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

Identification code	jesusccd
Empirical formula	C19 H24 N2 O2
Formula weight	312.40
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, P 21 21 21
Unit cell dimensions	a = 7.021(2) A alpha = 90 deg. b = 13.024(4) A beta = 90 deg. c = 18.216(7) A gamma = 90 deg.
Volume	1665.7(9) A^3
Z, Calculated density	4, 1.246 Mg/m^3
Absorption coefficient	0.081 mm^-1
F(000)	672
Crystal size	0.4 x 0.3 x 0.2 mm
Theta range for data collection	2.73 to 28.58 deg.
Limiting indices	0<=h<=9, 0<=k<=17, 0<=l<=24
Reflections collected / unique	2315 / 2315 [R(int) = 0.0000]
Completeness to theta = 28.58	94.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2315 / 0 / 237
Goodness-of-fit on F^2	1.094
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1443
R indices (all data)	R1 = 0.0570, wR2 = 0.1471
Absolute structure parameter	0(10)
Extinction coefficient	0.049(13)
Largest diff. peak and hole	0.340 and -0.207 e.A^-3

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for jesusccd.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	4527(3)	499(2)	-92(1)	45(1)
O(1)	5595(3)	1628(1)	-972(1)	51(1)
O(2)	11144(3)	1524(1)	268(1)	51(1)
C(2)	5714(3)	822(2)	-629(1)	36(1)
C(3)	7259(3)	-539(2)	-1469(1)	32(1)
N(4)	5459(3)	-1089(2)	-1598(1)	36(1)
C(5)	9332(4)	1093(2)	142(2)	47(1)
C(6)	9256(3)	541(2)	-587(1)	35(1)
C(7)	7307(3)	19(2)	-710(1)	30(1)
C(8)	6835(3)	-720(2)	-96(1)	33(1)
C(9)	7797(4)	-1563(2)	165(1)	44(1)
C(10)	7104(6)	-2075(2)	773(2)	59(1)
C(11)	5471(6)	-1756(3)	1106(2)	67(1)
C(12)	4455(5)	-913(3)	850(2)	61(1)
C(13)	5167(3)	-400(2)	245(1)	40(1)
C(14)	7800(5)	117(2)	-2143(1)	50(1)
C(15)	6701(5)	-314(2)	-2805(1)	52(1)
C(16)	4607(6)	-50(2)	-2702(2)	61(1)
C(17)	3993(4)	-426(2)	-1933(2)	48(1)
C(18)	9770(30)	-2134(14)	-3484(8)	82(5)
C(19)	9022(15)	-1629(13)	-2926(6)	53(3)
C(18)	10178(14)	-1741(10)	-3226(8)	84(3)
C(19)	8655(17)	-2092(11)	-2960(4)	63(2)
C(20)	6839(5)	-1490(3)	-2840(1)	51(1)
C(21)	5874(5)	-1911(2)	-2132(1)	45(1)

Table 3. Bond lengths [A] and angles [deg] for jesusccd.

N(1)-C(2)	1.352(4)
N(1)-C(13)	1.397(4)
N(1)-H(1)	1.0125
O(1)-C(2)	1.224(3)
O(2)-C(5)	1.409(3)
O(2)-H(2)	0.8183
C(2)-C(7)	1.538(3)
C(3)-N(4)	1.471(3)
C(3)-C(14)	1.542(3)
C(3)-C(7)	1.563(3)
C(3)-H(3)	1.0080
N(4)-C(17)	1.476(3)
N(4)-C(21)	1.477(3)
C(5)-C(6)	1.512(3)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.544(3)
C(6)-H(6A)	1.0274
C(6)-H(6B)	1.0646

