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Table S1. Crystal data and structure refinement for (1S,2S-(-)-saldpen)MnN (2)

Empirical formula	C ₂₈ H ₂₂ Mn N ₃ O ₂ (C ₂ H ₃ N) _{1.5}
Formula weight	549.01
Crystallization solvent	Acetonitrile
Crystal shape	Rectangular
Crystal size	0.4 × 0.4 × 0.2 mm
Crystal color	Green
Data Collection	
Preliminary photos	
Type of diffractometer	CAD-4
Wavelength	0.71073 Å MoK α
Data collection temperature	160 K
Lattice determination from	25 reflections
Theta range for reflections used in lattice determination	12.8 to 13.6 deg.
Unit cell dimensions	$a = 20.924(4)$ Å $\alpha = 90$ deg. $b = 18.197(5)$ Å $\beta = 124.60(2)$ deg. $c = 17.238(3)$ Å $\gamma = 90$ deg.
Volume	5403(2) Å ³
Z	8
Crystal system and space group	Monoclinic C2
Density (calculated)	1.350 g/cm ³
Absorption coefficient	0.525 mm ⁻¹
F(000)	2280
Theta range for data collection	1.63 to 24.98 deg.
Index ranges	0 ≤ h ≤ 24, -21 ≤ k ≤ 21, -20 ≤ l ≤ 20
Data collection scan type	Omega scans
Reflections collected	12275
Independent reflections	9295 [R(merge) = 0.028 GOF(merge) = 1.10]
Absorption correction	Psi scan (not applied)
Max. and min. transmission	0.96 and 1.06
Number of standards	3 reflections measured every 60 min.
Variation of standards	1.2%
Structure solution and Refinement	
Structure solution program	SHELXS-86 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier maps
Hydrogen placement	Calculated positions
Structure refinement program	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full matrix least-squares on F ²
Data / restraints / parameters	9294 / 1 / 694
Treatment of hydrogen atoms	Riding atoms
Goodness-of-fit on F ²	1.488
Final R indices [I > 2σ(I)]	R1 = 0.0504, wR2 = 0.0895
R indices (all data)	R1 = 0.0649, wR2 = 0.0932
Max shift/error	0.000
Average shift/error	0.000
Absolute structure parameter	-0.01(2)
Largest diff. peak and hole	0.599 and -0.327 Å ³
Disorder present	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (2). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	<u>x</u>	<u>y</u>	<u>z</u>	<u>U(eq)</u>
MnA	3974(1)	3057(1)	3484(1)	25(1)
O(1A)	4692(2)	3699(2)	3454(2)	30(1)
O(2A)	4625(2)	2316(2)	3501(2)	33(1)
N(1A)	3232(2)	3095(2)	2509(2)	29(1)
N(2A)	3805(2)	3795(2)	4184(2)	22(1)
N(3A)	3621(2)	2393(2)	4055(2)	24(1)
C(1A)	3958(2)	4487(2)	4228(3)	28(1)
C(2A)	3713(2)	1692(2)	4142(3)	26(1)
C(3A)	3467(2)	3512(2)	4694(3)	27(1)
C(4A)	3091(2)	2772(2)	4241(3)	26(1)
C(11A)	4658(3)	4422(3)	3446(3)	26(1)
C(12A)	5014(2)	4818(3)	3084(3)	32(1)
C(13A)	5029(3)	5571(3)	3096(3)	38(1)
C(14A)	4689(3)	5975(3)	3456(3)	38(1)
C(15A)	4340(3)	5614(3)	3814(3)	35(1)
C(16A)	4301(3)	4831(2)	3805(3)	28(1)
C(21A)	4531(3)	1592(3)	3515(3)	28(1)
C(22A)	4865(3)	1123(3)	3187(3)	38(1)
C(23A)	4788(3)	378(3)	3178(3)	40(1)
C(24A)	4391(3)	46(3)	3520(3)	39(1)
C(25A)	4058(3)	499(3)	3852(3)	34(1)
C(26A)	4115(2)	1264(3)	3845(3)	27(1)
C(31A)	2908(2)	4036(2)	4691(3)	22(1)
C(32A)	2269(2)	4306(2)	3836(3)	31(1)
C(33A)	1770(3)	4802(3)	3832(3)	39(1)
C(34A)	1887(3)	5045(3)	4662(3)	38(1)
C(35A)	2508(3)	4777(3)	5509(3)	39(1)
C(36A)	3018(3)	4270(3)	5518(3)	36(1)
C(41A)	2872(3)	2346(2)	4809(3)	26(1)
C(42A)	2122(3)	2058(3)	4368(3)	35(1)
C(43A)	1910(3)	1673(3)	4889(4)	46(1)
C(44A)	2418(3)	1586(3)	5839(4)	45(1)
C(45A)	3175(3)	1863(3)	6284(3)	47(1)
C(46A)	3391(3)	2241(3)	5773(3)	36(1)
MnB	463(1)	3241(1)	1576(1)	28(1)
O(1B)	1039(2)	4001(2)	1465(2)	30(1)
O(2B)	1199(2)	2611(2)	1588(2)	31(1)
N(1B)	685(2)	3193(2)	2588(2)	35(1)
N(2B)	-440(2)	3895(2)	1044(2)	24(1)
N(3B)	-358(2)	2497(2)	885(2)	24(1)
C(1B)	-455(2)	4587(2)	938(3)	29(1)
C(2B)	-243(3)	1808(2)	829(3)	29(1)
C(3B)	-1133(2)	3491(2)	875(3)	26(1)
C(4B)	-1173(2)	2773(2)	377(3)	24(1)
C(11B)	907(3)	4708(3)	1406(3)	27(1)
C(12B)	1517(3)	5194(3)	1601(3)	33(1)
C(13B)	1397(3)	5950(3)	1531(3)	37(1)

