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Table V **Fractional Atomic Coordinates (x10⁴) and Thermal**
Parameters (Å² x 10³) for 4b.

	x	y	z	U(eq)
W	7667 (1)	7636 (1)	1612 (1)	41 (1)
C(01)	5590 (15)	7449 (10)	355 (6)	38 (3)
N(1)	5960 (12)	6895 (8)	960 (6)	40 (3)
N(2)	7425 (13)	8672 (8)	673 (6)	38 (3)
C(3)	3708 (17)	6216 (12)	111 (8)	53 (4)
C(02)	6358 (14)	8404 (10)	208 (7)	34 (3)
C(1)	5187 (16)	6039 (11)	1131 (7)	45 (4)
C(4)	4457 (15)	7112 (10)	-97 (7)	36 (3)
C(12)	8814 (17)	8531 (12)	2257 (8)	49 (4)
C(7)	5974 (14)	9007 (10)	-408 (7)	38 (3)
O(11)	7277 (14)	6288 (9)	2983 (6)	68 (4)
O(12)	9490 (15)	9046 (9)	2648 (6)	79 (4)
C(5)	4144 (18)	7737 (12)	-690 (8)	57 (4)
C(8)	6764 (17)	9941 (11)	-520 (7)	47 (4)
C(11)	7416 (18)	6781 (12)	2483 (9)	53 (4)
C(10)	8117 (17)	9570 (11)	547 (8)	50 (4)
C(6)	4874 (17)	8658 (13)	-860 (7)	53 (4)
C(9)	7811 (18)	10211 (11)	-48 (8)	53 (4)
C(2)	4053 (17)	5683 (12)	721 (8)	54 (4)
Cl	5663 (5)	8728 (3)	1985 (2)	56 (1)
S	9881 (5)	7334 (4)	-318 (2)	69 (1)
C(13)	9868 (17)	7558 (12)	1333 (9)	56 (4)
C(14)	8741 (16)	5977 (15)	1515 (9)	66 (5)
C(15)	9133 (19)	6683 (13)	999 (10)	62 (5)
C(16)	8957 (17)	6451 (13)	247 (9)	59 (5)
O(16)	8243 (16)	5758 (9)	27 (7)	88 (5)
C(19)	8616 (23)	8350 (18)	-1832 (11)	90 (7)
C(18)	8260 (25)	7255 (19)	-1563 (14)	114 (10)
C(17)	9502 (28)	6728 (18)	-1160 (11)	105 (9)
C(20)	7518 (28)	8914 (25)	-2344 (13)	140 (11)
C(03)	11066 (21)	8039 (15)	1357 (9)	76 (6)

Table VI Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4b.

	x	y	z	U(eq)
H(3)	2956(17)	5974(12)	-170(8)	63
H(1)	5424(16)	5670(11)	1542(7)	54
H(5)	3401(18)	7523(12)	-988(8)	68
H(8)	6572(17)	10370(11)	-911(7)	57
H(10)	8830(17)	9785(11)	862(8)	61
H(6)	4638(17)	9038(13)	-1268(7)	63
H(9)	8333(18)	10830(11)	-119(8)	63
H(2)	3534(17)	5091(12)	857(8)	65
H(14A)	9450(16)	5793(15)	1873(9)	79
H(14B)	8147(16)	5380(15)	1367(9)	79
H(19A)	9497(23)	8297(18)	-2072(11)	108
H(19B)	8778(23)	8816(18)	-1430(11)	108
H(18A)	7974(25)	6801(19)	-1957(14)	137
H(18B)	7472(25)	7312(19)	-1255(14)	137
H(17A)	10331(28)	6775(18)	-1442(11)	126
H(17B)	9296(28)	5974(18)	-1093(11)	126
H(20A)	7820(121)	9634(67)	-2436(93)	210
H(20B)	6618(60)	8932(159)	-2132(52)	210
H(20C)	7444(177)	8522(107)	-2778(46)	210
H(03A)	11788(21)	7799(15)	1080(9)	91
H(03B)	11209(21)	8627(15)	1652(9)	91

