')	30.2(7)
N(1')-C(7')-C(8')-N(4')	145.5(6)
N(1')-C(7')-C(8')-C(11')	-89.3(8)
N(1')-C(7')-S(14')-C(5')	-133.7(5)
N(1')-C(15')-C(17')-C(21')	-0.9(11)
N(1')-C(15')-C(17')-C(22')	-124.4(9)
N(1')-C(15')-C(17')-C(23')	117.2(8)
C(2')-N(1')-C(7')-C(8')	-30.3(8)
C(2')-N(1')-C(7')-C(12')	-153.7(6)
C(2')-N(1')-C(7')-S(14')	81.3(6)
C(2')-N(1')-C(15')-O(16')	-106.0(9)
C(2')-N(1')-C(15')-C(17')	85.9(9)
C(2')-N(3')-C(8')-N(4')	-134.9(7)
C(2')-N(3')-C(8')-C(7')	-23.3(9)
C(2')-N(3')-C(8')-C(11')	97.5(8)
N(4')-C(5')-N(6')-C(18')	176.6(7)
N(4')-C(5')-S(14')-C(7')	14.8(6)
C(5')-N(4')-C(8')-N(3')	86.3(7)
C(5')-N(4')-C(8')-C(7')	-20.5(9)
C(5')-N(4')-C(8')-C(11')	-146.3(7)
C(5')-N(6')-C(18')-O(19')	-19.1(14)
C(5')-N(6')-C(18')-C(20')	162.5(8)
N(6')-C(5')-S(14')-C(7')	-164.4(8)
N(6')-C(18')-C(20')-C(24')	-179.5(10)
N(6')-C(18')-C(20')-C(25')	-66.6(12)
N(6')-C(18')-C(20')-C(26')	50.9(14)
C(7')-N(1')-C(2')-N(3')	16.8(8)
C(7')-N(1')-C(2')-S(13')	-160.6(6)
C(7')-N(1')-C(15')-O(16')	35.2(10)
C(7')-N(1')-C(15')-C(17')	-133.0(8)
C(8')-N(4')-C(5')-N(6')	-179.6(7)
C(8')-N(4')-C(5')-S(14')	1.2(8)
C(8')-C(7')-S(14')-C(5')	-24.8(5)
C(9')-N(3')-C(8')-N(4')	54.9(9)
C(9')-N(3')-C(8')-C(7')	166.4(7)

C(9')-N(3')-C(8')-C(11')	-72.7(10)
C(10')-N(4')-C(5')-N(6')	4.5(11)
C(10')-N(4')-C(5')-S(14')	-174.7(5)
C(10')-N(4')-C(8')-N(3')	-98.0(8)
C(10')-N(4')-C(8')-C(7')	155.2(7)
C(10')-N(4')-C(8')-C(11')	29.3(9)
C(12')-C(7')-C(8')-N(3')	151.1(7)
C(12')-C(7')-C(8')-N(4')	-93.6(8)
C(12')-C(7')-C(8')-C(11')	31.6(10)
C(12')-C(7')-S(14')-C(5')	100.6(6)
S(13')-C(2')-N(3')-C(8')	-177.0(6)
S(13')-C(2')-N(3')-C(9')	-6.9(12)
S(14')-C(5')-N(6')-C(18')	-4.3(12)
S(14')-C(7')-C(8')-N(3')	-86.6(6)
S(14')-C(7')-C(8')-N(4')	28.7(7)
S(14')-C(7')-C(8')-C(11')	153.9(6)
C(15')-N(1')-C(2')-N(3')	160.9(7)
C(15')-N(1')-C(2')-S(13')	-16.5(11)
C(15')-N(1')-C(7')-C(8')	-175.4(7)
C(15')-N(1')-C(7')-C(12')	61.2(9)
C(15')-N(1')-C(7')-S(14')	-63.8(8)
O(16')-C(15')-C(17')-C(21')	-168.3(8)
O(16')-C(15')-C(17')-C(22')	68.2(11)
O(16')-C(15')-C(17')-C(23')	-50.2(11)
O(19')-C(18')-C(20')-C(24')	2.0(15)
O(19')-C(18')-C(20')-C(25')	115.0(12)
O(19')-C(18')-C(20')-C(26')	-127.6(13)