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C(7)-C(8)	1.512(3)
C(8)-C(9)	1.374(3)
C(8)-C(13)	1.389(3)
C(9)-C(10)	1.381(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.362(6)
C(10)-H(10)	0.9300
C(11)-C(12)	1.390(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.382(4)
C(12)-H(12)	0.9300
C(14)-C(15)	1.538(4)
C(14)-H(14A)	1.0976
C(14)-H(14B)	0.9036
C(15)-C(16)	1.522(5)
C(15)-C(20)	1.535(4)
C(15)-H(15)	1.1116
C(16)-C(17)	1.546(5)
C(16)-H(16A)	0.8244
C(16)-H(16B)	0.9108
C(17)-H(17A)	1.0051
C(17)-H(17B)	1.0557
C(18)-C(19)	1.32(2)
C(18)-H(181)	0.9379
C(18)-H(182)	0.9379
C(19)-C(20)	1.552(11)
C(19)-H(191)	0.9300
C(18)-C(19)	1.259(16)
C(18)-H(183)	0.9302
C(18)-H(184)	0.9302
C(19)-C(20)	1.513(8)
C(19)-H(192)	0.9300
C(20)-C(21)	1.556(4)
C(20)-H(20)	1.1675
C(21)-H(21A)	1.0885
C(21)-H(21B)	1.1506

C(2)-N(1)-C(13)	112.3(2)
C(2)-N(1)-H(1)	119.3
C(13)-N(1)-H(1)	128.0
C(5)-O(2)-H(2)	109.3
O(1)-C(2)-N(1)	126.4(2)
O(1)-C(2)-C(7)	125.7(2)
N(1)-C(2)-C(7)	107.8(2)
N(4)-C(3)-C(14)	110.79(18)
N(4)-C(3)-C(7)	112.70(17)
C(14)-C(3)-C(7)	116.17(19)
N(4)-C(3)-H(3)	104.8
C(14)-C(3)-H(3)	102.9
C(7)-C(3)-H(3)	108.3
C(3)-N(4)-C(17)	112.32(18)
C(3)-N(4)-C(21)	106.8(2)
C(17)-N(4)-C(21)	106.8(2)
O(2)-C(5)-C(6)	111.3(2)
O(2)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
O(2)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
C(5)-C(6)-C(7)	111.55(19)
C(5)-C(6)-H(6A)	110.6

C(7)-C(6)-H(6A)	107.2
C(5)-C(6)-H(6B)	111.1
C(7)-C(6)-H(6B)	105.4
H(6A)-C(6)-H(6B)	110.8
C(8)-C(7)-C(2)	101.69(18)
C(8)-C(7)-C(6)	111.62(18)
C(2)-C(7)-C(6)	109.34(17)
C(8)-C(7)-C(3)	110.69(17)
C(2)-C(7)-C(3)	112.63(18)
C(6)-C(7)-C(3)	110.59(18)
C(9)-C(8)-C(13)	119.9(2)
C(9)-C(8)-C(7)	131.1(2)
C(13)-C(8)-C(7)	108.9(2)
C(8)-C(9)-C(10)	119.4(3)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	120.4(3)
C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(10)-C(11)-C(12)	121.6(3)
C(10)-C(11)-H(11)	119.2
C(12)-C(11)-H(11)	119.2
C(13)-C(12)-C(11)	117.6(3)
C(13)-C(12)-H(12)	121.2
C(11)-C(12)-H(12)	121.2
C(12)-C(13)-C(8)	121.1(3)
C(12)-C(13)-N(1)	129.7(3)
C(8)-C(13)-N(1)	109.0(2)
C(15)-C(14)-C(3)	107.3(2)
C(15)-C(14)-H(14A)	114.0
C(3)-C(14)-H(14A)	111.9
C(15)-C(14)-H(14B)	103.8
C(3)-C(14)-H(14B)	113.4
H(14A)-C(14)-H(14B)	106.3
C(16)-C(15)-C(20)	107.0(3)
C(16)-C(15)-C(14)	107.8(3)
C(20)-C(15)-C(14)	111.4(2)
C(16)-C(15)-H(15)	117.9
C(20)-C(15)-H(15)	104.2
C(14)-C(15)-H(15)	108.6
C(15)-C(16)-C(17)	108.0(2)
C(15)-C(16)-H(16A)	114.5
C(17)-C(16)-H(16A)	111.1
C(15)-C(16)-H(16B)	96.4
C(17)-C(16)-H(16B)	112.6
H(16A)-C(16)-H(16B)	113.4
N(4)-C(17)-C(16)	111.5(2)
N(4)-C(17)-H(17A)	92.2
C(16)-C(17)-H(17A)	116.5
N(4)-C(17)-H(17B)	113.5
C(16)-C(17)-H(17B)	108.1
H(17A)-C(17)-H(17B)	114.6
C(18)-C(19)-C(20)	121.9(16)
C(20)-C(19)-H(191)	119.1
C(19)-C(18)-H(183)	120.0
C(19)-C(18)-H(184)	120.0
H(183)-C(18)-H(184)	120.0
C(18)-C(19)-C(20)	125.7(13)
C(18)-C(19)-H(192)	117.2
C(20)-C(19)-H(192)	117.1
C(19)-C(20)-C(15)	125.2(7)