Table VII **Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4b.**

	U11	U22	U33	U23	U13	U12
W	41 (1)	40 (1)	41 (1)	-4 (1)	1 (1)	-7 (1)
C (01)	44 (8)	36 (7)	34 (7)	-11 (6)	6 (6)	-7 (7)
N (1)	43 (8)	39 (6)	38 (7)	-2 (5)	3 (6)	0 (6)
N (2)	42 (8)	37 (6)	37 (6)	-10 (5)	9 (6)	-8 (6)
C (3)	42 (10)	57 (10)	59 (10)	0 (8)	-8 (8)	-18 (8)
C (02)	33 (8)	35 (7)	33 (7)	-8 (6)	10 (6)	-3 (6)
C (1)	47 (10)	44 (8)	43 (8)	17 (7)	-2 (7)	-14 (7)
C (4)	38 (9)	36 (7)	33 (7)	-6 (6)	11 (6)	-2 (6)
C (12)	40 (10)	59 (10)	49 (9)	8 (8)	9 (8)	0 (8)
C (7)	23 (8)	38 (8)	54 (9)	-4 (6)	14 (7)	-10 (6)
O (11)	81 (10)	71 (8)	52 (7)	28 (6)	-11 (7)	3 (7)
O (12)	84 (10)	77 (8)	76 (8)	-33 (7)	-11 (8)	-21 (8)
C (5)	54 (11)	64 (10)	52 (9)	-16 (8)	-9 (8)	12 (9)
C (8)	64 (12)	41 (8)	37 (8)	-5 (6)	13 (8)	-11 (8)
C (11)	47 (10)	52 (9)	58 (10)	-13 (8)	-5 (8)	2 (8)
C (10)	49 (11)	49 (9)	53 (10)	0 (7)	5 (8)	-4 (8)
C (6)	52 (11)	69 (11)	38 (8)	-3 (7)	10 (8)	1 (9)
C (9)	61 (12)	39 (8)	59 (10)	-4 (7)	18 (9)	-14 (8)
C (2)	52 (11)	45 (9)	66 (11)	-10 (8)	7 (9)	-26 (8)
Cl	62 (3)	52 (2)	56 (2)	3 (2)	15 (2)	3 (2)
S	62 (3)	75 (3)	71 (3)	-23 (2)	12 (2)	-22 (3)
C (13)	41 (10)	60 (10)	66 (10)	-9 (8)	-8 (8)	-17 (9)
C (14)	9 (8)	101 (14)	88 (13)	-19 (11)	5 (8)	5 (9)
C (15)	54 (12)	49 (10)	82 (13)	-14 (9)	-23 (10)	-3 (9)
C (16)	32 (10)	57 (10)	87 (13)	-30 (9)	15 (9)	-10 (8)
O (16)	108 (12)	65 (8)	94 (10)	-38 (7)	23 (9)	-46 (8)
C (19)	70 (16)	123 (19)	80 (15)	-38 (13)	22 (12)	-14 (14)
C (18)	63 (16)	133 (21)	147 (24)	-72 (19)	27 (16)	-35 (16)
C (17)	116 (22)	114 (18)	89 (16)	-49 (14)	59 (16)	-40 (17)
C (20)	84 (19)	217 (31)	118 (22)	-49 (21)	-18 (17)	-11 (21)
C (03)	75 (15)	90 (13)	60 (11)	-2 (10)	-13 (11)	-7 (12)

Table VIII Bond lengths (Å) and angles (°) for 4b.

W-C(12)	1.964 (17)	W-C(11)	1.993 (18)
W-C(13)	2.181 (17)	W-C(15)	2.197 (19)
W-N(1)	2.213 (11)	W-N(2)	2.211 (11)
W-C(14)	2.318 (18)	W-Cl	2.468 (4)
C(01)-N(1)	1.38 (2)	C(01)-C(02)	1.43 (2)
C(01)-C(4)	1.42 (2)	N(1)-C(1)	1.34 (2)
N(2)-C(10)	1.32 (2)	N(2)-C(02)	1.36 (2)
C(3)-C(2)	1.37 (2)	C(3)-C(4)	1.39 (2)
C(02)-C(7)	1.43 (2)	C(1)-C(2)	1.38 (2)
C(4)-C(5)	1.39 (2)	C(12)-O(12)	1.16 (2)
C(7)-C(8)	1.41 (2)	C(7)-C(6)	1.40 (2)
O(11)-C(11)	1.15 (2)	C(5)-C(6)	1.39 (2)
C(8)-C(9)	1.36 (2)	C(10)-C(9)	1.41 (2)
S-C(16)	1.79 (2)	S-C(17)	1.80 (2)
C(13)-C(03)	1.29 (2)	C(13)-C(15)	1.43 (2)
C(14)-C(15)	1.38 (2)	C(15)-C(16)	1.47 (2)
C(16)-O(16)	1.17 (2)	C(19)-C(18)	1.50 (3)
C(19)-C(20)	1.57 (3)	C(18)-C(17)	1.54 (3)
C(12)-W-C(11)	82.1 (6)	C(12)-W-C(13)	70.1 (6)
C(11)-W-C(13)	108.8 (7)	C(12)-W-C(15)	106.9 (6)
C(11)-W-C(15)	104.4 (7)	C(13)-W-C(15)	38.2 (6)
C(12)-W-N(1)	166.0 (5)	C(11)-W-N(1)	97.9 (5)
C(13)-W-N(1)	122.5 (5)	C(15)-W-N(1)	86.8 (5)
C(12)-W-N(2)	102.4 (5)	C(11)-W-N(2)	166.7 (6)
C(13)-W-N(2)	84.5 (5)	C(15)-W-N(2)	86.4 (6)
N(1)-W-N(2)	74.7 (4)	C(12)-W-C(14)	108.6 (6)
C(11)-W-C(14)	69.8 (6)	C(13)-W-C(14)	60.7 (6)
C(15)-W-C(14)	35.4 (6)	N(1)-W-C(14)	84.3 (5)
N(2)-W-C(14)	119.4 (5)	C(12)-W-Cl	85.7 (5)
C(11)-W-Cl	86.5 (5)	C(13)-W-Cl	148.6 (4)
C(15)-W-Cl	164.2 (4)	N(1)-W-Cl	80.3 (3)
N(2)-W-Cl	81.4 (3)	C(14)-W-Cl	149.6 (4)
N(1)-C(01)-C(02)	117.5 (12)	N(1)-C(01)-C(4)	121.7 (12)
C(02)-C(01)-C(4)	120.7 (12)	C(1)-N(1)-C(01)	118.3 (12)
C(1)-N(1)-W	126.5 (9)	C(01)-N(1)-W	114.9 (8)
C(10)-N(2)-C(02)	116.9 (12)	C(10)-N(2)-W	127.0 (10)
C(02)-N(2)-W	115.8 (8)	C(2)-C(3)-C(4)	121.5 (14)
N(2)-C(02)-C(01)	116.9 (12)	N(2)-C(02)-C(7)	124.5 (12)
C(01)-C(02)-C(7)	118.7 (12)	N(1)-C(1)-C(2)	122.8 (13)
C(3)-C(4)-C(5)	125.6 (14)	C(3)-C(4)-C(01)	116.8 (12)
C(5)-C(4)-C(01)	117.5 (13)	O(12)-C(12)-W	178.9 (14)
C(8)-C(7)-C(6)	123.8 (14)	C(8)-C(7)-C(02)	115.9 (13)
C(6)-C(7)-C(02)	120.4 (12)	C(6)-C(5)-C(4)	124 (2)
C(9)-C(8)-C(7)	119.2 (14)	O(11)-C(11)-W	180 (2)
N(2)-C(10)-C(9)	122 (2)	C(5)-C(6)-C(7)	118.9 (14)
C(8)-C(9)-C(10)	121.1 (14)	C(3)-C(2)-C(1)	118.9 (14)
C(16)-S-C(17)	100.9 (9)	C(03)-C(13)-C(15)	142 (2)
C(03)-C(13)-W	146 (2)	C(15)-C(13)-W	71.5 (10)
C(15)-C(14)-W	67.5 (11)	C(14)-C(15)-C(13)	108 (2)
C(14)-C(15)-C(16)	123 (2)	C(13)-C(15)-C(16)	128 (2)
C(14)-C(15)-W	77.1 (12)	C(13)-C(15)-W	70.3 (10)
C(16)-C(15)-W	124.9 (12)	O(16)-C(16)-C(15)	123 (2)
O(16)-C(16)-S	122 (2)	C(15)-C(16)-S	115.1 (12)
C(18)-C(19)-C(20)	118 (2)	C(19)-C(18)-C(17)	112 (2)
C(18)-C(17)-S	113 (2)		