Crystal structure of 2,6,6-trimethyl-2-hydroxybicyclo[3.1.1]-3-heptanone oxime, $C_{10}H_{17}NO_2$

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Abstract

$C_{10}H_{17}NO_2$, triclinic, $P1$ (No. 1), $a = 7.197(2)$ Å, $b = 12.928(3)$ Å, $c = 17.966(4)$ Å, $\alpha = 87.14(1)^\circ$, $\beta = 81.75(2)^\circ$, $\gamma = 79.78(2)^\circ$, $V = 1627.5$ Å³, $Z = 6$, $R_g(F) = 0.035$, $wR_{ref}(F^2) = 0.077$, $T = 298$ K.

Source of material

The title compound was synthesized through the oxidation of α -pinene by potassium permanganate in 90% aqueous acetone at 273 K – 283 K and then the reaction of intermediate 2,6,6-trimethyl-2-hydroxybicyclo[3.1.1]-3-heptanone with hydroxylamine hydrochloride. The single crystals were grown by recrystallization from ethyl acetate-petroleum.

Discussion

As a part of a work on the ligand behaviour and reactivity of aminoalcohols, here we report the characterization of a precursor of aminoalcohols, 2,6,6-trimethyl-2-hydroxybicyclo[3.1.1]-3-heptanone oxime.

The distance C3–N1 is equal to 1.270(3) Å, clearly indicating a double bond. The bond lengths of C1–C2, C1–C6, C2–C3, C4–C5, C5–C6, C6–C8, C1–C7, C2–C10, C3–C4, C5–C7, C6–C9 are 1.515(4) Å, 1.570(4) Å, 1.523(4) Å, 1.512(4) Å, 1.536(4) Å, 1.526(4) Å, 1.535(4) Å, 1.511(4) Å, 1.514(4) Å, 1.536(4) Å, 1.508(4) Å, respectively; these data suggest that single bonds exist between every two carbon atoms and the C2=C3 double bond have disappeared [1]. The distance O1–C2 is equal to 1.451(3) Å, which verify the appearance of hydroxy group [2,3]. The distance O2–N1 is equal to 1.403(3) Å, which confirms the existence of another hydroxy group. The atoms C1, C5, C6 and C7 constitute a four-membered ring. The bond an-

gles $\angle C1-C7-C5$, $\angle C7-C1-C6$, $\angle C7-C5-C6$ and $\angle C5-C6-C1$ are 86.2(2)°, 87.3(2)°, 88.5(2)° and 85.0(2)°, respectively, and other C–C–C bond angle is about 109°. The bond angle $\angle C3-N1-O2$ is 111.5°. Every unit cell is composed of six molecules, there are twelve intermolecular hydrogen bonds in a unit cell, the hydrogen bond length is between 2.6 Å to 2.9 Å, and the hydrogen bond angle is in the range of 149° – 173°. The structural differences among the six independent molecules are not significant.

Table 1. Data collection and handling.

Crystal:	colorless plate, size 0.20 × 0.52 × 0.80 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	0.77 cm ⁻¹
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6444, 6240
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4274
$N(param)_{refined}$:	734
Programs:	SHELXTL-plus [4], SHELXL-93 [5], ORTEP3 [6]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(10)	1a	0.4029	-0.2323	1.4908	0.072
H(20)	1a	0.3495	-0.0994	1.2694	0.080
H(110)	1a	0.4544	-0.4323	1.5934	0.075
H(120)	1a	0.4286	-0.2917	1.3468	0.099
H(210)	1a	0.4238	-0.5225	1.6888	0.080
H(220)	1a	0.5072	-0.2097	1.6205	0.094
H(310)	1a	0.2338	-0.0661	1.1690	0.093
H(320)	1a	0.2225	-0.0886	0.9328	0.113
H(410)	1a	0.2152	0.0355	1.0707	0.078
H(420)	1a	0.2669	0.3040	0.8948	0.107
H(510)	1a	0.2666	0.0992	0.9153	0.089
H(520)	1a	0.3551	0.3337	0.7388	0.092
H(1)	1a	0.7559	-0.1340	1.5553	0.060
H(4A)	1a	0.6276	0.0339	1.3448	0.069
H(4B)	1a	0.4305	0.0588	1.3963	0.069
H(5)	1a	0.6685	0.1237	1.4549	0.071
H(7A)	1a	0.5874	0.0402	1.5744	0.080
H(7B)	1a	0.4324	0.0008	1.5320	0.080
H(8A)	1a	1.0524	-0.0481	1.5310	0.102
H(8B)	1a	0.8880	0.0455	1.5558	0.102
H(8C)	1a	1.0378	0.0586	1.4850	0.102
H(9A)	1a	1.0176	-0.0130	1.3661	0.090
H(9B)	1a	0.8923	-0.0996	1.3620	0.090
H(9C)	1a	1.0682	-0.1228	1.4063	0.090
H(10A)	1a	0.7770	-0.3065	1.4867	0.077
H(10B)	1a	0.8671	-0.2486	1.4155	0.077