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C(19)-C(20)-C(19)	24.7(3)
C(15)-C(20)-C(19)	100.6(7)
C(19)-C(20)-C(21)	107.7(4)
C(15)-C(20)-C(21)	106.9(2)
C(19)-C(20)-C(21)	118.2(5)
C(19)-C(20)-H(20)	109.6
C(15)-C(20)-H(20)	105.6
C(19)-C(20)-H(20)	125.3
C(21)-C(20)-H(20)	98.7
N(4)-C(21)-C(20)	112.1(2)
N(4)-C(21)-H(21A)	102.7
C(20)-C(21)-H(21A)	114.4
N(4)-C(21)-H(21B)	104.2
C(20)-C(21)-H(21B)	110.9
H(21A)-C(21)-H(21B)	112.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for jesusccd. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	29(1)	53(1)	55(1)	-16(1)	3(1)	7(1)
O(1)	57(1)	37(1)	59(1)	-7(1)	-18(1)	7(1)
O(2)	30(1)	52(1)	71(1)	-27(1)	-4(1)	1(1)
C(2)	32(1)	33(1)	44(1)	-10(1)	-9(1)	4(1)
C(3)	34(1)	36(1)	26(1)	-4(1)	-1(1)	1(1)
N(4)	39(1)	36(1)	32(1)	-4(1)	-2(1)	-6(1)
C(5)	36(1)	64(2)	42(1)	-20(1)	3(1)	-11(1)
C(6)	31(1)	42(1)	31(1)	-6(1)	1(1)	-3(1)
C(7)	30(1)	33(1)	27(1)	-5(1)	-2(1)	2(1)
C(8)	36(1)	38(1)	25(1)	-6(1)	1(1)	-3(1)
C(9)	54(2)	41(1)	38(1)	-1(1)	-5(1)	5(1)
C(10)	86(2)	45(1)	45(1)	8(1)	-12(2)	-13(2)
C(11)	95(3)	63(2)	43(2)	7(1)	4(2)	-35(2)
C(12)	57(2)	75(2)	51(2)	-14(2)	22(1)	-22(2)
C(13)	35(1)	44(1)	39(1)	-13(1)	6(1)	-6(1)
C(14)	58(2)	61(2)	31(1)	5(1)	-4(1)	-23(1)
C(15)	68(2)	57(2)	30(1)	9(1)	-10(1)	-17(2)
C(16)	78(2)	44(1)	60(2)	7(1)	-29(2)	4(2)
C(17)	39(1)	50(1)	57(2)	-9(1)	-13(1)	0(1)
C(18)	105(11)	76(8)	66(7)	-24(5)	-3(7)	38(8)
C(19)	54(5)	48(7)	56(5)	-18(4)	22(4)	-11(4)
C(18)	83(6)	79(5)	89(8)	-8(6)	18(5)	-2(5)
C(19)	85(5)	56(5)	49(3)	-2(3)	10(3)	3(4)
C(20)	62(2)	65(2)	28(1)	-8(1)	-6(1)	2(2)
C(21)	64(2)	35(1)	35(1)	-6(1)	-6(1)	-1(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for jesusccd.