Table 14. Anisotropic displacement parameters (Å^2 x 10^3) for **7** and **7'**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
7						
N(1)	51(5)	28(4)	51(5)	-3(3)	2(4)	-1(3)
C(2)	52(6)	24(4)	74(7)	5(4)	5(5)	-3(4)
N(3)	66(5)	21(4)	79(6)	-3(4)	19(4)	1(3)
N(4)	58(5)	23(4)	68(6)	1(4)	14(4)	16(3)
C(5)	34(5)	25(4)	59(7)	-10(4)	8(5)	-3(4)
N(6)	77(6)	47(5)	63(7)	-9(5)	20(5)	3(4)
C(7)	57(6)	24(4)	52(6)	-1(4)	15(5)	7(4)
C(8)	38(6)	25(4)	68(7)	7(4)	11(5)	9(4)
C(9)	88(7)	20(4)	93(8)	-3(4)	16(6)	-2(4)
C(10)	92(8)	41(5)	84(8)	-13(5)	27(6)	7(5)
C(11)	69(7)	31(5)	99(8)	-2(5)	26(6)	-2(4)
C(12)	44(6)	29(4)	85(7)	7(4)	9(5)	-5(4)
S(13)	74(2)	42(1)	99(2)	12(1)	31(2)	-7(1)
S(14)	47(1)	23(1)	64(2)	-2(1)	6(1)	6(1)
C(15)	55(6)	50(6)	55(7)	-18(5)	10(5)	-14(5)
O(16)	93(5)	37(4)	79(5)	-9(3)	5(4)	17(3)
C(17)	52(7)	67(7)	68(8)	-2(5)	6(6)	2(5)
C(18)	67(7)	47(6)	55(8)	-4(5)	-3(6)	-1(5)
O(19)	104(6)	72(5)	72(5)	2(4)	12(4)	40(4)

C(20)	86(8)	48(6)	70(8)	-5(5)	0(6)	-4(5)
C(21)	97(9)	102(9)	79(9)	-2(6)	15(7)	-6(7)
C(22)	132(11)	77(8)	81(9)	9(6)	-30(7)	23(7)
C(23)	99(9)	93(8)	88(9)	-14(7)	-1(7)	-29(7)
C(24)	171(14)	96(9)	86(9)	13(7)	-6(9)	42(9)
C(25)	142(14)	159(14)	147(14)	40(10)	32(11)	-52(11)
C(26)	219(17)	88(9)	72(9)	-16(7)	-9(9)	-31(9)
7'						
N(1')	63(5)	22(4)	67(5)	-3(3)	14(4)	0(3)
C(2')	58(6)	25(4)	62(6)	-7(4)	8(5)	-1(4)
N(3')	55(5)	19(3)	73(5)	-6(3)	16(4)	9(3)
N(4')	71(5)	20(4)	71(6)	-1(4)	24(5)	0(3)
C(5')	65(6)	33(5)	41(6)	1(5)	0(5)	11(4)
N(6')	89(7)	45(5)	76(8)	3(5)	9(5)	9(5)
C(7')	44(5)	19(4)	59(6)	-8(4)	9(5)	-4(3)
C(8')	45(6)	15(4)	63(7)	7(4)	21(5)	5(4)
C(9')	83(8)	21(5)	113(9)	4(5)	17(6)	11(4)
C(10')	95(8)	24(5)	93(8)	13(5)	22(6)	4(5)
C(11')	59(6)	28(5)	99(8)	-6(5)	15(5)	-19(4)
C(12')	44(6)	22(4)	90(7)	-2(4)	-8(5)	0(4)
S(13')	76(2)	47(1)	104(2)	-11(1)	33(2)	4(1)
S(14')	48(2)	25(1)	67(2)	-4(1)	6(1)	-7(1)
C(15')	39(6)	37(5)	76(8)	10(5)	10(5)	7(4)
O(16')	96(5)	35(4)	91(5)	7(3)	-8(4)	-21(3)
C(17')	69(8)	72(7)	62(8)	5(5)	2(6)	8(5)
C(18')	69(8)	36(6)	84(9)	-7(5)	4(6)	-4(5)
O(19')	90(6)	87(5)	92(6)	-18(4)	5(5)	-32(4)
C(20')	78(8)	83(8)	68(8)	-15(7)	6(6)	-3(6)
C(21')	72(7)	78(7)	98(9)	-19(6)	-5(6)	-8(6)
C(22')	94(9)	117(10)	88(9)	2(7)	31(8)	0(7)
C(23')	103(9)	70(7)	96(9)	11(6)	-10(7)	26(6)
C(24')	216(19)	165(15)	75(10)	-36(9)	-25(10)	-44(13)
C(25')	134(14)	182(16)	145(14)	-89(12)	26(10)	-3(11)
C(26')	370(30)	115(12)	60(9)	15(8)	-10(12)	37(14)