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Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(10C)	1a	0.6926	-0.3041	1.4108	0.077
H(11)	1a	0.1863	-0.6095	1.5996	0.062
H(14A)	1a	0.5035	-0.5610	1.3788	0.084
H(14B)	1a	0.2971	-0.5241	1.3579	0.084
H(15)	1a	0.3216	-0.7041	1.4040	0.077
H(17A)	1a	0.5234	-0.6487	1.5074	0.081
H(17B)	1a	0.4019	-0.7412	1.5282	0.081
H(18A)	1a	-0.0756	-0.6976	1.5520	0.099
H(18B)	1a	0.1218	-0.7691	1.5278	0.099
H(18C)	1a	-0.0230	-0.7385	1.4696	0.099
H(19A)	1a	-0.0808	-0.5637	1.4151	0.090
H(19B)	1a	0.0135	-0.4735	1.4407	0.090
H(19C)	1a	-0.1445	-0.5182	1.4958	0.090
H(11A)	1a	0.1202	-0.4090	1.6302	0.075
H(11B)	1a	0.0118	-0.3992	1.5597	0.075
H(11C)	1a	0.1654	-0.3286	1.5648	0.075
H(21)	1a	0.6483	-0.5920	1.8429	0.067
H(24A)	1a	0.3995	-0.2644	1.8088	0.075
H(24B)	1a	0.6154	-0.2535	1.7949	0.075
H(25)	1a	0.5412	-0.3248	1.9211	0.068
H(27A)	1a	0.4220	-0.4874	1.9295	0.076
H(27B)	1a	0.3323	-0.4408	1.8557	0.076
H(28A)	1a	0.8369	-0.4441	1.9678	0.143
H(28B)	1a	0.9038	-0.5537	1.9301	0.143
H(28C)	1a	0.6927	-0.5219	1.9683	0.143
H(29A)	1a	0.8832	-0.3799	1.7717	0.135
H(29B)	1a	1.0158	-0.4726	1.8076	0.135
H(29C)	1a	0.9631	-0.3631	1.8461	0.135
H(21A)	1a	0.7814	-0.6200	1.7002	0.089
H(21B)	1a	0.8886	-0.5271	1.7101	0.089
H(21C)	1a	0.7627	-0.5218	1.6452	0.089
H(31)	1a	0.0275	-0.2605	1.2592	0.071
H(34A)	1a	0.3076	-0.3185	1.0303	0.103
H(34B)	1a	0.0944	-0.3098	1.0172	0.103
H(35)	1a	0.1715	-0.452	1.1078	0.092
H(37A)	1a	0.2719	-0.4019	1.2215	0.103
H(37B)	1a	0.3576	-0.3151	1.1666	0.103
H(38A)	1a	-0.2053	-0.4019	1.2609	0.159

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(38B)	1a	0.0101	-0.4543	1.2536	0.159
H(38C)	1a	-0.1223	-0.4869	1.2001	0.159
H(39A)	1a	-0.1789	-0.2510	1.0899	0.163
H(39B)	1a	-0.3146	-0.2627	1.1651	0.163
H(39C)	1a	-0.2587	-0.3558	1.1090	0.163
H(31A)	1a	-0.1312	-0.0709	1.2290	0.099
H(31B)	1a	-0.2062	-0.1088	1.1591	0.099
H(31C)	1a	-0.0824	-0.0195	1.1494	0.099
H(41)	1a	0.4804	0.0855	1.1966	0.065
H(44A)	1a	0.1836	0.3586	1.0839	0.084
H(44B)	1a	0.3930	0.3718	1.0519	0.084
H(45)	1a	0.3586	0.3762	1.1880	0.078
H(47A)	1a	0.1501	0.2210	1.1861	0.087
H(47B)	1a	0.2624	0.2267	1.2562	0.087
H(48A)	1a	0.7484	0.1807	1.2374	0.096
H(48B)	1a	0.5485	0.2345	1.2768	0.096
H(48C)	1a	0.6931	0.3036	1.2364	0.096
H(49A)	1a	0.7687	0.3097	1.1016	0.090
H(49B)	1a	0.6728	0.2471	1.0497	0.090
H(49C)	1a	0.8229	0.1869	1.0987	0.090
H(41A)	1a	0.5637	-0.0251	1.0748	0.082
H(41B)	1a	0.6666	0.0662	1.0388	0.082
H(41C)	1a	0.5138	0.0276	0.9980	0.082
H(51)	1a	-0.0657	-0.0319	0.8670	0.071
H(54A)	1a	0.3197	0.0904	0.6887	0.087
H(54B)	1a	0.1270	0.1614	0.6743	0.087
H(55)	1a	0.1029	-0.0216	0.6629	0.081
H(57A)	1a	0.1407	-0.1320	0.7727	0.085
H(57B)	1a	0.2855	-0.0560	0.7863	0.085
H(58A)	1a	-0.3307	-0.0470	0.7857	0.134
H(58B)	1a	-0.1443	-0.1214	0.7521	0.134
H(58C)	1a	-0.2646	-0.0463	0.6987	0.134
H(59A)	1a	-0.2588	0.1472	0.6948	0.138
H(59B)	1a	-0.1691	0.1936	0.7575	0.138
H(59C)	1a	-0.3504	0.1411	0.7792	0.138
H(51A)	1a	-0.1021	0.1356	0.9500	0.124
H(51B)	1a	-0.1842	0.1904	0.8789	0.124
H(51C)	1a	-0.0234	0.2337	0.9117	0.124

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	1a	0.4510(3)	-0.1919(2)	1.5128(1)	0.077(2)	0.068(2)	0.042(1)	-0.032(1)	-0.009(1)	0.015(1)
O(2)	1a	0.4154(3)	-0.0723(2)	1.2938(1)	0.077(2)	0.083(2)	0.053(1)	-0.036(1)	-0.032(1)	0.029(1)
O(11)	1a	0.4545(3)	-0.4881(2)	1.5736(1)	0.075(2)	0.057(1)	0.061(1)	-0.018(1)	-0.023(1)	0.000(1)
O(12)	1a	0.3997(4)	-0.3500(2)	1.3564(1)	0.137(2)	0.079(2)	0.044(1)	-0.057(2)	-0.014(1)	0.015(1)
O(21)	1a	0.4384(3)	-0.5340(2)	1.7331(1)	0.088(2)	0.065(1)	0.060(1)	-0.043(1)	-0.023(1)	0.015(1)
O(22)	1a	0.4928(4)	-0.2294(2)	1.6647(1)	0.139(2)	0.041(1)	0.055(1)	-0.018(1)	-0.016(2)	0.016(1)
O(31)	1a	0.2291(4)	-0.1250(2)	1.1875(1)	0.111(2)	0.076(2)	0.065(1)	-0.049(2)	-0.049(2)	0.025(1)
O(32)	1a	0.2197(5)	-0.1412(2)	0.9601(1)	0.186(3)	0.054(1)	0.038(1)	-0.022(2)	0.003(2)	0.006(1)
O(41)	1a	0.2225(3)	0.0736(2)	1.1050(1)	0.084(2)	0.057(1)	0.060(1)	-0.029(1)	-0.014(1)	0.005(1)
O(42)	1a	0.2853(5)	0.3123(2)	0.9379(1)	0.166(3)	0.048(1)	0.067(2)	-0.030(2)	-0.050(2)	0.019(1)
O(51)	1a	0.2287(4)	0.0529(2)	0.8951(1)	0.133(2)	0.048(1)	0.054(1)	-0.032(1)	-0.039(2)	0.012(1)
O(52)	1a	0.3114(4)	0.2822(2)	0.7293(1)	0.105(2)	0.081(2)	0.058(1)	-0.057(2)	-0.022(1)	0.028(1)
N(1)	1a	0.4770(3)	-0.1430(2)	1.3506(1)	0.054(2)	0.059(2)	0.040(1)	-0.019(1)	-0.011(1)	0.016(1)
N(11)	1a	0.3508(4)	-0.3625(2)	1.4347(1)	0.081(2)	0.059(2)	0.045(2)	-0.027(2)	-0.014(1)	0.008(1)
N(21)	1a	0.5444(4)	-0.3395(2)	1.6695(1)	0.068(2)	0.042(1)	0.049(2)	-0.016(1)	-0.004(1)	0.008(1)
N(31)	1a	0.1536(4)	-0.1115(2)	1.0338(1)	0.091(2)	0.048(1)	0.035(1)	-0.013(1)	-0.013(1)	0.002(1)
N(41)	1a	0.3326(4)	0.2138(2)	0.9735(1)	0.106(2)	0.044(2)	0.053(2)	-0.025(2)	-0.022(2)	0.012(1)
N(51)	1a	0.2264(4)	0.2395(2)	0.7962(1)	0.064(2)	0.050(2)	0.048(1)	-0.019(1)	-0.011(1)	0.019(1)
C(1)	1a	0.7042(4)	-0.0971(2)	1.5118(2)	0.062(2)	0.052(2)	0.038(2)	-0.010(2)	-0.012(2)	0.000(1)
C(2)	1a	0.6161(4)	-0.1645(2)	1.4648(2)	0.053(2)	0.042(2)	0.040(2)	-0.010(2)	-0.009(2)	0.007(1)
C(3)	1a	0.5465(4)	-0.0979(2)	1.3987(2)	0.042(2)	0.046(2)	0.038(2)	-0.012(1)	-0.007(1)	0.006(1)
C(4)	1a	0.5581(5)	0.0181(2)	1.3932(2)	0.066(2)	0.046(2)	0.062(2)	-0.010(2)	-0.015(2)	0.011(2)
C(5)	1a	0.6566(5)	0.0493(2)	1.4554(2)	0.073(2)	0.044(2)	0.062(2)	-0.012(2)	-0.012(2)	-0.007(2)
C(6)	1a	0.8401(5)	-0.0290(2)	1.4637(2)	0.053(2)	0.058(2)	0.057(2)	-0.017(2)	-0.010(2)	-0.008(2)
C(7)	1a	0.5658(5)	0.0059(2)	1.5304(2)	0.076(3)	0.067(2)	0.056(2)	-0.012(2)	-0.001(2)	-0.018(2)
C(8)	1a	0.9663(6)	0.0104(3)	1.5135(2)	0.086(3)	0.089(3)	0.095(3)	-0.034(2)	-0.035(2)	-0.006(2)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(9)	1a	0.9660(5)	-0.0698(3)	1.3931(2)	0.062(2)	0.087(3)	0.078(2)	-0.024(2)	-0.001(2)	-0.008(2)
C(10)	1a	0.7505(5)	-0.2651(2)	1.4424(2)	0.077(2)	0.048(2)	0.071(2)	-0.005(2)	-0.027(2)	-0.001(2)
C(11)	1a	0.2333(4)	-0.5901(2)	1.5478(2)	0.063(2)	0.045(2)	0.048(2)	-0.012(2)	-0.007(2)	0.006(1)
C(12)	1a	0.2847(4)	-0.4804(2)	1.5379(2)	0.054(2)	0.044(2)	0.047(2)	-0.011(2)	-0.012(2)	0.004(1)
C(13)	1a	0.3374(5)	-0.4579(2)	1.4543(2)	0.066(2)	0.049(2)	0.047(2)	-0.021(2)	-0.010(2)	0.001(2)
C(14)	1a	0.3696(6)	-0.5459(2)	1.3993(2)	0.089(3)	0.063(2)	0.060(2)	-0.024(2)	-0.002(2)	-0.008(2)
C(15)	1a	0.3093(5)	-0.6445(2)	1.4371(2)	0.088(3)	0.045(2)	0.059(2)	-0.015(2)	-0.002(2)	-0.009(2)
C(16)	1a	0.1139(5)	-0.6171(2)	1.4873(2)	0.065(2)	0.041(2)	0.063(2)	-0.015(2)	-0.012(2)	0.003(2)
C(17)	1a	0.3996(5)	-0.6694(2)	1.5094(2)	0.069(2)	0.044(2)	0.087(3)	-0.001(2)	-0.011(2)	-0.003(2)
C(18)	1a	0.0261(6)	-0.7146(3)	1.5114(2)	0.109(3)	0.061(2)	0.087(3)	-0.039(2)	-0.017(2)	-0.002(2)
C(19)	1a	-0.0385(6)	-0.5356(3)	1.4569(2)	0.080(3)	0.064(2)	0.088(3)	-0.018(2)	-0.029(2)	0.001(2)
C(110)	1a	0.1314(5)	-0.3966(2)	1.5767(2)	0.079(3)	0.047(2)	0.060(2)	-0.012(2)	-0.004(2)	-0.002(2)
C(21)	1a	0.6190(5)	-0.5168(2)	1.8302(2)	0.074(2)	0.043(2)	0.050(2)	-0.005(2)	-0.015(2)	0.008(1)
C(22)	1a	0.6033(4)	-0.4922(2)	1.7481(2)	0.047(2)	0.041(2)	0.048(2)	-0.012(1)	-0.004(2)	0.003(1)
C(23)	1a	0.5593(4)	-0.3735(2)	1.7363(2)	0.044(2)	0.042(2)	0.044(2)	-0.013(1)	0.002(1)	0.005(1)
C(24)	1a	0.5285(5)	-0.3036(2)	1.8034(2)	0.087(3)	0.044(2)	0.052(2)	-0.005(2)	-0.004(2)	0.002(1)
C(25)	1a	0.5601(5)	-0.3662(2)	1.8755(2)	0.073(2)	0.057(2)	0.040(2)	-0.016(2)	-0.001(2)	-0.000(1)
C(26)	1a	0.7424(5)	-0.4474(3)	1.8644(2)	0.060(2)	0.072(2)	0.065(2)	-0.003(2)	-0.022(2)	-0.006(2)
C(27)	1a	0.4471(5)	-0.4567(3)	1.8795(2)	0.067(2)	0.079(2)	0.043(2)	-0.022(2)	0.001(2)	0.013(2)
C(28)	1a	0.7993(8)	-0.4964(4)	1.9398(2)	0.150(5)	0.109(3)	0.103(3)	0.009(3)	-0.074(3)	-0.007(3)
C(29)	1a	0.9175(6)	-0.4125(4)	1.8181(3)	0.055(3)	0.166(5)	0.127(4)	-0.031(3)	-0.015(3)	-0.047(3)
C(210)	1a	0.7747(5)	-0.5451(3)	1.6962(2)	0.085(3)	0.060(2)	0.070(2)	0.003(2)	-0.002(2)	-0.012(2)
C(31)	1a	0.0649(5)	-0.2685(2)	1.2049(2)	0.075(2)	0.061(2)	0.044(2)	-0.022(2)	-0.003(2)	0.008(2)
C(32)	1a	0.0778(4)	-0.1657(2)	1.1614(2)	0.056(2)	0.051(2)	0.039(2)	-0.011(2)	-0.012(2)	0.001(1)
C(33)	1a	0.1365(4)	-0.1894(2)	1.0785(2)	0.056(2)	0.041(2)	0.040(2)	-0.003(2)	-0.007(1)	0.002(1)
C(34)	1a	0.1765(7)	-0.3016(2)	1.0541(2)	0.138(4)	0.043(2)	0.061(2)	-0.003(2)	0.023(2)	-0.002(2)
C(35)	1a	0.1439(6)	-0.3774(2)	1.1201(2)	0.118(3)	0.036(2)	0.066(2)	-0.012(2)	0.014(2)	0.001(2)
C(36)	1a	-0.0439(6)	-0.3421(3)	1.1691(2)	0.082(3)	0.076(2)	0.067(2)	-0.039(2)	0.002(2)	-0.003(2)
C(37)	1a	0.2460(6)	-0.3467(3)	1.1839(2)	0.093(3)	0.058(2)	0.104(3)	-0.007(2)	-0.019(3)	0.037(2)
C(38)	1a	-0.0952(8)	-0.4296(4)	1.2264(3)	0.182(5)	0.114(4)	0.107(3)	-0.089(4)	0.041(4)	0.000(3)
C(39)	1a	-0.2146(7)	-0.2989(4)	1.1297(3)	0.100(4)	0.148(5)	0.181(5)	-0.058(4)	-0.034(4)	-0.044(4)
C(310)	1a	-0.1021(6)	-0.0837(3)	1.1761(2)	0.093(3)	0.071(2)	0.073(2)	0.006(2)	-0.002(2)	-0.010(2)
C(41)	1a	0.4392(5)	0.1465(2)	1.1647(2)	0.072(2)	0.050(2)	0.042(2)	-0.016(2)	-0.009(2)	0.006(1)
C(42)	1a	0.3941(5)	0.1192(2)	1.0878(2)	0.067(2)	0.042(2)	0.045(2)	-0.018(2)	-0.007(2)	0.003(1)
C(43)	1a	0.3457(5)	0.2224(2)	1.0432(2)	0.072(2)	0.041(2)	0.048(2)	-0.015(2)	-0.012(2)	-0.000(1)
C(44)	1a	0.3163(6)	0.3257(2)	1.0813(2)	0.096(3)	0.042(2)	0.073(2)	-0.005(2)	-0.024(2)	-0.008(2)
C(45)	1a	0.3712(5)	0.3113(2)	1.1604(2)	0.087(3)	0.052(2)	0.057(2)	-0.009(2)	-0.010(2)	-0.015(2)
C(46)	1a	0.5621(5)	0.2354(2)	1.1612(2)	0.072(2)	0.055(2)	0.049(2)	-0.023(2)	-0.006(2)	-0.004(2)
C(47)	1a	0.2717(6)	0.2255(3)	1.2019(2)	0.079(3)	0.089(3)	0.053(2)	-0.028(2)	0.004(2)	-0.015(2)
C(48)	1a	0.6459(6)	0.2389(3)	1.2349(2)	0.097(3)	0.080(2)	0.068(2)	-0.025(2)	-0.019(2)	-0.003(2)
C(49)	1a	0.7214(5)	0.2457(3)	1.0968(2)	0.082(3)	0.072(2)	0.074(2)	-0.029(2)	-0.001(2)	-0.004(2)
C(410)	1a	0.5487(5)	0.0397(2)	1.0460(2)	0.093(3)	0.045(2)	0.067(2)	-0.006(2)	-0.014(2)	-0.002(2)
C(51)	1a	0.0001(5)	0.0073(2)	0.8265(2)	0.071(2)	0.047(2)	0.062(2)	-0.025(2)	-0.003(2)	0.009(2)
C(52)	1a	0.0778(5)	0.0998(2)	0.8527(2)	0.069(2)	0.043(2)	0.046(2)	-0.017(2)	-0.001(2)	0.002(1)
C(53)	1a	0.1673(4)	0.1554(2)	0.7842(2)	0.048(2)	0.042(2)	0.042(2)	-0.011(1)	-0.011(1)	0.009(1)
C(54)	1a	0.1858(6)	0.1091(3)	0.7083(2)	0.086(3)	0.090(3)	0.050(2)	-0.038(2)	-0.014(2)	0.006(2)
C(55)	1a	0.0929(5)	0.0126(3)	0.7111(2)	0.083(3)	0.069(2)	0.060(2)	-0.027(2)	-0.021(2)	-0.006(2)
C(56)	1a	-0.1059(5)	0.0325(3)	0.7558(2)	0.058(2)	0.053(2)	0.102(3)	-0.020(2)	-0.029(2)	0.009(2)
C(57)	1a	0.1581(5)	-0.0598(2)	0.7761(2)	0.086(3)	0.048(2)	0.083(2)	-0.009(2)	-0.035(2)	-0.007(2)
C(58)	1a	-0.2222(6)	-0.0536(3)	0.7473(3)	0.096(3)	0.093(3)	0.167(5)	-0.051(3)	-0.053(3)	0.013(3)
C(59)	1a	-0.2328(6)	0.1384(3)	0.7459(3)	0.073(3)	0.081(3)	0.198(5)	-0.004(2)	-0.059(3)	0.011(3)
C(510)	1a	-0.0716(6)	0.1714(3)	0.9029(2)	0.117(4)	0.084(3)	0.103(3)	-0.043(3)	0.052(3)	-0.036(2)

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