	x	y	z	U(eq)
H(5A)	8380	1633	149	57
H(5B)	9035	613	533	57
H(9)	8904	-1786	-65	53
H(10)	7756	-2642	955	71
H(11)	5025	-2111	1514	81
H(12)	3336	-701	1078	73
H(181)	8976	-2418	-3840	99
H(182)	11080	-2206	-3522	99
H(191)	9829	-1349	-2574	63
H(183)	10249	-1056	-3368	100
H(184)	11231	-2167	-3281	100
H(192)	8647	-2781	-2826	76
H(1)	3402	943	51	60
H(2)	11180	2101	91	60
H(3)	8265	-1091	-1468	60
H(6A)	9457	1049	-1012	60
H(6B)	10276	-63	-609	60
H(14A)	9348	151	-2223	60
H(14B)	7396	774	-2111	60
H(15)	7414	-51	-3316	60
H(16A)	4351	563	-2759	60
H(16B)	4157	-458	-3069	60
H(17A)	3015	-989	-1918	60
H(17B)	3653	224	-1612	60
H(20)	5695	-1746	-3267	60
H(21A)	6756	-2437	-1816	60
H(21B)	4405	-2257	-2264	60

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Table 1. Bond lengths [A] for jesusccd.

N(1)-C(2)	1.352(4)
N(1)-C(13)	1.397(4)
N(1)-H(1)	1.0125
O(1)-C(2)	1.224(3)
O(2)-C(5)	1.409(3)
O(2)-H(2)	0.8183
C(2)-C(7)	1.538(3)
C(3)-N(4)	1.471(3)
C(3)-C(14)	1.542(3)
C(3)-C(7)	1.563(3)
C(3)-H(3)	1.0080
N(4)-C(17)	1.476(3)
N(4)-C(21)	1.477(3)
C(5)-C(6)	1.512(3)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.544(3)
C(6)-H(6A)	1.0274
C(6)-H(6B)	1.0646
C(7)-C(8)	1.512(3)
C(8)-C(9)	1.374(3)
C(8)-C(13)	1.389(3)
C(9)-C(10)	1.381(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.362(6)
C(10)-H(10)	0.9300
C(11)-C(12)	1.390(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.382(4)
C(12)-H(12)	0.9300
C(14)-C(15)	1.538(4)
C(14)-H(14A)	1.0976
C(14)-H(14B)	0.9036
C(15)-C(16)	1.522(5)
C(15)-C(20)	1.535(4)
C(15)-H(15)	1.1116
C(16)-C(17)	1.546(5)
C(16)-H(16A)	0.8244
C(16)-H(16B)	0.9108
C(17)-H(17A)	1.0051
C(17)-H(17B)	1.0557
C(18)-C(19)	1.32(2)
C(18)-H(181)	0.9379
C(18)-H(182)	0.9379
C(19)-C(20)	1.552(11)
C(19)-H(191)	0.9300
C(18)-C(19)	1.259(16)
C(18)-H(183)	0.9302
C(18)-H(184)	0.9302
C(19)-C(20)	1.513(8)
C(19)-H(192)	0.9300
C(20)-C(21)	1.556(4)
C(20)-H(20)	1.1675
C(21)-H(21A)	1.0885
C(21)-H(21B)	1.1506

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Table 2. Angles [deg] for jesusccd.

