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Fraktionelle Atomkoordinaten x, y, z ($\times 10^4$) und äquivalente isotrope Temperaturfaktoren U_{eq} ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
O(1)	2397(6)	4491(5)	-848(2)	53(6)
O(2)	864(7)	5440(7)	-767(4)	67(6)
O(3)	3498(5)	6970(6)	-1486(2)	56(4)
C(1)	1616(11)	5702(9)	-1357(4)	68(10)
C(2)	823(8)	7512(9)	-125(4)	61(7)
C(3)	1455(7)	9109(8)	-285(3)	57(6)
C(4)	2048(7)	8196(7)	-1108(3)	52(6)
C(5)	2887(7)	6766(7)	-711(3)	55(6)
C(6)	4180(10)	5168(13)	-1411(6)	63(11)
C(7)	3263(6)	7072(7)	424(3)	33(5)
C(8)	3811(7)	8988(8)	674(4)	72(7)
C(9)	4140(8)	9328(10)	1720(4)	92(8)
C(10)	3916(7)	7765(10)	2519(3)	79(6)
C(11)	3381(7)	5869(10)	2276(3)	67(7)
C(12)	3042(8)	5524(9)	1236(3)	55(7)

Bindungslängen [$\text{\AA}$] und -winkel [$^\circ$]

O(1)-C(5)	1.461(8)	O(2)-C(1)-C(4)	109.6(6)
O(1)-C(1)	1.47(2)	O(1)-C(1)-C(4)	89.7(8)
O(2)-C(2)	1.394(6)	C(3)-C(2)-O(2)	113.7(8)
O(2)-C(1)	1.40(2)	C(2)-C(3)-C(4)	110.5(5)
O(3)-C(5)	1.377(9)	C(3)-C(4)-C(1)	99.9(7)
O(3)-C(6)	1.431(12)	C(3)-C(4)-C(5)	117.9(4)
C(1)-C(4)	1.543(9)	C(1)-C(4)-C(5)	86.8(6)
C(2)-C(3)	1.323(12)	O(3)-C(5)-O(1)	110.2(4)
C(3)-C(4)	1.485(10)	O(3)-C(5)-C(7)	114.4(8)
C(4)-C(5)	1.553(12)	O(1)-C(5)-C(7)	111.7(3)
C(5)-C(7)	1.501(7)	O(3)-C(5)-C(4)	107.9(4)
C(7)-C(8)	1.367(9)	O(1)-C(5)-C(4)	89.7(6)
C(7)-C(12)	1.376(6)	C(7)-C(5)-C(4)	120.2(5)
C(8)-C(9)	1.379(9)	C(8)-C(7)-C(12)	118.6(5)
C(9)-C(10)	1.370(8)	C(8)-C(7)-C(5)	119.7(4)
C(10)-C(11)	1.346(11)	C(12)-C(7)-C(5)	121.6(6)
C(11)-C(12)	1.378(7)	C(9)-C(8)-C(7)	120.2(6)
C(5)-O(1)-C(1)	93.1(5)	C(10)-C(9)-C(8)	120.5(7)
C(2)-O(2)-C(1)	106.2(7)	C(11)-C(10)-C(9)	119.6(5)
C(5)-O(3)-C(6)	114.1(5)	C(10)-C(11)-C(12)	120.4(5)
O(2)-C(1)-O(1)	112.8(5)	C(7)-C(12)-C(11)	120.7(7)

Torsionswinkel [°]

C(2)-O(2)-C(1)-O(1)	94.9(6)	C(1)-C(4)-C(5)-O(3)	104.8(5)
C(2)-O(2)-C(1)-C(4)	-3.3(10)	C(3)-C(4)-C(5)-O(1)	93.2(5)
C(5)-O(1)-C(1)-O(2)	-117.9(5)	C(1)-C(4)-C(5)-O(1)	-6.4(5)
C(5)-O(1)-C(1)-C(4)	-6.7(6)	C(3)-C(4)-C(5)-C(7)	-21.9(9)
C(1)-O(2)-C(2)-C(3)	2.7(11)	C(1)-C(4)-C(5)-C(7)	-121.5(6)
O(2)-C(2)-C(3)-C(4)	-9.1(10)	O(3)-C(5)-C(7)-C(8)	47.8(8)
C(2)-C(3)-C(4)-C(1)	-1.1(8)	O(1)-C(5)-C(7)-C(8)	173.9(8)
C(2)-C(3)-C(4)-C(5)	-92.8(8)	C(4)-C(5)-C(7)-C(8)	-83.1(10)
O(2)-C(1)-C(4)-C(3)	2.7(9)	O(3)-C(5)-C(7)-C(12)	-134.8(7)
O(1)-C(1)-C(4)-C(3)	-111.5(6)	O(1)-C(5)-C(7)-C(12)	-8.8(11)
O(2)-C(1)-C(4)-C(5)	120.5(8)	C(4)-C(5)-C(7)-C(12)	94.2(8)
O(1)-C(1)-C(4)-C(5)	6.3(5)	C(12)-C(7)-C(8)-C(9)	.7(14)
C(6)-O(3)-C(5)-O(1)	-64.7(8)	C(5)-C(7)-C(8)-C(9)	178.1(9)
C(6)-O(3)-C(5)-C(7)	62.2(7)	C(7)-C(8)-C(9)-C(10)	0(2)
C(6)-O(3)-C(5)-C(4)	-161.1(6)	C(8)-C(9)-C(10)-C(11)	1(2)
C(1)-O(1)-C(5)-O(3)	-102.3(7)	C(9)-C(10)-C(11)-C(12)	-1(2)
C(1)-O(1)-C(5)-C(7)	129.4(7)	C(8)-C(7)-C(12)-C(11)	-1.3(14)
C(1)-O(1)-C(5)-C(4)	6.7(5)	C(5)-C(7)-C(12)-C(11)	-178.6(8)
C(3)-C(4)-C(5)-O(3)	-155.6(5)	C(10)-C(11)-C(12)-C(7)	2(2)

Anisotrope Temperaturfaktoren ($\text{\AA}^2 \times 10^3$). Form des Exponenten des anisotropen Temperaturfaktors: $-2\pi^2(h^2a^2 \times 2U_{11} + \dots + 2hka \times b \times U_{12})$.

	U11	U22	U33	U23	U13	U12
O(1)	67(19)	39(2)	52(2)	1(1)	-5(3)	-2(3)
O(2)	60(20)	56(2)	84(3)	13(2)	11(5)	-26(4)
O(3)	56(14)	64(2)	48(2)	1(2)	11(3)	5(4)
C(1)	105(31)	49(3)	48(3)	-5(2)	-10(6)	-15(6)
C(2)	69(22)	55(3)	61(3)	-2(2)	25(5)	10(5)
C(3)	82(20)	42(2)	48(2)	-1(2)	5(4)	11(4)
C(4)	69(20)	43(2)	43(2)	12(2)	-6(4)	-2(4)
C(5)	88(20)	33(2)	44(2)	4(2)	8(4)	-3(4)
C(6)	39(34)	89(5)	60(4)	-2(3)	9(6)	22(7)
C(7)	16(16)	37(2)	45(2)	2(2)	-5(4)	2(3)
C(8)	99(21)	50(3)	64(3)	6(2)	-7(4)	-18(4)
C(9)	138(25)	59(3)	77(3)	13(3)	-12(6)	-20(5)
C(10)	115(19)	74(3)	47(2)	-16(2)	-8(4)	10(6)
C(11)	86(22)	73(3)	41(2)	8(2)	-8(4)	2(5)
C(12)	68(24)	49(2)	49(2)	3(2)	-1(4)	-12(5)

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H-Atomkoordinaten x, y, z ($\times 10^4$) und isotrope Temperaturfaktoren ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(1)	1309(53)	5101(71)	-2120(34)	57(14)
H(2)	238(57)	7531(71)	361(31)	46(15)
H(3)	1504(58)	10620(76)	30(31)	57(14)
H(4)	2115(54)	9201(73)	-1651(32)	54(14)
H(6A)	4467(64)	5262(89)	-2076(46)	78(18)
H(6B)	4460(96)	5264(125)	-873(59)	115(33)
H(6C)	3801(69)	3329(115)	-1471(43)	114(23)
H(8)	3934(54)	10128(80)	107(37)	76(17)
H(9)	4581(65)	10686(85)	1926(35)	69(16)
H(10)	4133	8013	3225	40
H(11)	3093(56)	4783(75)	2815(36)	61(14)
H(12)	2670(51)	4234(63)	1054(25)	28(11)

Fractionelle Atomkoordinaten x, y, z , ($\times 10^4$) und äquivalente isotrope Temperaturfaktoren U_{eq} ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
O(1)	1669(2)	-1223(1)	8065(1)	43(1)
O(2)	-1484(3)	593(2)	7009(2)	89(1)
O(3)	-392(2)	-747(2)	6245(1)	62(1)
C(1)	1175(3)	-1210(2)	9031(2)	41(1)
C(2)	2481(3)	-1377(2)	9968(2)	44(1)
C(3)	3074(3)	-191(2)	10258(2)	48(1)
C(4)	2188(3)	613(2)	9704(2)	46(1)
C(5)	854(3)	105(2)	8918(1)	40(1)
C(6)	1120(3)	-44(2)	7834(1)	36(1)
C(7)	-410(3)	-25(2)	7001(2)	43(1)
C(8)	-1769(4)	-751(3)	5395(2)	70(1)
C(9)	2285(3)	736(2)	7507(1)	35(1)
C(10)	2082(3)	1931(2)	7496(2)	46(1)
C(11)	3122(4)	2659(2)	7191(2)	54(1)
C(12)	4374(4)	2198(2)	6889(2)	57(1)
C(13)	4590(4)	1014(3)	6895(2)	54(1)
C(14)	3541(3)	276(2)	7201(2)	44(1)
C(15)	3497(4)	-2443(2)	10135(2)	60(1)
C(16)	2345(4)	-2269(2)	10765(2)	58(1)

Bindungslängen [$\text{\AA}$] und -winkel [$^\circ$]

O(1)-C(6)	1.446(2)	C(3)-C(2)-C(15)	123.7(2)
O(1)-C(1)	1.469(2)	C(1)-C(2)-C(15)	122.5(2)
O(2)-C(7)	1.185(3)	C(3)-C(2)-C(16)	121.6(2)
O(3)-C(7)	1.315(3)	C(1)-C(2)-C(16)	120.4(2)
O(3)-C(8)	1.446(3)	C(15)-C(2)-C(16)	59.2(2)
C(1)-C(2)	1.494(3)	C(4)-C(3)-C(2)	112.2(2)
C(1)-C(5)	1.538(3)	C(3)-C(4)-C(5)	112.3(2)
C(2)-C(3)	1.476(3)	C(4)-C(5)-C(1)	102.8(2)
C(2)-C(15)	1.499(3)	C(4)-C(5)-C(6)	115.9(2)
C(2)-C(16)	1.509(3)	C(1)-C(5)-C(6)	85.2(2)
C(3)-C(4)	1.314(3)	O(1)-C(6)-C(9)	113.8(2)
C(4)-C(5)	1.491(3)	O(1)-C(6)-C(7)	111.1(2)
C(5)-C(6)	1.544(3)	C(9)-C(6)-C(7)	108.6(2)
C(6)-C(9)	1.508(3)	O(1)-C(6)-C(5)	91.24(14)
C(6)-C(7)	1.524(3)	C(9)-C(6)-C(5)	118.9(2)
C(9)-C(14)	1.377(3)	C(7)-C(6)-C(5)	112.3(2)
C(9)-C(10)	1.384(3)	O(2)-C(7)-O(3)	123.2(2)
C(10)-C(11)	1.376(4)	O(2)-C(7)-C(6)	112.4(2)
C(11)-C(12)	1.372(4)	C(14)-C(9)-C(10)	119.3(2)
C(12)-C(13)	1.373(4)	C(14)-C(9)-C(6)	120.9(2)
C(13)-C(14)	1.389(4)	C(10)-C(9)-C(6)	119.8(2)
C(15)-C(16)	1.487(4)	C(11)-C(10)-C(9)	120.7(3)
C(6)-O(1)-C(1)	91.41(14)	C(12)-C(11)-C(10)	119.8(3)
C(7)-O(3)-C(8)	116.4(2)	C(11)-C(12)-C(13)	120.0(3)

O(1)-C(1)-C(2)	114.2(2)	C(12)-C(13)-C(14)	120.4(3)
O(1)-C(1)-C(5)	90.6(2)	C(9)-C(14)-C(13)	119.7(2)
C(2)-C(1)-C(5)	107.1(2)	C(16)-C(15)-C(2)	60.7(2)
C(3)-C(2)-C(1)	104.6(2)	C(15)-C(16)-C(2)	60.1(2)

Torsionswinkel [°]

C(6)-O(1)-C(1)-C(2)	-118.7(2)	C(8)-O(3)-C(7)-C(6)	-177.3(2)
C(6)-O(1)-C(1)-C(5)	-9.7(2)	O(1)-C(6)-C(7)-O(2)	139.0(2)
O(1)-C(1)-C(2)-C(3)	88.5(2)	C(9)-C(6)-C(7)-O(2)	-95.1(3)
C(5)-C(1)-C(2)-C(3)	-10.2(2)	C(5)-C(6)-C(7)-O(2)	38.4(3)
O(1)-C(1)-C(2)-C(15)	-59.3(3)	O(1)-C(6)-C(7)-O(3)	-43.2(2)
C(5)-C(1)-C(2)-C(15)	-158.0(2)	C(9)-C(6)-C(7)-O(3)	82.7(2)
O(1)-C(1)-C(2)-C(16)	-130.1(2)	C(5)-C(6)-C(7)-O(3)	-143.8(2)
C(5)-C(1)-C(2)-C(16)	131.2(2)	O(1)-C(6)-C(9)-C(14)	16.3(2)
C(1)-C(2)-C(3)-C(4)	7.5(3)	C(7)-C(6)-C(9)-C(14)	-108.0(2)
C(15)-C(2)-C(3)-C(4)	154.8(2)	C(5)-C(6)-C(9)-C(14)	122.0(2)
C(16)-C(2)-C(3)-C(4)	-133.4(2)	O(1)-C(6)-C(9)-C(10)	-164.8(2)
C(2)-C(3)-C(4)-C(5)	-1.5(3)	C(7)-C(6)-C(9)-C(10)	70.9(2)
C(3)-C(4)-C(5)-C(1)	-5.0(3)	C(5)-C(6)-C(9)-C(10)	-59.1(3)
C(3)-C(4)-C(5)-C(6)	-95.8(2)	C(14)-C(9)-C(10)-C(11)	-.3(3)
O(1)-C(1)-C(5)-C(4)	-106.3(2)	C(6)-C(9)-C(10)-C(11)	-179.3(2)
C(2)-C(1)-C(5)-C(4)	9.3(2)	C(9)-C(10)-C(11)-C(12)	.2(3)
O(1)-C(1)-C(5)-C(6)	9.1(2)	C(10)-C(11)-C(12)-C(13)	-.2(4)
C(2)-C(1)-C(5)-C(6)	124.7(2)	C(11)-C(12)-C(13)-C(14)	.4(4)
C(1)-O(1)-C(6)-C(9)	132.2(2)	C(10)-C(9)-C(14)-C(13)	.5(3)
C(1)-O(1)-C(6)-C(7)	-104.9(2)	C(6)-C(9)-C(14)-C(13)	179.4(2)
C(1)-O(1)-C(6)-C(5)	9.7(2)	C(12)-C(13)-C(14)-C(9)	-.5(3)
C(4)-C(5)-C(6)-O(1)	92.6(2)	C(3)-C(2)-C(15)-C(16)	109.6(3)
C(1)-C(5)-C(6)-O(1)	-9.2(2)	C(1)-C(2)-C(15)-C(16)	-108.6(3)
C(4)-C(5)-C(6)-C(9)	-25.6(3)	C(16)-C(2)-C(15)-C(16)	.000(3)
C(1)-C(5)-C(6)-C(9)	-127.5(2)	C(2)-C(15)-C(16)-C(2)	.000(3)
C(4)-C(5)-C(6)-C(7)	-153.9(2)	C(3)-C(2)-C(16)-C(15)	-113.1(3)
C(1)-C(5)-C(6)-C(7)	104.2(2)	C(1)-C(2)-C(16)-C(15)	112.0(3)
C(8)-O(3)-C(7)-O(2)	.6(4)	C(15)-C(2)-C(16)-C(15)	.000(3)

Anisotrope Temperaturfaktoren ($\text{\AA}^2 \times 10^3$). Form des Exponenten des anisotropen Temperaturfaktors: $-2\pi^2(h^2a^2 \times 2U_{11} + \dots + 2hka \times b \times U_{12})$.

	U11	U22	U33	U23	U13	U12
O(1)	54(1)	41(1)	35(1)	1(1)	12(1)	7(1)
O(2)	56(2)	122(2)	75(1)	-32(1)	-11(1)	38(1)
O(3)	61(1)	72(1)	43(1)	-14(1)	-7(1)	12(1)
C(1)	40(2)	48(1)	35(1)	1(1)	10(1)	-7(1)
C(2)	43(2)	51(1)	36(1)	5(1)	7(1)	-2(1)
C(3)	46(2)	63(2)	35(1)	-2(1)	7(1)	-12(1)
C(4)	59(2)	46(1)	36(1)	-6(1)	16(1)	-10(1)
C(5)	39(2)	49(1)	35(1)	1(1)	13(1)	1(1)

C(6)	36(2)	40(1)	33(1)	1(1)	9(1)	5(1)
C(7)	43(2)	45(1)	39(1)	0(1)	9(1)	-1(1)
C(8)	73(3)	75(2)	45(1)	-8(1)	-16(1)	-3(2)
C(9)	31(2)	47(1)	27(1)	1(1)	4(1)	2(1)
C(10)	48(2)	48(1)	44(1)	3(1)	15(1)	2(1)
C(11)	63(2)	51(1)	49(1)	4(1)	15(1)	-6(1)
C(12)	55(2)	69(2)	45(1)	6(1)	10(1)	-17(2)
C(13)	32(2)	83(2)	49(1)	1(1)	13(1)	3(2)
C(14)	38(2)	53(1)	42(1)	4(1)	9(1)	6(1)
C(15)	58(2)	64(2)	57(2)	6(1)	11(2)	8(2)
C(16)	62(2)	65(2)	45(1)	16(1)	10(1)	-1(2)

H-Atomkoordinaten x, y, z ($\times 10^4$) und isotrope Temperaturfaktoren ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(1)	262(25)	-1754(19)	8978(15)	41(6)
H(3)	4008(31)	-37(22)	10788(20)	66(7)
H(4)	2339(26)	1399(21)	9760(17)	53(7)
H(5)	-194(31)	402(19)	8937(17)	49(7)
H(8A)	-1473(34)	-1271(26)	4934(24)	84(10)
H(8B)	-1909(40)	14(30)	5076(26)	105(11)
H(8C)	-2671(45)	-1097(32)	5653(29)	114(14)
H(10)	1258(31)	2254(21)	7707(19)	56(8)
H(11)	3013(31)	3505(26)	7176(21)	76(8)
H(12)	5107(30)	2720(22)	6695(18)	59(8)
H(13)	5440(32)	679(20)	6725(18)	53(8)
H(14)	3677(25)	-526(20)	7202(16)	42(6)
H(15A)	4612(36)	-2289(22)	10455(22)	72(9)
H(15B)	3237(29)	-3014(23)	9610(20)	64(8)
H(16A)	1336(33)	-2746(22)	10601(19)	65(8)
H(16B)	2763(29)	-2065(21)	11502(21)	66(7)