C(14B)	698(3)	6262(3)	1271(3)	37(1)
C(15B)	103(3)	5802(3)	1074(3)	35(1)
C(16B)	195(3)	5032(2)	1144(3)	28(1)
C(21B)	1193(3)	1890(3)	1640(3)	26(1)
C(22B)	1895(3)	1496(3)	2033(3)	33(1)
C(23B)	1917(3)	747(3)	2076(3)	35(1)
C(24B)	1243(3)	334(3)	1711(3)	36(1)
C(25B)	553(3)	694(3)	1303(3)	36(1)
C(26B)	505(3)	1469(3)	1268(3)	27(1)
C(31B)	-1885(2)	3902(2)	366(3)	24(1)
C(32B)	-2172(3)	4175(3)	874(3)	39(1)
C(33B)	-2877(3)	4543(3)	410(4)	46(1)
C(34B)	-3286(3)	4664(3)	-544(4)	43(1)
C(35B)	-3000(3)	4415(3)	-1043(3)	39(1)
C(36B)	-2299(3)	4047(2)	-591(3)	29(1)
C(41B)	-1727(2)	2224(2)	348(3)	22(1)
C(42B)	-1582(2)	1911(2)	1177(3)	29(1)
C(43B)	-2089(3)	1401(2)	1130(3)	36(1)
C(44B)	-2752(3)	1197(3)	270(3)	36(1)
C(45B)	-2903(3)	1508(3)	-550(3)	37(1)
C(46B)	-2394(3)	2021(2)	-515(3)	30(1)
C(50)	-2443(5)	3501(4)	2569(5)	73(2)
N(50)	-2202(3)	4044(3)	2961(4)	82(2)
C(51)	-2735(6)	2849(4)	2041(7)	172(5)
C(60)	5042(4)	3213(4)	1604(5)	74(2)
N(60)	5582(4)	3486(4)	1714(7)	162(4)
C(61)	4367(3)	2894(3)	1463(4)	65(2)
C(70)	128(4)	3147(4)	4021(4)	67(2)
N(70)	-490(4)	2927(3)	3461(4)	97(2)
C(71)	905(3)	3414(3)	4724(4)	75(2)

Table S3. Bond lengths [Å] and angles [deg] for (2).

MnA-N(1A)	1.509(3)
MnA-O(2A)	1.905(3)
MnA-O(1A)	1.927(3)
MnA-N(3A)	1.949(4)
MnA-N(2A)	1.967(3)
O(1A)-C(11A)	1.317(5)
O(2A)-C(21A)	1.336(6)
N(2A)-C(1A)	1.289(5)
N(2A)-C(3A)	1.499(5)
N(3A)-C(2A)	1.286(5)
N(3A)-C(4A)	1.487(5)
C(1A)-C(16A)	1.427(6)
C(2A)-C(26A)	1.437(6)
C(3A)-C(31A)	1.507(6)
C(3A)-C(4A)	1.531(5)
C(4A)-C(41A)	1.510(6)
C(11A)-C(12A)	1.410(6)
C(11A)-C(16A)	1.422(6)
C(12A)-C(13A)	1.370(6)