C(2)-N(1)-C(13)	112.3(2)
C(2)-N(1)-H(1)	119.3
C(13)-N(1)-H(1)	128.0
C(5)-O(2)-H(2)	109.3
O(1)-C(2)-N(1)	126.4(2)
O(1)-C(2)-C(7)	125.7(2)
N(1)-C(2)-C(7)	107.8(2)
N(4)-C(3)-C(14)	110.79(18)
N(4)-C(3)-C(7)	112.70(17)
C(14)-C(3)-C(7)	116.17(19)
N(4)-C(3)-H(3)	104.8
C(14)-C(3)-H(3)	102.9
C(7)-C(3)-H(3)	108.3
C(3)-N(4)-C(17)	112.32(18)
C(3)-N(4)-C(21)	106.8(2)
C(17)-N(4)-C(21)	106.8(2)
O(2)-C(5)-C(6)	111.3(2)
O(2)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
O(2)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
C(5)-C(6)-C(7)	111.55(19)
C(5)-C(6)-H(6A)	110.6
C(7)-C(6)-H(6A)	107.2
C(5)-C(6)-H(6B)	111.1
C(7)-C(6)-H(6B)	105.4
H(6A)-C(6)-H(6B)	110.8
C(8)-C(7)-C(2)	101.69(18)
C(8)-C(7)-C(6)	111.62(18)
C(2)-C(7)-C(6)	109.34(17)
C(8)-C(7)-C(3)	110.69(17)
C(2)-C(7)-C(3)	112.63(18)
C(6)-C(7)-C(3)	110.59(18)
C(9)-C(8)-C(13)	119.9(2)
C(9)-C(8)-C(7)	131.1(2)
C(13)-C(8)-C(7)	108.9(2)
C(8)-C(9)-C(10)	119.4(3)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	120.4(3)
C(11)-C(10)-H(10)	119.8
C(9)-C(10)-H(10)	119.8
C(10)-C(11)-C(12)	121.6(3)
C(10)-C(11)-H(11)	119.2
C(12)-C(11)-H(11)	119.2
C(13)-C(12)-C(11)	117.6(3)
C(13)-C(12)-H(12)	121.2
C(11)-C(12)-H(12)	121.2
C(12)-C(13)-C(8)	121.1(3)
C(12)-C(13)-N(1)	129.7(3)
C(8)-C(13)-N(1)	109.0(2)
C(15)-C(14)-C(3)	107.3(2)
C(15)-C(14)-H(14A)	114.0
C(3)-C(14)-H(14A)	111.9
C(15)-C(14)-H(14B)	103.8
C(3)-C(14)-H(14B)	113.4
H(14A)-C(14)-H(14B)	106.3

C(16)-C(15)-C(20)	107.0(3)
C(16)-C(15)-C(14)	107.8(3)
C(20)-C(15)-C(14)	111.4(2)
C(16)-C(15)-H(15)	117.9
C(20)-C(15)-H(15)	104.2
C(14)-C(15)-H(15)	108.6
C(15)-C(16)-C(17)	108.0(2)
C(15)-C(16)-H(16A)	114.5
C(17)-C(16)-H(16A)	111.1
C(15)-C(16)-H(16B)	96.4
C(17)-C(16)-H(16B)	112.6
H(16A)-C(16)-H(16B)	113.4
N(4)-C(17)-C(16)	111.5(2)
N(4)-C(17)-H(17A)	92.2
C(16)-C(17)-H(17A)	116.5
N(4)-C(17)-H(17B)	113.5
C(16)-C(17)-H(17B)	108.1
H(17A)-C(17)-H(17B)	114.6
C(18)-C(19)-C(20)	121.9(16)
C(20)-C(19)-H(191)	119.1
C(19)-C(18)-H(183)	120.0
C(19)-C(18)-H(184)	120.0
H(183)-C(18)-H(184)	120.0
C(18)-C(19)-C(20)	125.7(13)
C(18)-C(19)-H(192)	117.2
C(20)-C(19)-H(192)	117.1
C(19)-C(20)-C(15)	125.2(7)
C(19)-C(20)-C(19)	24.7(3)
C(15)-C(20)-C(19)	100.6(7)
C(19)-C(20)-C(21)	107.7(4)
C(15)-C(20)-C(21)	106.9(2)
C(19)-C(20)-C(21)	118.2(5)
C(19)-C(20)-H(20)	109.6
C(15)-C(20)-H(20)	105.6
C(19)-C(20)-H(20)	125.3
C(21)-C(20)-H(20)	98.7
N(4)-C(21)-C(20)	112.1(2)
N(4)-C(21)-H(21A)	102.7
C(20)-C(21)-H(21A)	114.4
N(4)-C(21)-H(21B)	104.2
C(20)-C(21)-H(21B)	110.9
H(21A)-C(21)-H(21B)	112.0

Symmetry transformations used to generate equivalent atoms: