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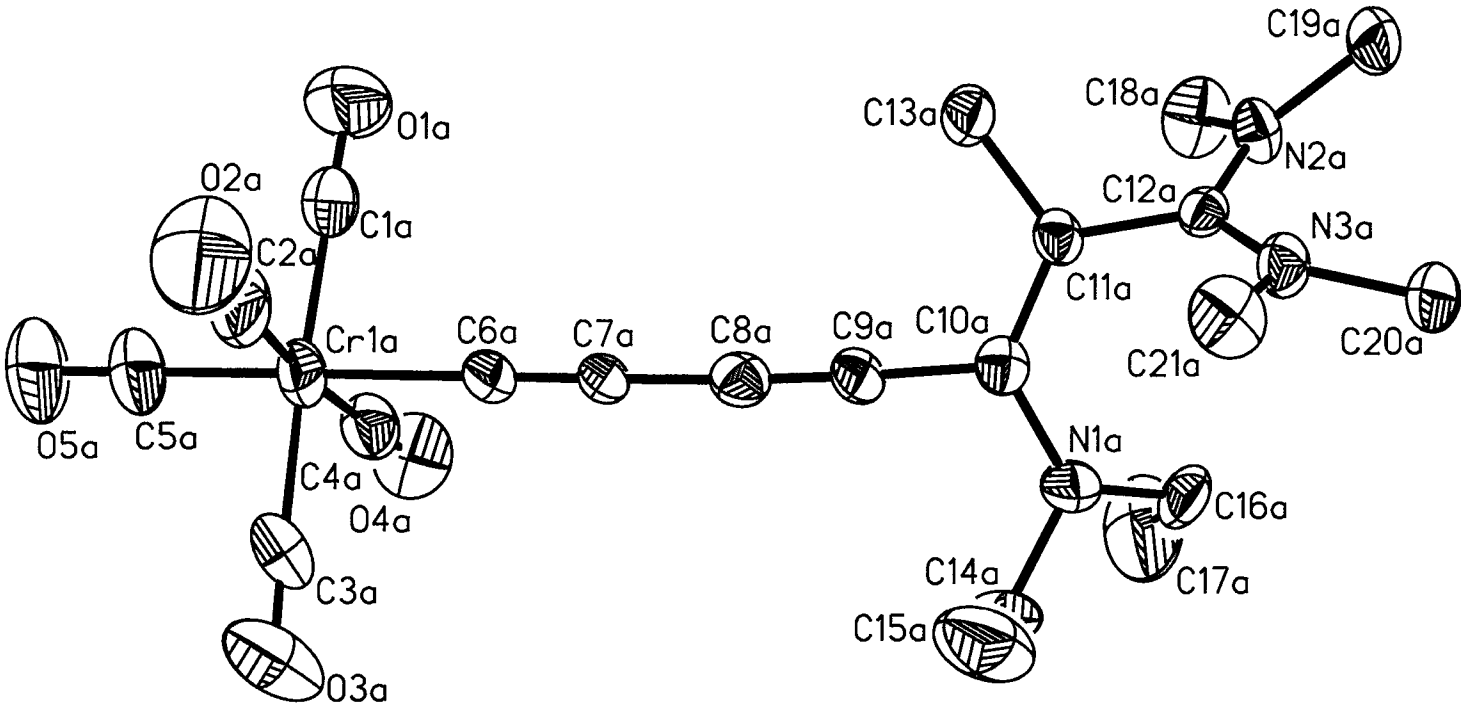
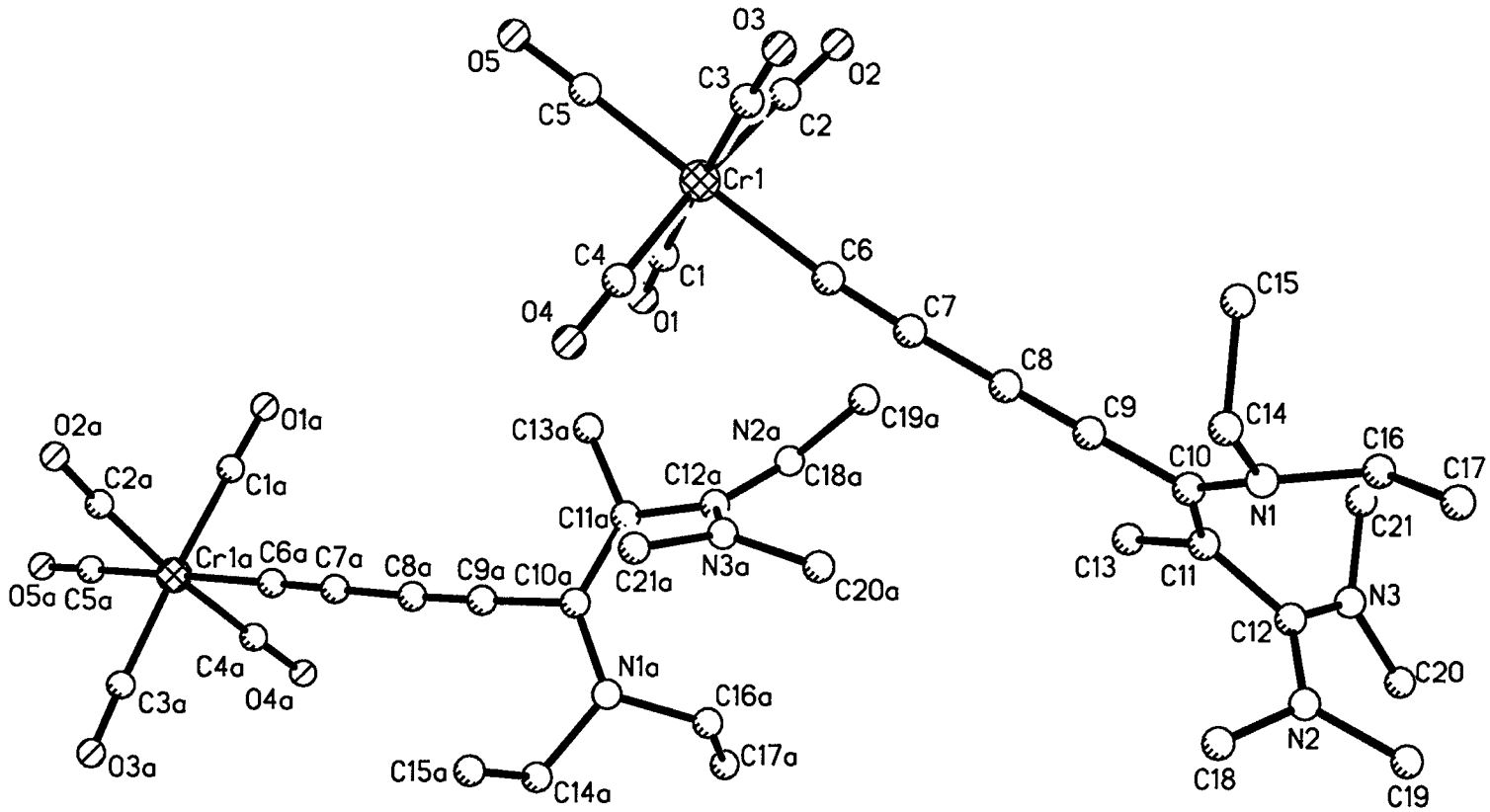


Compound **5a** (molecule 2)



Arrangement of the two independent molecules of **5a** in the unit cell

Crystal Data

Name of Structure	Compound 5a
Empirical Formula	$C_{21}\ H_{25}\ Cr\ N_3\ O_5$
Color; Habit	orange prism
Crystal Size (mm)	0.3 x 0.3 x 0.3
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 15.940(2) Å
	$\underline{b}$ = 9.4320(10) Å
	$\underline{c}$ = 30.905(3) Å
	β = 90.130(10)°
Volume	4644.8(9) $Å^3$
Z	8
Formula weight	451.4
Density(calc.)	1.291 g/cm^3
Absorption Coefficient	0.512 mm^{-1}
F(000)	1888

Data Collection

Diffractometer Used	Siemens P4
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	244
Monochromator	Highly oriented graphite crystal
2θ Range	4.0 to 54.0°
Scan Type	Wyckoff
Scan Speed	Variable; 4.00 to 30.00°/min. in ω
Scan Range (ω)	1.50°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections
Index Ranges	$0 \leq h \leq 19$, $0 \leq k \leq 11$ $-38 \leq \ell \leq 38$
Reflections Collected	10068
Independent Reflections	9121 (R_{int} = 5.02%)
Observed Reflections	4325 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement

System Used	Siemens SHELXTL PLUS (VMS)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.00010F^2$
Number of Parameters refined	541
Final R indices (obs. data)	R = 7.01 %, wR = 6.31 %
R Indices (all data)	R = 14.57 %, wR = 7.40 %
Goodness-of-Fit	1.54
Largest and Mean Δ/σ	0.0011, 0.0002
Data-to-Parameter Ratio	8.0:1
Largest Difference Peak	0.52 eÅ^{-3}
Largest Difference Hole	-0.43 eÅ^{-3}

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Cr(1)	6054(1)	7301(1)	-445(1)	31(1)
C(1)	5669(4)	6941(8)	122(2)	39(3)
O(1)	5443(3)	6713(6)	466(2)	63(2)
C(2)	6312(4)	5362(9)	-495(2)	39(3)
O(2)	6488(3)	4180(6)	-522(2)	63(2)
C(3)	6487(4)	7601(8)	-1005(2)	39(3)
O(3)	6760(3)	7769(6)	-1347(2)	74(2)
C(4)	5872(4)	9281(9)	-369(2)	45(3)
O(4)	5769(3)	10461(6)	-321(2)	72(3)
C(5)	4972(4)	7037(8)	-663(2)	39(3)
O(5)	4301(3)	6870(5)	-788(2)	56(2)
C(6)	7239(3)	7528(7)	-203(2)	31(2)
C(7)	7959(4)	7569(7)	-70(2)	33(2)
C(8)	8780(4)	7548(7)	72(2)	33(2)
C(9)	9505(4)	7535(7)	188(2)	36(2)
C(10)	10363(3)	7521(7)	327(2)	33(2)
C(11)	10512(3)	7075(7)	745(2)	29(2)
C(12)	11332(4)	7232(8)	964(2)	28(2)
C(13)	9824(4)	6513(8)	1031(2)	50(3)
N(1)	10960(3)	7949(6)	33(2)	35(2)
C(14)	10677(4)	8590(8)	-373(2)	48(3)
C(15)	10487(5)	7568(9)	-730(2)	67(3)
C(16)	11768(4)	7222(9)	9(2)	62(3)
C(17)	12449(5)	8001(11)	-186(3)	92(4)
N(2)	11685(3)	8506(6)	1006(2)	34(2)
C(18)	11191(5)	9814(8)	946(2)	54(3)
C(19)	12588(4)	8754(8)	1058(2)	55(3)
N(3)	11690(3)	6076(6)	1127(2)	32(2)
C(20)	12243(4)	6069(8)	1506(2)	50(3)
C(21)	11497(4)	4651(7)	967(2)	43(3)
Cr(1A)	1139(1)	8180(1)	2729(1)	47(1)
C(1A)	1138(5)	6261(12)	2545(3)	78(4)
O(1A)	1147(4)	5115(8)	2437(3)	123(4)
C(2A)	623(5)	8709(11)	2208(3)	65(4)
O(2A)	319(4)	8991(9)	1880(2)	108(3)
C(3A)	1200(5)	10116(10)	2897(3)	55(3)
O(3A)	1256(4)	11251(7)	3004(2)	93(3)
C(4A)	1719(5)	7573(9)	3219(3)	50(3)
O(4A)	2094(4)	7182(6)	3518(2)	75(3)
C(5A)	112(5)	7903(9)	3004(2)	58(3)
O(5A)	-520(3)	7722(7)	3179(2)	83(3)
C(6A)	2278(4)	8467(8)	2440(2)	39(3)
C(7A)	2974(4)	8600(7)	2282(2)	35(2)
C(8A)	3787(4)	8678(7)	2122(2)	35(2)
C(9A)	4478(4)	8684(7)	1988(2)	31(2)
C(10A)	5341(4)	8553(7)	1847(2)	30(2)
C(11A)	5527(3)	7474(7)	1563(2)	29(2)
C(12A)	6333(4)	7369(7)	1344(2)	27(2)
C(13A)	4870(4)	6370(7)	1457(2)	39(3)
N(1A)	5903(3)	9503(6)	2025(2)	42(2)
C(14A)	5594(5)	10792(8)	2238(2)	57(3)
C(15A)	5268(6)	11860(9)	1923(3)	80(4)
C(16A)	6754(4)	9071(8)	2147(2)	48(3)
C(17A)	6807(5)	8502(12)	2602(3)	98(5)

N(2A)	6726(3)	6115(6)	1340(2)	34(2)
C(18A)	6590(4)	5064(8)	1682(2)	55(3)
C(19A)	7255(4)	5607(7)	988(2)	48(3)
N(3A)	6667(3)	8461(6)	1135(2)	34(2)
C(20A)	7574(4)	8660(8)	1076(2)	49(3)
C(21A)	6161(4)	9668(8)	985(2)	49(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Cr(1)-C(1)	1.889 (7)	Cr(1)-C(2)	1.881 (8)
Cr(1)-C(3)	1.886 (7)	Cr(1)-C(4)	1.904 (9)
Cr(1)-C(5)	1.866 (7)	Cr(1)-C(6)	2.041 (6)
C(1)-O(1)	1.144 (9)	C(2)-O(2)	1.153 (10)
C(3)-O(3)	1.155 (9)	C(4)-O(4)	1.134 (10)
C(5)-O(5)	1.148 (8)	C(6)-C(7)	1.219 (8)
C(7)-C(8)	1.379 (8)	C(8)-C(9)	1.209 (9)
C(9)-C(10)	1.433 (8)	C(10)-C(11)	1.380 (9)
C(10)-N(1)	1.379 (8)	C(11)-C(12)	1.478 (8)
C(11)-C(13)	1.506 (9)	C(12)-N(2)	1.333 (9)
C(12)-N(3)	1.329 (9)	N(1)-C(14)	1.461 (8)
N(1)-C(16)	1.461 (9)	C(14)-C(15)	1.496 (10)
C(16)-C(17)	1.443 (11)	N(2)-C(18)	1.474 (9)
N(2)-C(19)	1.467 (8)	N(3)-C(20)	1.465 (8)
N(3)-C(21)	1.465 (9)	Cr(1A)-C(1A)	1.896 (11)
Cr(1A)-C(2A)	1.874 (9)	Cr(1A)-C(3A)	1.901 (9)
Cr(1A)-C(4A)	1.862 (8)	Cr(1A)-C(5A)	1.865 (7)
Cr(1A)-C(6A)	2.043 (6)	C(1A)-O(1A)	1.132 (14)
C(2A)-O(2A)	1.153 (11)	C(3A)-O(3A)	1.125 (12)
C(4A)-O(4A)	1.162 (10)	C(5A)-O(5A)	1.158 (9)
C(6A)-C(7A)	1.220 (9)	C(7A)-C(8A)	1.389 (9)
C(8A)-C(9A)	1.179 (9)	C(9A)-C(10A)	1.449 (9)
C(10A)-C(11A)	1.377 (9)	C(10A)-N(1A)	1.381 (8)
C(11A)-C(12A)	1.458 (8)	C(11A)-C(13A)	1.512 (9)
C(12A)-N(2A)	1.339 (9)	C(12A)-N(3A)	1.328 (8)
N(1A)-C(14A)	1.469 (10)	N(1A)-C(16A)	1.464 (8)
C(14A)-C(15A)	1.493 (11)	C(16A)-C(17A)	1.506 (11)
N(2A)-C(18A)	1.467 (9)	N(2A)-C(19A)	1.457 (8)
N(3A)-C(20A)	1.470 (8)	N(3A)-C(21A)	1.468 (9)

Table 3. Bond angles (°)

C(1)-Cr(1)-C(2)	88.4(3)	C(1)-Cr(1)-C(3)	177.0(3)
C(2)-Cr(1)-C(3)	89.4(3)	C(1)-Cr(1)-C(4)	90.7(3)
C(2)-Cr(1)-C(4)	175.5(3)	C(3)-Cr(1)-C(4)	91.3(3)
C(1)-Cr(1)-C(5)	90.5(3)	C(2)-Cr(1)-C(5)	92.4(3)
C(3)-Cr(1)-C(5)	91.6(3)	C(4)-Cr(1)-C(5)	92.0(3)
C(1)-Cr(1)-C(6)	89.0(3)	C(2)-Cr(1)-C(6)	86.0(3)
C(3)-Cr(1)-C(6)	88.8(3)	C(4)-Cr(1)-C(6)	89.6(3)
C(5)-Cr(1)-C(6)	178.3(3)	Cr(1)-C(1)-O(1)	179.3(5)
Cr(1)-C(2)-O(2)	178.4(6)	Cr(1)-C(3)-O(3)	179.0(6)
Cr(1)-C(4)-O(4)	179.6(7)	Cr(1)-C(5)-O(5)	178.6(6)
Cr(1)-C(6)-C(7)	175.4(6)	C(6)-C(7)-C(8)	177.1(7)
C(7)-C(8)-C(9)	178.8(7)	C(8)-C(9)-C(10)	180.0(10)
C(9)-C(10)-C(11)	116.5(5)	C(9)-C(10)-N(1)	117.4(5)
C(11)-C(10)-N(1)	126.1(5)	C(10)-C(11)-C(12)	123.2(5)
C(10)-C(11)-C(13)	122.2(5)	C(12)-C(11)-C(13)	114.3(5)
C(11)-C(12)-N(2)	120.5(6)	C(11)-C(12)-N(3)	118.0(6)
N(2)-C(12)-N(3)	121.4(5)	C(10)-N(1)-C(14)	118.3(5)
C(10)-N(1)-C(16)	120.3(5)	C(14)-N(1)-C(16)	115.0(5)
N(1)-C(14)-C(15)	115.3(6)	N(1)-C(16)-C(17)	116.4(7)
C(12)-N(2)-C(18)	121.1(5)	C(12)-N(2)-C(19)	124.6(6)
C(18)-N(2)-C(19)	113.8(5)	C(12)-N(3)-C(20)	124.3(6)
C(12)-N(3)-C(21)	122.3(5)	C(20)-N(3)-C(21)	113.1(5)
C(1A)-Cr(1A)-C(2A)	89.8(4)	C(1A)-Cr(1A)-C(3A)	176.8(4)
C(2A)-Cr(1A)-C(3A)	90.1(4)	C(1A)-Cr(1A)-C(4A)	87.1(4)
C(2A)-Cr(1A)-C(4A)	175.2(4)	C(3A)-Cr(1A)-C(4A)	92.8(3)
C(1A)-Cr(1A)-C(5A)	90.1(4)	C(2A)-Cr(1A)-C(5A)	92.6(3)
C(3A)-Cr(1A)-C(5A)	93.1(4)	C(4A)-Cr(1A)-C(5A)	91.2(3)
C(1A)-Cr(1A)-C(6A)	89.8(3)	C(2A)-Cr(1A)-C(6A)	88.7(3)
C(3A)-Cr(1A)-C(6A)	87.0(3)	C(4A)-Cr(1A)-C(6A)	87.5(3)
C(5A)-Cr(1A)-C(6A)	178.7(3)	Cr(1A)-C(1A)-O(1A)	179.2(8)
Cr(1A)-C(2A)-O(2A)	177.5(8)	Cr(1A)-C(3A)-O(3A)	177.8(8)
Cr(1A)-C(4A)-O(4A)	178.4(7)	Cr(1A)-C(5A)-O(5A)	179.1(6)
Cr(1A)-C(6A)-C(7A)	177.0(6)	C(6A)-C(7A)-C(8A)	176.0(7)
C(7A)-C(8A)-C(9A)	177.2(7)	C(8A)-C(9A)-C(10A)	174.0(7)
C(9A)-C(10A)-C(11A)	117.4(6)	C(9A)-C(10A)-N(1A)	116.2(5)
C(11A)-C(10A)-N(1A)	126.4(5)	C(10A)-C(11A)-C(12A)	122.5(6)
C(10A)-C(11A)-C(13A)	119.8(5)	C(12A)-C(11A)-C(13A)	117.7(5)
C(11A)-C(12A)-N(2A)	118.5(6)	C(11A)-C(12A)-N(3A)	121.9(6)
N(2A)-C(12A)-N(3A)	119.6(5)	C(10A)-N(1A)-C(14A)	119.9(5)
C(10A)-N(1A)-C(16A)	121.4(6)	C(14A)-N(1A)-C(16A)	115.2(5)
N(1A)-C(14A)-C(15A)	112.5(6)	N(1A)-C(16A)-C(17A)	113.0(6)
C(12A)-N(2A)-C(18A)	121.3(5)	C(12A)-N(2A)-C(19A)	124.7(5)
C(18A)-N(2A)-C(19A)	113.8(5)	C(12A)-N(3A)-C(20A)	123.6(5)
C(12A)-N(3A)-C(21A)	122.3(5)	C(20A)-N(3A)-C(21A)	113.7(5)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cr(1)	20(1)	40(1)	33(1)	1(1)	-4(1)	-3(1)
C(1)	29(4)	48(5)	41(5)	4(4)	-3(3)	-1(4)
O(1)	58(3)	87(5)	45(3)	-12(3)	2(3)	8(3)
C(2)	22(4)	44(5)	52(5)	0(4)	-5(3)	-8(4)
O(2)	58(4)	39(4)	92(4)	16(3)	-6(3)	-9(3)
C(3)	41(4)	42(5)	35(4)	0(4)	-6(3)	-10(4)
O(3)	93(4)	92(5)	38(3)	6(4)	14(3)	4(3)
C(4)	32(4)	49(6)	53(5)	-3(4)	6(4)	-3(5)
O(4)	61(4)	40(4)	114(5)	0(3)	5(3)	-3(4)
C(5)	37(4)	45(5)	37(4)	5(4)	-4(3)	-2(4)
O(5)	27(3)	65(4)	76(4)	0(3)	-19(3)	-1(3)
C(6)	24(3)	40(5)	31(4)	0(3)	0(3)	-7(3)
C(7)	25(3)	41(5)	32(4)	0(3)	1(3)	-6(3)
C(8)	30(4)	38(5)	31(4)	1(3)	1(3)	-9(3)
C(9)	30(4)	49(5)	30(4)	-7(4)	2(3)	-8(4)
C(10)	21(3)	39(5)	38(4)	-5(3)	-2(3)	-6(4)
C(11)	21(3)	32(4)	32(4)	3(3)	3(3)	-2(3)
C(12)	26(3)	40(5)	19(3)	3(4)	5(3)	-1(3)
C(13)	38(4)	66(6)	47(5)	0(4)	8(4)	13(4)
N(1)	23(3)	56(4)	25(3)	0(3)	-5(2)	8(3)
C(14)	37(4)	66(6)	41(5)	5(4)	0(3)	9(4)
C(15)	52(5)	104(8)	45(5)	-1(5)	-7(4)	-21(5)
C(16)	34(4)	115(8)	38(4)	17(5)	13(3)	27(5)
C(17)	39(5)	157(10)	82(7)	11(6)	6(4)	42(7)
N(2)	26(3)	37(4)	38(4)	-1(3)	-6(3)	0(3)
C(18)	59(5)	36(5)	67(6)	5(4)	-8(4)	4(4)
C(19)	41(5)	57(6)	66(5)	-18(4)	-12(4)	-6(4)
N(3)	31(3)	35(4)	29(3)	0(3)	-1(3)	3(3)
C(20)	55(5)	59(6)	37(4)	0(4)	-18(4)	9(4)
C(21)	42(4)	47(5)	41(5)	2(4)	3(4)	1(4)
Cr(1A)	31(1)	63(1)	47(1)	1(1)	12(1)	-9(1)
C(1A)	41(5)	90(8)	103(8)	-21(5)	30(5)	-42(7)
O(1A)	97(5)	89(6)	183(8)	-30(5)	40(5)	-73(6)
C(2A)	40(5)	108(8)	49(5)	1(5)	8(4)	-18(6)
O(2A)	93(5)	179(8)	52(4)	1(5)	-6(4)	-2(5)
C(3A)	51(5)	55(6)	58(6)	19(5)	14(4)	-5(5)
O(3A)	123(6)	62(5)	93(5)	24(4)	24(4)	-18(4)
C(4A)	45(5)	51(6)	54(5)	0(4)	13(4)	-3(5)
O(4A)	78(4)	75(5)	73(4)	3(4)	-5(3)	20(4)
C(5A)	39(4)	82(7)	53(5)	11(5)	12(4)	7(5)
O(5A)	52(3)	121(6)	76(4)	10(4)	27(3)	16(4)
C(6A)	33(4)	46(5)	38(4)	3(4)	1(3)	-16(4)
C(7A)	32(4)	46(5)	28(4)	-5(3)	8(3)	-16(3)
C(8A)	40(4)	38(5)	26(4)	-2(4)	1(3)	-4(3)
C(9A)	34(4)	39(5)	20(3)	-1(3)	5(3)	-2(3)
C(10A)	30(4)	37(5)	22(4)	0(3)	0(3)	3(3)
C(11A)	28(3)	36(4)	22(3)	0(3)	4(3)	1(3)
C(12A)	27(3)	33(5)	20(3)	-6(3)	0(3)	-2(3)
C(13A)	29(4)	53(5)	34(4)	-3(4)	0(3)	-6(4)
N(1A)	36(3)	49(4)	41(4)	-2(3)	-2(3)	-20(3)
C(14A)	66(5)	49(6)	57(5)	-11(5)	6(4)	-26(5)
C(15A)	115(8)	41(6)	83(7)	4(6)	27(6)	-8(5)
C(16A)	30(4)	71(6)	43(5)	-21(4)	0(3)	-15(4)
C(17A)	62(6)	170(12)	61(6)	4(7)	-15(5)	-4(7)
N(2A)	30(3)	33(4)	38(4)	7(3)	8(3)	5(3)

C(18A)	56(5)	46(5)	62(6)	1(4)	1(4)	21(5)
C(19A)	32(4)	42(5)	69(6)	3(4)	12(4)	-12(4)
N(3A)	32(3)	38(4)	33(3)	-4(3)	8(3)	4(3)
C(20A)	44(5)	48(5)	54(5)	-15(4)	23(4)	-6(4)
C(21A)	63(5)	48(5)	35(5)	1(4)	6(4)	15(4)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(13A)	9311	6445	869	80
H(13B)	9982	5590	1133	80
H(13C)	9744	7135	1274	80
H(14A)	11105	9226	-472	80
H(14B)	10183	9140	-315	80
H(15A)	10308	8062	-985	80
H(15B)	10983	7028	-793	80
H(15C)	10050	6941	-635	80
H(16A)	11691	6374	-158	80
H(16B)	11930	6945	297	80
H(17A)	12954	7446	-191	80
H(17B)	12299	8263	-476	80
H(17C)	12539	8840	-16	80
H(18A)	10608	9581	917	80
H(18B)	11269	10419	1193	80
H(18C)	11378	10294	690	80
H(19A)	12866	7859	1095	80
H(19B)	12800	9216	804	80
H(19C)	12691	9341	1306	80
H(20A)	12346	7030	1594	80
H(20B)	11985	5561	1740	80
H(20C)	12764	5623	1432	80
H(21A)	11130	4729	721	80
H(21B)	12004	4179	882	80
H(21C)	11225	4116	1190	80
H(13D)	4367	6554	1618	80
H(13E)	4746	6394	1153	80
H(13F)	5085	5452	1533	80
H(14C)	6040	11210	2404	80
H(14D)	5153	10540	2435	80
H(15D)	5071	12684	2075	80
H(15E)	5710	12127	1730	80
H(15F)	4814	11451	1761	80
H(16C)	7116	9881	2126	80
H(16D)	6951	8366	1948	80
H(17D)	7375	8242	2669	80
H(17E)	6620	9210	2803	80
H(17F)	6453	7682	2623	80
H(18D)	6239	5466	1903	80
H(18E)	6320	4245	1561	80
H(18F)	7118	4793	1806	80
H(19D)	7316	6354	779	80
H(19E)	7797	5347	1098	80
H(19F)	6999	4799	853	80
H(20D)	7861	7834	1182	80
H(20E)	7697	8787	775	80
H(20F)	7759	9478	1235	80
H(21D)	5579	9463	1034	80
H(21E)	6315	10507	1142	80
H(21F)	6254	9817	682	80

Table 6. Torsion Angles (deg) for Compound 5a

C2	CR1	C1	O1	35.2(***)	C3	CR1	C1	O1	-9.0(***)	C4	CR1	C1	O1	-140.3(***)
C5	CR1	C1	O1	127.6(***)	C6	CR1	C1	O1	-50.7(***)	C1	CR1	C2	O2	-90.6(***)
C3	CR1	C2	O2	87.4(***)	C4	CR1	C2	O2	-11.3(***)	C5	CR1	C2	O2	179.0(***)
C6	CR1	C2	O2	-1.5(***)	C1	CR1	C3	O3	13.4(***)	C2	CR1	C3	O3	-30.9(***)
C4	CR1	C3	O3	144.7(***)	C5	CR1	C3	O3	-123.3(***)	C6	CR1	C3	O3	55.1(***)
C1	CR1	C4	O4	70.4(***)	C2	CR1	C4	O4	-8.8(***)	C3	CR1	C4	O4	-107.4(***)
C5	CR1	C4	O4	160.9(***)	C6	CR1	C4	O4	-18.6(***)	C1	CR1	C5	O5	3.7(***)
C2	CR1	C5	O5	92.2(***)	C3	CR1	C5	O5	-178.4(***)	C4	CR1	C5	O5	-87.0(***)
C6	CR1	C5	O5	76.6(***)	C1	CR1	C6	C7	102.8(6.8)	C2	CR1	C6	C7	14.2(6.8)
C3	CR1	C6	C7	-75.3(6.8)	C4	CR1	C6	C7	-166.5(6.8)	C5	CR1	C6	C7	29.8(***)
CR1	C6	C7	C8	2.1(***)	C6	C7	C8	C9	73.6(***)	C7	C8	C9	C10	140.0(***)
C8	C9	C10	C11	50.7(***)	C8	C9	C10	N1	-129.4(***)	C9	C10	C11	C12	-168.9(0.6)
C9	C10	C11	C13	5.0(0.9)	N1	C10	C11	C12	11.2(1.1)	N1	C10	C11	C13	-174.9(0.6)
C9	C10	N1	C14	9.3(0.9)	C9	C10	N1	C16	-141.4(0.6)	C11	C10	N1	C14	-170.8(0.6)
C11	C10	N1	C16	38.6(1.0)	C10	C11	C12	N2	57.1(0.9)	C10	C11	C12	N3	-124.7(0.7)
C13	C11	C12	N2	-117.2(0.6)	C13	C11	C12	N3	61.0(0.8)	C10	C11	C13	H13A	5.2(0.7)
C10	C11	C13	H13B	124.9(0.5)	C10	C11	C13	H13C	-115.3(0.6)	C12	C11	C13	H13A	179.6(0.4)
C12	C11	C13	H13B	-60.7(0.5)	C12	C11	C13	H13C	59.2(0.6)	C11	C12	N2	C18	16.7(0.8)
C11	C12	N2	C19	-155.4(0.6)	N3	C12	N2	C18	-161.5(0.6)	N3	C12	N2	C19	26.5(0.9)
C11	C12	N3	C20	-149.8(0.6)	C11	C12	N3	C21	23.6(0.8)	N2	C12	N3	C20	28.4(0.9)
N2	C12	N3	C21	-158.2(0.6)	C10	N1	C14	H14A	152.0(0.4)	C10	N1	C14	H14B	35.2(0.6)
C10	N1	C14	C15	-86.9(0.7)	C16	N1	C14	H14A	-55.8(0.6)	C16	N1	C14	H14B	-172.6(0.4)
C16	N1	C14	C15	65.2(0.8)	C10	N1	C16	H16A	80.8(0.5)	C10	N1	C16	H16B	-35.6(0.6)
C10	N1	C16	C17	-158.9(0.6)	C14	N1	C16	H16A	-70.7(0.5)	C14	N1	C16	H16B	172.9(0.4)
C14	N1	C16	C17	49.6(0.9)	N1	C14	C15	H15A	-179.8(0.4)	N1	C14	C15	H15B	-59.2(0.5)
N1	C14	C15	H15C	60.1(0.5)	H14A	C14	C15	H15A	-58.5(0.2)	H14A	C14	C15	H15B	62.1(0.2)
H14A	C14	C15	H15C	-178.7(0.0)	H14B	C14	C15	H15A	58.1(0.2)	H14B	C14	C15	H15B	178.7(0.0)
H14B	C14	C15	H15C	-62.1(0.2)	N1	C16	C17	H17A	-179.4(0.4)	N1	C16	C17	H17B	-58.3(0.6)
N1	C16	C17	H17C	60.7(0.6)	H16A	C16	C17	H17A	-58.8(0.3)	H16A	C16	C17	H17B	62.3(0.3)
H16A	C16	C17	H17C	-178.7(0.0)	H16B	C16	C17	H17A	57.5(0.3)	H16B	C16	C17	H17B	178.6(0.0)
H16B	C16	C17	H17C	-62.3(0.3)	C12	N2	C18	H18A	7.7(0.6)	C12	N2	C18	H18B	127.8(0.5)
C12	N2	C18	H18C	-112.3(0.5)	C19	N2	C18	H18A	-179.4(0.4)	C19	N2	C18	H18B	-59.3(0.5)
C19	N2	C18	H18C	60.5(0.5)	C12	N2	C19	H19A	-7.5(0.6)	C12	N2	C19	H19B	112.1(0.5)
C12	N2	C19	H19C	-127.6(0.5)	C18	N2	C19	H19A	179.9(0.4)	C18	N2	C19	H19B	-60.5(0.5)
C18	N2	C19	H19C	59.8(0.5)	C12	N3	C20	H20A	-6.2(0.6)	C12	N3	C20	H20B	113.9(0.5)
C12	N3	C20	H20C	-125.7(0.5)	C21	N3	C20	H20A	179.8(0.4)	C21	N3	C20	H20B	-60.1(0.5)
C21	N3	C20	H20C	60.3(0.5)	C12	N3	C21	H21A	5.3(0.6)	C12	N3	C21	H21B	125.2(0.5)
C12	N3	C21	H21C	-114.5(0.5)	C20	N3	C21	H21A	179.4(0.4)	C20	N3	C21	H21B	-60.6(0.5)
C20	N3	C21	H21C	59.7(0.5)	C2A	CR1A	C1A	O1A	126.5(***)	C3A	CR1A	C1A	O1A	38.3(***)
C4A	CR1A	C1A	O1A	-49.8(***)	C5A	CR1A	C1A	O1A	-140.9(***)	C6A	CR1A	C1A	O1A	37.7(***)
C1A	CR1A	C2A	O2A	-27.3(***)	C3A	CR1A	C2A	O2A	149.5(***)	C4A	CR1A	C2A	O2A	23.5(***)
C5A	CR1A	C2A	O2A	-117.4(***)	C6A	CR1A	C2A	O2A	62.5(***)	C1A	CR1A	C3A	O3A	-67.9(***)
C2A	CR1A	C3A	O3A	-156.0(***)	C4A	CR1A	C3A	O3A	20.1(***)	C5A	CR1A	C3A	O3A	111.4(***)
C6A	CR1A	C3A	O3A	-67.3(***)	C1A	CR1A	C4A	O4A	58.8(***)	C2A	CR1A	C4A	O4A	8.0(***)
C3A	CR1A	C4A	O4A	-118.0(***)	C5A	CR1A	C4A	O4A	148.9(***)	C6A	CR1A	C4A	O4A	-31.1(***)
C1A	CR1A	C5A	O5A	77.5(***)	C2A	CR1A	C5A	O5A	167.3(***)	C3A	CR1A	C5A	O5A	-102.5(***)
C4A	CR1A	C5A	O5A	-9.6(***)	C6A	CR1A	C5A	O5A	-9.1(***)	C1A	CR1A	C6A	C7A	-70.2(***)
C2A	CR1A	C6A	C7A	-160.1(***)	C3A	CR1A	C6A	C7A	109.8(***)	C4A	CR1A	C6A	C7A	16.9(***)
C5A	CR1A	C6A	C7A	16.4(***)	CR1A	C6A	C7A	C8A	9.3(***)	C6A	C7A	C8A	C9A	40.4(***)
C7A	C8A	C9A	C10A	-26.5(***)	C8A	C9A	C10A	C11A	68.8(6.4)	C8A	C9A	C10A	N1A	-109.1(6.3)
C9A	C10A	C11A	C12A	169.7(0.6)	C9A	C10A	C11A	C13A	-8.1(0.9)	N1A	C10A	C11A	C12A	-12.7(1.0)
N1A	C10A	C11A	C13A	169.5(0.6)	C9A	C10A	N1A	C14A	-16.9(0.8)	C9A	C10A	N1A	C16A	141.0(0.6)
C11A	C10A	N1A	C14A	165.5(0.6)	C11A	C10A	N1A	C16A	-36.6(0.9)	C10A	C11A	C12A	N2A	132.9(0.6)
C10A	C11A	C12A	N3A	-50.0(0.9)	C13A	C11A	C12A	N2A	-49.2(0.8)	C13A	C11A	C12A	N3A	127.9(0.6)
C10A	C11A	C13A	H13D	-1.5(0.6)	C10A	C11A	C13A	H13E	119.0(0.5)	C10A	C11A	C13A	H13F	-121.4(0.5)
C12A	C11A	C13A	H13D	-179.4(0.4)	C12A	C11A	C13A	H13E	-59.0(0.5)	C12A	C11A	C13A	H13F	60.7(0.5)
C11A	C12A	N2A	C18A	-26.7(0.8)	C11A	C12A	N2A	C19A	147.5(0.6)	N3A	C12A	N2A	C18A	156.1(0.6)
N3A	C12A	N2A	C19A	-29.7(0.9)	C11A	C12A	N3A	C20A	152.1(0.6)	C11A	C12A	N3A	C21A	-20.5(0.9)

N2A	C12A	N3A	C20A	-30.8(0.9)	N2A	C12A	N3A	C21A	156.6(0.6)	C10A	N1A	C14A	H14C	165.9(0.4)
C10A	N1A	C14A	H14D	48.1(0.6)	C10A	N1A	C14A	C15A	-72.8(0.8)	C16A	N1A	C14A	H14C	6.7(0.6)
C16A	N1A	C14A	H14D	-111.1(0.5)	C16A	N1A	C14A	C15A	128.0(0.7)	C10A	N1A	C16A	H16C	151.9(0.4)
C10A	N1A	C16A	H16D	34.4(0.6)	C10A	N1A	C16A	C17A	-88.0(0.8)	C14A	N1A	C16A	H16C	-49.3(0.5)
C14A	N1A	C16A	H16D	-166.8(0.4)	C14A	N1A	C16A	C17A	70.9(0.8)	N1A	C14A	C15A	H15D	179.9(0.4)
N1A	C14A	C15A	H15E	-60.0(0.6)	N1A	C14A	C15A	H15F	59.7(0.6)	H14C	C14A	C15A	H15D	-58.7(0.3)
H14C	C14A	C15A	H15E	61.4(0.3)	H14C	C14A	C15A	H15F	-178.9(0.0)	H14D	C14A	C15A	H15D	58.8(0.3)
H14D	C14A	C15A	H15E	178.9(0.0)	H14D	C14A	C15A	H15F	-61.4(0.3)	N1A	C16A	C17A	H17D	-179.4(0.4)
N1A	C16A	C17A	H17E	-58.8(0.6)	N1A	C16A	C17A	H17F	60.8(0.6)	H16C	C16A	C17A	H17D	-59.2(0.3)
H16C	C16A	C17A	H17E	61.4(0.2)	H16C	C16A	C17A	H17F	-179.0(0.0)	H16D	C16A	C17A	H17D	58.4(0.3)
H16D	C16A	C17A	H17E	179.0(0.0)	H16D	C16A	C17A	H17F	-61.4(0.2)	C12A	N2A	C18A	H18D	-5.3(0.6)
C12A	N2A	C18A	H18E	114.5(0.5)	C12A	N2A	C18A	H18F	-125.5(0.5)	C19A	N2A	C18A	H18D	179.9(0.4)
C19A	N2A	C18A	H18E	-60.3(0.5)	C19A	N2A	C18A	H18F	59.7(0.5)	C12A	N2A	C19A	H19D	5.7(0.6)
C12A	N2A	C19A	H19E	125.5(0.5)	C12A	N2A	C19A	H19F	-113.9(0.5)	C18A	N2A	C19A	H19D	-179.7(0.4)
C18A	N2A	C19A	H19E	-59.9(0.5)	C18A	N2A	C19A	H19F	60.7(0.5)	C12A	N3A	C20A	H20D	6.7(0.6)
C12A	N3A	C20A	H20E	126.4(0.5)	C12A	N3A	C20A	H20F	-113.2(0.5)	C21A	N3A	C20A	H20D	179.8(0.4)
C21A	N3A	C20A	H20E	-60.5(0.5)	C21A	N3A	C20A	H20F	59.9(0.5)	C12A	N3A	C21A	H21D	-6.7(0.6)
C12A	N3A	C21A	H21E	113.3(0.5)	C12A	N3A	C21A	H21F	-126.4(0.5)	C20A	N3A	C21A	H21D	-179.9(0.4)
C20A	N3A	C21A	H21E	-59.9(0.5)	C20A	N3A	C21A	H21F	60.4(0.5)					

Table 7. Non-Bonded Distances (Angstrom) for Compound 5a

Second atoms generated by transformation: 0.00000 +X 0.00000 +Y 0.00000 +Z

H16B-H16A	1.551	H14B-H14A	1.551	H14D-H14C	1.553	H16D-H16C	1.553	H15C-H15A	1.567	H21C-H21A	1.568
H17B-H17A	1.568	H19B-H19A	1.568	H17C-H17B	1.568	H18F-H18E	1.568	H15E-H15D	1.568	H19C-H19B	1.568
H18C-H18B	1.568	H13B-H13A	1.568	H17C-H17A	1.568	H15F-H15E	1.568	H13C-H13A	1.568	H20C-H20A	1.568
H19C-H19A	1.568	H21C-H21B	1.568	H20C-H20B	1.568	H20B-H20A	1.568	H15C-H15B	1.568	H15F-H15D	1.568
H21B-H21A	1.568	H20F-H20D	1.568	H21F-H21D	1.568	H13F-H13D	1.568	H18B-H18A	1.568	H21E-H21D	1.568
H18C-H18A	1.568	H18E-H18D	1.568	H17F-H17E	1.568	H15B-H15A	1.568	H18F-H18D	1.568	H19F-H19D	1.568
H20E-H20D	1.568	H17F-H17D	1.568	H13C-H13B	1.568	H13F-H13E	1.568	H17E-H17D	1.568	H19E-H19D	1.568
H19F-H19E	1.568	H20F-H20E	1.568	H21F-H21E	1.568	H13E-H13D	1.568	H20A-H19A	1.918	C17 -H16A	1.954
H17C-C16	1.961	C17 -H16B	1.976	H16A-N1	1.978	H17B-C16	1.983	H14A-N1	1.984	H19D-N2A	1.985
H16B-N1	1.986	H14B-N1	1.987	H16C-N1A	1.989	H20A-N3	1.994	H21A-N3	1.995	H19A-N2	1.997
H21D-N3A	1.998	H20D-N3A	1.998	H19F-N2A	1.999	H16D-N1A	1.999	H20C-N3	1.999	H18E-N2A	2.000
H17A-C16	2.000	H14D-N1A	2.000	H19E-N2A	2.000	H19B-N2	2.001	H21C-N3	2.002	H14C-N1A	2.002
H18D-N2A	2.004	H21F-N3A	2.005	H18F-N2A	2.006	H21B-N3	2.006	H18C-N2	2.008	H18B-N2	2.008
H20E-N3A	2.009	H21E-N3A	2.009	H20B-N3	2.010	H20F-N3A	2.011	C15 -H14A	2.011	H19C-N2	2.011
H18A-N2	2.012	H15C-C14	2.018	C15 -H14B	2.019	C15A-H14D	2.020	C15A-H14C	2.022	H15E-C14A	2.023
H15F-C14A	2.024	C17A-H16C	2.025	H15B-C14	2.025	H17F-C16A	2.027	H13B-C11	2.029	H15D-C14A	2.033
H13F-C11A	2.035	C17A-H16D	2.039	H13A-C11	2.041	H17E-C16A	2.041	H15A-C14	2.043	H13C-C11	2.044
H17D-C16A	2.045	H13E-C11A	2.045	H13D-C11A	2.050	H20D-H19D	2.060	H17B-H14A	2.108	H18D-H13F	2.164
H17A-H16A	2.254	H17C-H16B	2.254	H17B-H16A	2.254	H17A-H16B	2.273	H18E-H13F	2.276	H16B-C12	2.290
H16C-H14C	2.292	N3A -N2A	2.304	H15C-H14B	2.307	H15B-H14A	2.307	H15A-H14A	2.308	H16D-C12A	2.308
H15D-H14D	2.311	H15D-H14C	2.312	H15A-H14B	2.315	H15E-H14C	2.315	H15F-H14D	2.315	H13D-C9A	2.317
H17D-H16C	2.318	N3 -N2	2.322	H17F-H16D	2.326	H17E-H16C	2.326	H17D-H16D	2.330	C20 -H19A	2.336
H16A-H15B	2.346	H20A-C19	2.354	H20C-H19A	2.358	H20D-H19E	2.362	H13A-C9	2.363	H20E-H19D	2.374
H21A-H13B	2.376	H20D-C19A	2.387	C11 -C9	2.391	C20A-H19D	2.396	N1A -C9A	2.402	N1 -C9	2.402
N2A -C11A	2.404	N3 -C11	2.408	C11A-C9A	2.415	H13E-O1	2.416	H20A-H19C	2.417	H21A-C11	2.424
H21C-H13B	2.426	H14B-C9	2.427	H18A-C11	2.428	H17E-H14C	2.434	N3A -C11A	2.435	C14 -C10	2.438
N2 -C11	2.441	C21 -C20	2.444	H18D-C11A	2.444	C18 -C12	2.446	C18A-C12A	2.447	C21 -C12	2.449
C16A-H14C	2.449	C21A-C12A	2.450	C19A-C18A	2.450	N1 -C11	2.460	C21A-C20A	2.460	N1A -C11A	2.461
C15A-N1A	2.463	C19 -C18	2.464	C16 -C10	2.464	C16 -C14	2.465	C14A-C10A	2.466	C20A-C12A	2.467
C17 -N1	2.469	C18A-H13F	2.469	C20 -C12	2.472	H14D-C9A	2.475	C16A-C14A	2.477	C19A-C12A	2.477
C17A-N1A	2.477	H20D-N2A	2.478	C19 -C12	2.480	C16A-C10A	2.482	C12A-C10A	2.486	H21D-C11A	2.489
H21B-H20C	2.490	H21C-H20B	2.490	N3A -H19D	2.497	H18D-C12A	2.497	C15 -N1	2.498	H21A-C12	2.499
H19E-H18F	2.499	H19F-H18E	2.500	C13A-C10A	2.500	H21D-C12A	2.501	H18A-C12	2.502	C13 -C12	2.506
H19B-H18C	2.508	H19C-H18B	2.508	H21E-H20F	2.513	H21F-H20E	2.513	C12 -C10	2.515	H20A-N2	2.518
N3 -H19A	2.520	H14B-C10	2.520	H20D-C12A	2.525	C13 -C10	2.528	H20A-C12	2.534	H19D-C12A	2.535
C13A-C12A	2.541	H13D-C10A	2.542	H19A-C12	2.547	N3A -H16D	2.554	H16B-C10	2.558	H21E-H15E	2.563
C9A -C7A	2.567	H13A-C10	2.581	C17 -H14A	2.588	C9 -C7	2.588	H16D-C10A	2.589	C4A -C1A	2.590
H17B-H15B	2.591	H19B-H17C	2.591	H16C-C14A	2.597	C8 -C6	2.597	C8A -C6A	2.607	H17B-C14	2.623
C21 -H13B	2.624	C10A-C8A	2.624	C16 -H14A	2.626	H14D-C10A	2.629	C2 -C1	2.630	H21C-C20	2.641
C21 -H20C	2.642	C10 -C8	2.642	C19A-H18E	2.650	C3 -C2	2.650	H21B-C20	2.653	C19A-H18F	2.653
C21 -H20B	2.653	H15F-N1A	2.655	H15E-N1A	2.655	H19E-C18A	2.656	H16B-C11	2.657	H17C-N1	2.658
C19 -H18B	2.658	H19F-C18A	2.659	C5A -C4A	2.662	C2A -C1A	2.662	C5A -C1A	2.663	H19B-C18	2.663
H21F-C20A	2.664	H21E-C20A	2.665	C21A-H20F	2.666	C19 -H18C	2.666	C21A-H20E	2.667	C5 -C1	2.668
H17B-N1	2.669	N2 -H16B	2.669	H17F-N1A	2.670	C3A -C2A	2.671	H19C-C18	2.671	H17E-N1A	2.674
C6 -C2	2.676	H21D-C10A	2.682	C5 -C3	2.691	H15C-N1	2.693	H18A-C10	2.694	H16D-C11A	2.694
H15B-N1	2.697	C4 -C1	2.699	H13D-C8A	2.702	H13B-C12	2.703	C5A -C2A	2.703	C6A -C4A	2.704
C5 -C2	2.705	H13C-C12	2.710	C4 -C3	2.710	C5 -C4	2.713	H18D-C13A	2.716	C6A -C3A	2.716
N3 -H16B	2.720	H16A-C14	2.724	C4A -C3A	2.725	C5A -C3A	2.734	C14 -C9	2.738	C6A -C2A	2.741
H15C-C9	2.748	C6 -C3	2.750	H13F-C12A	2.754	H13E-C12A	2.754	H15F-C9A	2.755	C6 -C1	2.756
N2A -H13F	2.758	N3 -H13B	2.762	C14A-C9A	2.777	C6 -C4	2.782	C6A -C1A	2.782	C16 -H15B	2.783
C13A-C9A	2.801	H13A-C8	2.805	H16A-C10	2.813	H17E-C14A	2.816	C13 -C9	2.824	H16A-C15	2.839
H21A-C13	2.846	C21 -C11	2.855	C18A-C11A	2.858	N2A -H16D	2.858	C18 -C11	2.869	H15F-C10A	2.872
C20A-N2A	2.874	H20E-C7	2.885	C20A-H16D	2.886	N3A -C19A	2.887	C17A-H14C	2.896	C20 -N2	2.909
N3 -C19	2.911	C21A-C11A	2.915	C17 -C14	2.935	C20A-C19A	2.937	C20 -C19	2.939	H14B-C8	2.949
H14D-C8A	2.959	H21E-N1A	2.962	N2A -C13A	2.992	N1A -C12A	2.994	H18C-C12	3.010	N1 -C12	3.014
O5 -CR1	3.015	H20E-C8	3.015	N3 -C13	3.017	H18E-C12A	3.022	O5A -CR1A	3.023	O4A -CR1A	3.024
H21E-C12A	3.024	O3A -CR1A	3.025	H21C-C12	3.026	O2A -CR1A	3.026	O1A -CR1A	3.028	C16A-C12A	3.031

C16 -C12 3.032 O1 -CR1 3.033 O2 -CR1 3.034 H15C-C8 3.036 C16 -C11 3.037 H19B-C12 3.038
O4 -CR1 3.038 H20F-C12A 3.039 C16A-H14D 3.039 O3 -CR1 3.041 H19D-C7 3.044 H20B-C12 3.050
H19F-C12A 3.051 C16A-C11A 3.056 N3A -C10A 3.056 H17B-C15 3.061 H15C-C10 3.063 C21 -H16B 3.073
H18E-C13A 3.075 C16 -C15 3.078 C18A-C13A 3.083 H18F-C12A 3.084 H21B-C12 3.084 H21F-C12A 3.087
C19 -H16B 3.088 H18B-C12 3.090 C17A-C14A 3.107 N2 -C10 3.112 C12A-O1 3.120 C15A-C10A 3.131
C21A-C10A 3.149 N3A -N1A 3.167 C18 -C10 3.174 N3A -C16A 3.185 C21 -C13 3.200 C13A-O1 3.214
C21A-N1A 3.243 C15 -C9 3.243 C15A-C9A 3.256 C7 -CR1 3.257 C7A -CR1A 3.261 N2 -N1 3.261
C15 -C10 3.272 N3A -O1 3.282 C17A-C10A 3.299 N2 -C16 3.311 C18 -N1 3.347 C21A-O1 3.412
C13A-C8A 3.458 C11A-C8A 3.463 C14 -C8 3.465 C11 -C8 3.483 C14A-C8A 3.521 C13 -C8 3.535

Second atoms generated by transformation: 1.00000 +X 0.00000 +Y 0.00000 +Z
H17A-O5 2.887

Second atoms generated by transformation: -1.00000 +X 0.00000 +Y 0.00000 +Z
O1A -H20B 2.573 O2A -H13C 2.722 C7A -H20A 2.777 C1A -H20B 2.911 O2A -H18B 2.937 C6A -H20A 2.947
O2A -C18 3.298

Second atoms generated by transformation: 0.00000 +X -1.00000 +Y 0.00000 +Z
H18E-H15E 2.282 H18E-C15A 3.023

Second atoms generated by transformation: 1.00000 -X 2.00000 -Y 0.00000 -Z
H21E-O5 2.877 H15F-O3 2.909 O4 -O4 3.276 O4 -C4 3.388 C21A-O5 3.402 O4 -C1 3.413

Second atoms generated by transformation: 1.00000 -X 1.00000 -Y 0.00000 -Z
H19F-O5 2.609 H18E-O5 2.789 H13E-O2 2.821 O2 -O1 3.196 C2 -O1 3.414

Second atoms generated by transformation: 2.00000 -X 1.00000 -Y 0.00000 -Z
H21A-H15C 2.467 H19A-O2 2.811 H16B-O2 2.821 H17A-O2 2.825 H21B-C6 2.909 H21B-C3 2.957
H21B-C2 2.973 H21B-C7 3.003 C21 -H15C 3.062

Second atoms generated by transformation: 2.00000 -X 2.00000 -Y 0.00000 -Z
H18A-H14B 2.548 H14B-H14B 2.604 H19B-O4 2.745 H19C-O3 2.866 H19B-C4 2.882 H17C-O4 2.965
H18C-C7 2.977

Second atoms generated by transformation: 1.00000 -X 0.50000 +Y 0.50000 -Z
O5A -H21C 2.607 H20F-O4A 2.672 H14C-C8A 2.764 O3A -H13C 2.869 H14C-C7A 2.913 H17D-O1A 2.963
C14A-C8A 3.505

Second atoms generated by transformation: 1.00000 -X -0.50000 +Y 0.50000 -Z
H17F-H15D 2.605 H18F-C4A 2.798 H18F-C6A 2.812 H18F-C3A 2.848 H18F-O4A 2.941 H18F-C7A 3.038
H18F-CR1A 3.475

Second atoms generated by transformation: 0.00000 -X 0.50000 +Y 0.50000 -Z
O5A -O1A 3.116 C5A -O1A 3.197 C2A -O1A 3.308

Second atoms generated by transformation: -1.00000 +X 1.50000 -Y 0.50000 +Z
O4A -H15B 2.870