C(13A)-C(14A)	1.390(7)
C(14A)-C(15A)	1.363(6)
C(15A)-C(16A)	1.426(6)
C(21A)-C(22A)	1.410(6)
C(21A)-C(26A)	1.414(6)
C(22A)-C(23A)	1.364(7)
C(23A)-C(24A)	1.400(7)
C(24A)-C(25A)	1.393(6)
C(25A)-C(26A)	1.398(6)
C(31A)-C(36A)	1.376(6)
C(31A)-C(32A)	1.401(6)
C(32A)-C(33A)	1.377(6)
C(33A)-C(34A)	1.380(6)
C(34A)-C(35A)	1.379(6)
C(35A)-C(36A)	1.405(6)
C(41A)-C(46A)	1.388(6)
C(41A)-C(42A)	1.400(6)
C(42A)-C(43A)	1.397(6)
C(43A)-C(44A)	1.363(7)
C(44A)-C(45A)	1.404(7)
C(45A)-C(46A)	1.380(6)
MnB-N(1B)	1.531(3)
MnB-O(2B)	1.910(3)
MnB-O(1B)	1.912(3)
MnB-N(2B)	1.966(3)
MnB-N(3B)	1.971(3)
O(1B)-C(11B)	1.308(6)
O(2B)-C(21B)	1.316(5)
N(2B)-C(1B)	1.269(5)
N(2B)-C(3B)	1.500(5)
N(3B)-C(2B)	1.291(5)
N(3B)-C(4B)	1.494(5)
C(1B)-C(16B)	1.444(6)
C(2B)-C(26B)	1.433(6)
C(3B)-C(31B)	1.497(6)
C(3B)-C(4B)	1.540(5)
C(4B)-C(41B)	1.508(5)
C(11B)-C(16B)	1.417(6)
C(11B)-C(12B)	1.427(6)
C(12B)-C(13B)	1.391(7)
C(13B)-C(14B)	1.384(7)
C(14B)-C(15B)	1.374(6)
C(15B)-C(16B)	1.411(6)
C(21B)-C(22B)	1.414(6)
C(21B)-C(26B)	1.422(6)
C(22B)-C(23B)	1.365(6)
C(23B)-C(24B)	1.393(7)
C(24B)-C(25B)	1.363(6)
C(25B)-C(26B)	1.412(6)
C(31B)-C(36B)	1.384(6)
C(31B)-C(32B)	1.404(6)
C(32B)-C(33B)	1.386(7)
C(33B)-C(34B)	1.373(7)
C(34B)-C(35B)	1.374(6)

C(35B)-C(36B)	1.380(6)
C(41B)-C(46B)	1.393(6)
C(41B)-C(42B)	1.402(6)
C(42B)-C(43B)	1.378(6)
C(43B)-C(44B)	1.387(6)
C(44B)-C(45B)	1.382(6)
C(45B)-C(46B)	1.392(6)
C(50)-N(50)	1.141(7)
C(50)-C(51)	1.407(9)
C(60)-N(60)	1.147(7)
C(60)-C(61)	1.415(7)
C(70)-N(70)	1.159(7)
C(70)-C(71)	1.453(8)
N(1A)-MnA-O(2A)	108.9(2)
N(1A)-MnA-O(1A)	105.4(2)
O(2A)-MnA-O(1A)	82.39(13)
N(1A)-MnA-N(3A)	98.4(2)
O(2A)-MnA-N(3A)	91.56(14)
O(1A)-MnA-N(3A)	156.10(13)
N(1A)-MnA-N(2A)	102.8(2)
O(2A)-MnA-N(2A)	148.22(14)
O(1A)-MnA-N(2A)	90.91(14)
N(3A)-MnA-N(2A)	82.11(13)
C(11A)-O(1A)-MnA	124.7(3)
C(21A)-O(2A)-MnA	125.9(3)
C(1A)-N(2A)-C(3A)	119.0(3)
C(1A)-N(2A)-MnA	125.3(3)
C(3A)-N(2A)-MnA	115.6(2)
C(2A)-N(3A)-C(4A)	121.1(4)
C(2A)-N(3A)-MnA	126.8(3)
C(4A)-N(3A)-MnA	111.3(2)
N(2A)-C(1A)-C(16A)	125.3(4)
N(3A)-C(2A)-C(26A)	125.1(4)
N(2A)-C(3A)-C(31A)	113.8(3)
N(2A)-C(3A)-C(4A)	106.3(3)
C(31A)-C(3A)-C(4A)	112.5(3)
N(3A)-C(4A)-C(41A)	116.1(3)
N(3A)-C(4A)-C(3A)	106.7(3)
C(41A)-C(4A)-C(3A)	112.2(4)
O(1A)-C(11A)-C(12A)	118.6(4)
O(1A)-C(11A)-C(16A)	123.8(4)
C(12A)-C(11A)-C(16A)	117.6(4)
C(13A)-C(12A)-C(11A)	121.3(5)
C(12A)-C(13A)-C(14A)	121.4(5)
C(15A)-C(14A)-C(13A)	119.2(5)
C(14A)-C(15A)-C(16A)	121.3(5)
C(11A)-C(16A)-C(15A)	119.2(4)
C(11A)-C(16A)-C(1A)	122.3(4)
C(15A)-C(16A)-C(1A)	118.4(4)
O(2A)-C(21A)-C(22A)	118.5(4)
O(2A)-C(21A)-C(26A)	123.8(4)
C(22A)-C(21A)-C(26A)	117.7(4)
C(23A)-C(22A)-C(21A)	121.5(5)

C(22A)-C(23A)-C(24A)	121.3(5)
C(25A)-C(24A)-C(23A)	118.2(5)
C(24A)-C(25A)-C(26A)	121.3(5)
C(25A)-C(26A)-C(21A)	119.9(4)
C(25A)-C(26A)-C(2A)	117.8(4)
C(21A)-C(26A)-C(2A)	122.2(4)
C(36A)-C(31A)-C(32A)	118.6(4)
C(36A)-C(31A)-C(3A)	121.3(4)
C(32A)-C(31A)-C(3A)	120.1(4)
C(33A)-C(32A)-C(31A)	120.2(4)
C(32A)-C(33A)-C(34A)	121.1(5)
C(35A)-C(34A)-C(33A)	119.4(5)
C(34A)-C(35A)-C(36A)	119.7(4)
C(31A)-C(36A)-C(35A)	120.9(4)
C(46A)-C(41A)-C(42A)	118.2(4)
C(46A)-C(41A)-C(4A)	121.9(4)
C(42A)-C(41A)-C(4A)	119.9(4)
C(43A)-C(42A)-C(41A)	120.4(4)
C(44A)-C(43A)-C(42A)	120.9(5)
C(43A)-C(44A)-C(45A)	119.0(5)
C(46A)-C(45A)-C(44A)	120.4(5)
C(45A)-C(46A)-C(41A)	121.0(4)
N(1B)-MnB-O(2B)	103.4(2)
N(1B)-MnB-O(1B)	110.7(2)
O(2B)-MnB-O(1B)	83.43(13)
N(1B)-MnB-N(2B)	98.9(2)
O(2B)-MnB-N(2B)	157.53(13)
O(1B)-MnB-N(2B)	90.47(14)
N(1B)-MnB-N(3B)	104.3(2)
O(2B)-MnB-N(3B)	90.88(14)
O(1B)-MnB-N(3B)	144.97(14)
N(2B)-MnB-N(3B)	81.75(13)
C(11B)-O(1B)-MnB	127.1(3)
C(21B)-O(2B)-MnB	124.0(3)
C(1B)-N(2B)-C(3B)	121.1(4)
C(1B)-N(2B)-MnB	127.4(3)
C(3B)-N(2B)-MnB	111.1(2)
C(2B)-N(3B)-C(4B)	118.9(3)
C(2B)-N(3B)-MnB	125.2(3)
C(4B)-N(3B)-MnB	115.9(3)
N(2B)-C(1B)-C(16B)	125.3(4)
N(3B)-C(2B)-C(26B)	125.0(4)
C(31B)-C(3B)-N(2B)	116.6(3)
C(31B)-C(3B)-C(4B)	113.0(3)
N(2B)-C(3B)-C(4B)	105.4(3)
N(3B)-C(4B)-C(41B)	113.4(3)
N(3B)-C(4B)-C(3B)	106.0(3)
C(41B)-C(4B)-C(3B)	112.2(3)
O(1B)-C(11B)-C(16B)	124.8(4)
O(1B)-C(11B)-C(12B)	118.1(4)
C(16B)-C(11B)-C(12B)	117.1(5)
C(13B)-C(12B)-C(11B)	119.9(5)
C(14B)-C(13B)-C(12B)	122.7(5)
C(15B)-C(14B)-C(13B)	118.2(5)

C(14B)-C(15B)-C(16B)	121.5(5)
C(15B)-C(16B)-C(11B)	120.6(4)
C(15B)-C(16B)-C(1B)	118.2(4)
C(11B)-C(16B)-C(1B)	121.2(4)
O(2B)-C(21B)-C(22B)	119.3(4)
O(2B)-C(21B)-C(26B)	123.6(4)
C(22B)-C(21B)-C(26B)	117.0(4)
C(23B)-C(22B)-C(21B)	121.7(4)
C(22B)-C(23B)-C(24B)	121.3(4)
C(25B)-C(24B)-C(23B)	118.6(5)
C(24B)-C(25B)-C(26B)	122.0(5)
C(25B)-C(26B)-C(21B)	119.3(4)
C(25B)-C(26B)-C(2B)	118.8(4)
C(21B)-C(26B)-C(2B)	121.9(4)
C(36B)-C(31B)-C(32B)	118.4(4)
C(36B)-C(31B)-C(3B)	122.1(4)
C(32B)-C(31B)-C(3B)	119.4(4)
C(33B)-C(32B)-C(31B)	120.1(5)
C(34B)-C(33B)-C(32B)	120.2(5)
C(33B)-C(34B)-C(35B)	120.0(5)
C(34B)-C(35B)-C(36B)	120.4(5)
C(35B)-C(36B)-C(31B)	120.7(4)
C(46B)-C(41B)-C(42B)	119.1(4)
C(46B)-C(41B)-C(4B)	119.7(4)
C(42B)-C(41B)-C(4B)	121.2(4)
C(43B)-C(42B)-C(41B)	120.0(4)
C(42B)-C(43B)-C(44B)	120.8(4)
C(45B)-C(44B)-C(43B)	119.5(4)
C(44B)-C(45B)-C(46B)	120.4(4)
C(45B)-C(46B)-C(41B)	120.1(4)
N(50)-C(50)-C(51)	176.4(8)
N(60)-C(60)-C(61)	178.6(8)
N(70)-C(70)-C(71)	179.4(7)

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (2). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	<u>U11</u>	<u>U22</u>	<u>U33</u>	<u>U23</u>	<u>U13</u>	<u>U12</u>
MnA	23(1)	31(1)	21(1)	1(1)	13(1)	0(1)
O(1A)	23(2)	38(2)	29(2)	3(2)	16(2)	-1(2)
O(2A)	32(2)	35(2)	40(2)	3(2)	26(2)	2(2)
N(1A)	30(2)	30(2)	26(2)	1(2)	16(2)	-3(2)
N(2A)	19(2)	28(2)	18(2)	1(2)	9(2)	-1(2)
N(3A)	22(2)	28(2)	19(2)	4(2)	11(2)	5(2)
C(1A)	21(2)	38(3)	16(2)	2(2)	5(2)	1(2)
C(2A)	21(2)	32(3)	20(2)	7(2)	9(2)	5(2)
C(3A)	23(2)	38(3)	19(2)	0(2)	12(2)	-1(2)
C(4A)	25(2)	26(2)	26(2)	3(2)	14(2)	1(2)
C(11A)	15(2)	36(3)	16(3)	-3(2)	2(2)	-5(2)
C(12A)	26(3)	43(3)	25(3)	-4(2)	13(2)	-11(2)

C(13A)	35(3)	42(3)	29(3)	4(2)	13(2)	-11(2)
C(14A)	40(3)	31(3)	30(3)	2(2)	12(3)	-6(2)
C(15A)	31(3)	43(3)	24(3)	1(2)	11(2)	-1(2)
C(16A)	23(3)	31(3)	20(2)	2(2)	7(2)	-6(2)
C(21A)	18(2)	36(3)	25(3)	2(2)	10(2)	5(2)
C(22A)	33(3)	42(3)	36(3)	-2(2)	20(3)	1(2)
C(23A)	31(3)	48(4)	38(3)	-8(2)	18(3)	4(2)
C(24A)	38(3)	32(3)	39(3)	0(2)	18(3)	5(2)
C(25A)	28(3)	36(3)	37(3)	5(2)	18(2)	6(2)
C(26A)	21(2)	31(3)	20(3)	5(2)	6(2)	6(2)
C(31A)	21(2)	22(2)	22(2)	-2(2)	12(2)	-4(2)
C(32A)	30(3)	35(3)	28(3)	-3(2)	17(2)	1(2)
C(33A)	36(3)	43(3)	35(3)	-1(2)	20(2)	3(2)
C(34A)	39(3)	43(3)	36(3)	-9(2)	23(3)	1(2)
C(35A)	50(3)	43(3)	33(3)	-17(2)	30(3)	-6(3)
C(36A)	38(3)	45(3)	28(3)	-5(2)	21(3)	-13(2)
C(41A)	29(3)	27(2)	29(3)	4(2)	21(2)	6(2)
C(42A)	31(3)	42(3)	31(3)	0(2)	17(2)	0(2)
C(43A)	32(3)	55(4)	57(4)	6(3)	28(3)	-6(3)
C(44A)	45(3)	53(3)	52(4)	6(3)	36(3)	1(3)
C(45A)	56(3)	54(3)	33(3)	13(2)	26(3)	1(3)
C(46A)	31(3)	40(3)	31(3)	8(2)	15(2)	3(2)
MnB	21(1)	34(1)	26(1)	1(1)	12(1)	-2(1)
O(1B)	22(2)	35(2)	35(2)	2(2)	16(2)	-5(2)
O(2B)	24(2)	34(2)	36(2)	8(2)	18(2)	2(2)
N(1B)	28(2)	42(2)	29(2)	5(2)	12(2)	2(2)
N(2B)	20(2)	27(2)	19(2)	2(2)	9(2)	0(2)
N(3B)	19(2)	30(2)	22(2)	2(2)	11(2)	0(2)
C(1B)	22(2)	41(3)	22(3)	-3(2)	12(2)	-4(2)
C(2B)	28(3)	33(3)	28(3)	1(2)	17(2)	1(2)
C(3B)	19(2)	34(3)	25(2)	0(2)	13(2)	-5(2)
C(4B)	20(2)	32(3)	20(2)	2(2)	11(2)	2(2)
C(11B)	29(3)	34(3)	18(3)	-6(2)	13(2)	-12(2)
C(12B)	35(3)	40(3)	29(3)	-3(2)	21(2)	-7(2)
C(13B)	46(3)	42(3)	30(3)	-10(2)	26(3)	-17(3)
C(14B)	45(3)	31(3)	40(3)	-7(2)	28(3)	-9(2)
C(15B)	39(3)	39(3)	27(3)	-1(2)	19(2)	-4(2)
C(16B)	29(3)	29(3)	20(2)	5(2)	11(2)	-2(2)
C(21B)	23(3)	34(3)	21(3)	5(2)	13(2)	4(2)
C(22B)	30(3)	42(3)	27(3)	2(2)	17(2)	3(2)
C(23B)	31(3)	45(3)	29(3)	4(2)	18(2)	12(2)
C(24B)	35(3)	45(3)	40(3)	2(2)	27(3)	13(2)
C(25B)	41(3)	34(3)	45(3)	3(2)	31(3)	1(2)
C(26B)	26(3)	37(3)	22(2)	2(2)	15(2)	6(2)
C(31B)	22(2)	24(2)	30(3)	3(2)	17(2)	-1(2)
C(32B)	39(3)	50(3)	35(3)	0(2)	25(3)	-1(3)
C(33B)	42(3)	52(3)	54(4)	-7(3)	33(3)	6(3)
C(34B)	28(3)	40(3)	55(4)	-5(3)	20(3)	6(2)
C(35B)	30(3)	38(3)	35(3)	-3(2)	10(3)	1(2)
C(36B)	24(3)	27(3)	31(3)	-3(2)	12(2)	-3(2)
C(41B)	17(2)	24(2)	22(2)	5(2)	10(2)	8(2)
C(42B)	23(2)	35(3)	28(3)	0(2)	14(2)	-1(2)
C(43B)	34(3)	39(3)	41(3)	6(2)	24(2)	-1(2)
C(44B)	24(3)	36(3)	46(3)	4(2)	19(3)	-5(2)

C(45B)	24(3)	36(3)	37(3)	-4(2)	8(2)	-4(2)
C(46B)	29(3)	30(3)	28(3)	1(2)	14(2)	8(2)
C(50)	113(6)	41(4)	104(6)	-5(3)	85(5)	-8(4)
N(50)	103(5)	86(4)	79(4)	8(3)	66(4)	4(4)
C(51)	293(14)	97(7)	275(13)	-93(8)	250(12)	-105(8)
C(60)	90(5)	50(4)	106(5)	-9(4)	71(4)	-6(4)
N(60)	135(7)	126(6)	280(11)	-26(6)	151(8)	-52(5)
C(61)	65(4)	74(5)	70(4)	-7(3)	46(3)	-2(3)
C(70)	91(5)	45(4)	76(4)	-14(4)	54(4)	4(4)
N(70)	96(5)	72(4)	116(5)	-42(4)	55(4)	-18(4)
C(71)	69(4)	83(5)	66(4)	-12(3)	36(4)	-11(4)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for (2).

	\bar{x}	\bar{y}	\bar{z}	$U(\text{eq})$
H(1AC)	3834(2)	4785(2)	4563(3)	80
H(2AA)	3504(2)	1442(2)	4420(3)	80
H(3AA)	3895(2)	3421(2)	5351(3)	80
H(4AA)	2609(2)	2876(2)	3627(3)	80
H(12A)	5242(2)	4564(3)	2833(3)	80
H(13A)	5271(3)	5817(3)	2857(3)	80
H(14A)	4701(3)	6486(3)	3454(3)	80
H(15A)	4123(3)	5883(3)	4068(3)	80
H(22A)	5145(3)	1326(3)	2971(3)	80
H(23A)	5004(3)	85(3)	2941(3)	80
H(24A)	4350(3)	-462(3)	3526(3)	80
H(25A)	3792(3)	287(3)	4082(3)	80
H(32A)	2181(2)	4150(2)	3270(3)	80
H(33A)	1346(3)	4976(3)	3260(3)	80
H(34A)	1551(3)	5386(3)	4651(3)	80
H(35A)	2589(3)	4932(3)	6073(3)	80
H(36A)	3436(3)	4090(3)	6090(3)	80
H(42A)	1764(3)	2123(3)	3724(3)	80
H(43A)	1414(3)	1473(3)	4585(4)	80
H(44A)	2266(3)	1347(3)	6186(4)	80
H(45A)	3534(3)	1791(3)	6927(3)	80
H(46A)	3892(3)	2429(3)	6079(3)	80
H(1BC)	-923(2)	4826(2)	710(3)	80
H(2BA)	-677(3)	1509(2)	476(3)	80
H(3BA)	-1015(2)	3356(2)	1494(3)	80
H(4BA)	-1354(2)	2890(2)	-273(3)	80
H(12B)	1995(3)	5005(3)	1774(3)	80
H(13B)	1802(3)	6258(3)	1664(3)	80
H(14B)	634(3)	6769(3)	1231(3)	80
H(15B)	-372(3)	6004(3)	890(3)	80
H(22B)	2354(3)	1754(3)	2267(3)	80
H(23B)	2392(3)	507(3)	2356(3)	80
H(24B)	1264(3)	-176(3)	1746(3)	80
H(25B)	99(3)	421(3)	1040(3)	80
H(32B)	-1889(3)	4109(3)	1523(3)	80

H(33B)	-3074(3)	4709(3)	745(4)	80
H(34B)	-3756(3)	4914(3)	-853(4)	80
H(35B)	-3279(3)	4495(3)	-1690(3)	80
H(36B)	-2104(3)	3894(2)	-932(3)	80
H(42B)	-1143(2)	2048(2)	1759(3)	80
H(43B)	-1986(3)	1191(2)	1682(3)	80
H(44B)	-3093(3)	853(3)	245(3)	80
H(45B)	-3348(3)	1374(3)	-1128(3)	80
H(46B)	-2499(3)	2228(2)	-1070(3)	80
H(51A)	-2896(6)	2522(4)	2337(7)	258
H(51B)	-2338(6)	2617(4)	2011(7)	258
H(51C)	-3172(6)	2962(4)	1415(7)	258
H(61A)	4487(3)	2695(3)	2047(4)	98
H(61B)	4184(3)	2509(3)	1003(4)	98
H(61C)	3971(3)	3263(3)	1242(4)	98
H(71A)	1198(3)	3034(3)	5178(4)	112
H(71B)	872(3)	3834(3)	5037(4)	112
H(71C)	1157(3)	3551(3)	4423(4)	112



