Supporting Information

One step transformation of tricyclopentabenzene(trindane, $C_{15}H_{18}$) to bicyclo(10.3.0)penta dec-1(12)ene-2, 6, 7, 11 tetra-one($C_{15}H_{18}O_4$) and its aldol product, 12-hydroxy-16-oxatetracyclo(10.3.1.$0^{1,5}$.$0^{7,11}$)hexadec-7(11)ene-2,6-dione($C_{15}H_{18}O_4$).

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Table 2. Crystal data and structure refinement for 1.

Identification code	oz4
Empirical formula	$C_{15}H_{18}O_4$
Formula weight	262.29
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.471(1) Å alpha = 73.02° b = 14.1580(10) Å beta = 89.26° c = 17.1210(10) Å gamma = 89.44°
Volume, Z	2659.1(2) $Å^3$, 8
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.775 mm^{-1}
F(000)	1120
Crystal size	0.36 x 0.30 x 0.07 mm
θ range for data collection	2.70 to 57.49°
Limiting indices	$-12 \le h \le 2$, $-14 \le k \le 14$, $-18 \le l \le 18$
Reflections collected	7699
Independent reflections	7213 (R_{int} = 0.0115)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7211 / 0 / 683
Goodness-of-fit on F^2	1.009
Final R indices [I>2σ(I)]	R1 = 0.0607, wR2 = 0.1414
R indices (all data)	R1 = 0.0980, wR2 = 0.1725
Extinction coefficient	0.0028(2)
Largest diff. peak and hole	0.869 and -0.751 $eÅ^{-3}$

Table 3. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1A)	6081	4072	3607	55(1)
C(1A)	5168(3)	3531(3)	4020(2)	41(1)
C(2A)	4164(3)	4216(3)	4051(2)	39(1)
C(3A)	3761(4)	4986(3)	3293(3)	62(1)
C(4A)	2725(4)	5474(3)	3564(3)	65(1)
C(5A)	2816(3)	5224(3)	4488(3)	49(1)
C(6A)	3626(3)	4338(3)	4705(2)	36(1)
C(7A)	3755(3)	3731(3)	5555(2)	37(1)
O(7A)	3668(3)	4100(2)	6123(2)	55(1)
C(8A)	3861(3)	2635(2)	5712(2)	35(1)
C(9A)	3846(3)	2049(3)	6619(2)	48(1)
C(10A)	5127(4)	2003(3)	6883(2)	56(1)
C(11A)	5809(4)	2045(3)	6136(2)	47(1)
O(11A)	6851(3)	1900(3)	6100(2)	78(1)
C(12A)	5031(3)	2334(3)	5379(2)	36(1)
O(13A)	5647(2)	3132(2)	4819(1)	37(1)
C(14A)	4872(4)	1491(3)	5010(3)	50(1)
C(15A)	4254(4)	1865(3)	4195(2)	53(1)
C(16A)	4919(4)	2724(3)	3628(2)	54(1)
O(1B)	2125(2)	6292(2)	-1189(2)	55(1)
C(1B)	2282(3)	5273(3)	-1036(2)	46(1)
C(2B)	2204(4)	4769(3)	-134(2)	52(1)
C(3B)	2860(5)	5159(5)	460(3)	86(2)
C(4B)	2524(6)	4481(5)	1284(3)	98(2)
C(5B)	1490(6)	3888(5)	1161(3)	94(2)
C(6B)	1475(4)	4054(3)	259(2)	55(1)
C(7B)	667(4)	3513(3)	-110(3)	59(1)
O(7B)	-310(3)	3280(2)	178(2)	82(1)
C(8B)	1126(4)	3151(3)	-805(3)	53(1)
C(9B)	269(5)	2508(4)	-1103(3)	80(2)
C(10B)	-427(5)	3212(4)	-1773(4)	90(2)
C(11B)	381(5)	4027(4)	-2159(3)	67(1)
O(11B)	283(4)	4609(3)	-2816(2)	108(2)
C(12B)	1406(4)	4013(3)	-1573(2)	49(1)
O(13B)	1336(2)	4969(2)	-1445(1)	43(1)
C(14B)	2554(4)	3872(3)	-1980(3)	67(1)
C(15B)	3574(4)	4090(4)	-1504(3)	70(1)
C(16B)	3442(4)	5120(3)	-1425(3)	60(1)
O(1D)	1595(2)	1045(2)	6095(2)	51(1)
C(1D)	584(3)	1589(3)	5785(2)	41(1)
C(2D)	-452(3)	908(3)	5965(2)	40(1)
C(3D)	-645(4)	220(4)	6810(3)	71(1)
C(4D)	-1731(4)	-333(4)	6749(3)	74(2)
C(5D)	-2000(3)	-130(3)	5846(3)	53(1)
C(6D)	-1200(3)	726(3)	5442(2)	38(1)
C(7D)	-1327(3)	1258(3)	4577(2)	38(1)
O(7D)	-1619(3)	837(2)	4081(2)	60(1)
C(8D)	-1222(3)	2371(3)	4333(2)	38(1)

C(9D)	-1489(3)	2881(3)	3436(2)	51(1)
C(10D)	-334(4)	2916(4)	2988(3)	61(1)
C(11D)	569(4)	2978(3)	3581(3)	52(1)
O(11D)	1574(3)	3189(3)	3437(2)	86(1)
C(12D)	32(3)	2710(3)	4452(2)	39(1)
O(13D)	787(2)	1941(2)	4918(2)	39(1)
C(14D)	23(4)	3584(3)	4795(3)	54(1)
C(15D)	-307(4)	3252(3)	5692(3)	55(1)
C(16D)	516(4)	2434(3)	6153(3)	54(1)
O(1H)	7035(3)	-1203(2)	1243(2)	59(1)
C(1H)	7123(4)	-183(3)	1109(2)	48(1)
C(2H)	7097(4)	337(3)	211(3)	55(1)
C(3H)	7874(5)	22(5)	-380(3)	93(2)
C(4H)	7522(7)	706(5)	-1209(3)	109(2)
C(5H)	6459(6)	1277(5)	-1092(3)	100(2)
C(6H)	6344(4)	1038(3)	-183(2)	60(1)
C(7H)	5438(5)	1535(3)	181(3)	59(1)
O(7H)	4469(3)	1713(2)	-117(2)	78(1)
C(8H)	5805(4)	1898(3)	888(2)	53(1)
C(9H)	4858(5)	2496(3)	1177(3)	76(2)
C(10H)	4146(5)	1751(4)	1805(3)	78(2)
C(11H)	4997(5)	973(3)	2213(3)	64(1)
O(11H)	4906(4)	389(3)	2875(2)	99(1)
C(12H)	6083(4)	1029(3)	1655(2)	51(1)
O(13H)	6102(2)	81(2)	1505(2)	47(1)
C(14H)	7179(4)	1206(3)	2083(3)	67(1)
C(15H)	8252(5)	1030(3)	1615(3)	73(2)
C(16H)	8230(4)	-8(3)	1529(3)	65(1)

Table 4. Bond lengths [Å] and angles [°] for 1.

O(1A)-C(1A)	1.366(3)	C(1A)-O(13A)	1.432(4)
C(1A)-C(2A)	1.509(5)	C(1A)-C(16A)	1.514(5)
C(2A)-C(6A)	1.326(5)	C(2A)-C(3A)	1.505(5)
C(3A)-C(4A)	1.503(6)	C(4A)-C(5A)	1.522(6)
C(5A)-C(6A)	1.512(5)	C(6A)-C(7A)	1.467(5)
C(7A)-O(7A)	1.232(4)	C(7A)-C(8A)	1.500(5)
C(8A)-C(9A)	1.531(5)	C(8A)-C(12A)	1.556(5)
C(9A)-C(10A)	1.538(6)	C(10A)-C(11A)	1.478(6)
C(11A)-O(11A)	1.215(5)	C(11A)-C(12A)	1.535(5)
C(12A)-O(13A)	1.436(4)	C(12A)-C(14A)	1.520(5)
C(14A)-C(15A)	1.521(6)	C(15A)-C(16A)	1.521(5)
O(1B)-C(1B)	1.400(5)	C(1B)-O(13B)	1.434(5)
C(1B)-C(2B)	1.503(5)	C(1B)-C(16B)	1.522(5)
C(2B)-C(6B)	1.334(6)	C(2B)-C(3B)	1.503(6)
C(3B)-C(4B)	1.505(7)	C(4B)-C(5B)	1.512(8)
C(5B)-C(6B)	1.493(6)	C(6B)-C(7B)	1.469(6)
C(7B)-O(7B)	1.227(5)	C(7B)-C(8B)	1.513(6)
C(8B)-C(9B)	1.536(6)	C(8B)-C(12B)	1.543(5)
C(9B)-C(10B)	1.512(7)	C(10B)-C(11B)	1.479(7)
C(11B)-O(11B)	1.191(6)	C(11B)-C(12B)	1.550(6)
C(12B)-O(13B)	1.435(5)	C(12B)-C(14B)	1.519(6)
C(14B)-C(15B)	1.519(7)	C(15B)-C(16B)	1.509(6)
O(1D)-C(1D)	1.407(4)	C(1D)-O(13D)	1.437(4)
C(1D)-C(2D)	1.509(5)	C(1D)-C(16D)	1.507(5)
C(2D)-C(6D)	1.327(5)	C(2D)-C(3D)	1.504(5)
C(3D)-C(4D)	1.499(6)	C(4D)-C(5D)	1.523(6)
C(5D)-C(6D)	1.518(5)	C(6D)-C(7D)	1.462(5)
C(7D)-O(7D)	1.222(4)	C(7D)-C(8D)	1.513(5)
C(8D)-C(9D)	1.528(5)	C(8D)-C(12D)	1.555(5)
C(9D)-C(10D)	1.517(6)	C(10D)-C(11D)	1.481(6)
C(11D)-O(11D)	1.199(5)	C(11D)-C(12D)	1.549(5)
C(12D)-O(13D)	1.437(4)	C(12D)-C(14D)	1.517(5)
C(14D)-C(15D)	1.513(6)	C(15D)-C(16D)	1.523(6)
O(1H)-C(1H)	1.400(5)	C(1H)-O(13H)	1.445(5)
C(1H)-C(2H)	1.499(6)	C(1H)-C(16H)	1.525(6)
C(2H)-C(6H)	1.339(6)	C(2H)-C(3H)	1.501(6)
C(3H)-C(4H)	1.522(8)	C(4H)-C(5H)	1.501(8)
C(5H)-C(6H)	1.498(6)	C(6H)-C(7H)	1.479(7)
C(7H)-O(7H)	1.223(5)	C(7H)-C(8H)	1.511(6)
C(8H)-C(9H)	1.535(6)	C(8H)-C(12H)	1.549(5)
C(9H)-C(10H)	1.506(7)	C(10H)-C(11H)	1.484(7)
C(11H)-O(11H)	1.196(5)	C(11H)-C(12H)	1.549(6)
C(12H)-O(13H)	1.438(4)	C(12H)-C(14H)	1.522(6)
C(14H)-C(15H)	1.519(7)	C(15H)-C(16H)	1.519(6)

O(1A)-C(1A)-O(13A)	101.5(3)	O(1A)-C(1A)-C(2A)	109.1(3)
O(13A)-C(1A)-C(2A)	110.0(3)	O(1A)-C(1A)-C(16A)	107.8(3)
O(13A)-C(1A)-C(16A)	111.4(3)	C(2A)-C(1A)-C(16A)	116.0(3)
C(6A)-C(2A)-C(3A)	110.2(4)	C(6A)-C(2A)-C(1A)	128.0(3)
C(3A)-C(2A)-C(1A)	121.1(3)	C(4A)-C(3A)-C(2A)	105.1(4)
C(3A)-C(4A)-C(5A)	105.7(3)	C(6A)-C(5A)-C(4A)	103.2(3)
C(2A)-C(6A)-C(7A)	127.3(3)	C(2A)-C(6A)-C(5A)	111.9(3)
C(7A)-C(6A)-C(5A)	120.9(3)	O(7A)-C(7A)-C(6A)	121.0(3)
O(7A)-C(7A)-C(8A)	121.2(3)	C(6A)-C(7A)-C(8A)	117.5(3)
C(7A)-C(8A)-C(9A)	114.0(3)	C(7A)-C(8A)-C(12A)	112.1(3)

C(9A)-C(8A)-C(12A)	104.5(3)	C(8A)-C(9A)-C(10A)	105.0(3)
C(11A)-C(10A)-C(9A)	104.8(3)	O(11A)-C(11A)-C(10A)	126.0(4)
O(11A)-C(11A)-C(12A)	122.9(4)	C(10A)-C(11A)-C(12A)	111.0(3)
O(13A)-C(12A)-C(14A)	110.4(3)	O(13A)-C(12A)-C(11A)	103.8(3)

C(14A)-C(12A)-C(11A)	112.4(3)	O(13A)-C(12A)-C(8A)	114.8(3)
C(14A)-C(12A)-C(8A)	111.8(3)	C(11A)-C(12A)-C(8A)	103.2(3)
C(1A)-O(13A)-C(12A)	117.3(3)	C(15A)-C(14A)-C(12A)	109.8(3)
C(14A)-C(15A)-C(16A)	110.3(3)	C(1A)-C(16A)-C(15A)	112.6(3)
O(1B)-C(1B)-O(13B)	104.8(3)	O(1B)-C(1B)-C(2B)	109.8(3)
O(13B)-C(1B)-C(2B)	110.1(3)	O(1B)-C(1B)-C(16B)	107.1(3)
O(13B)-C(1B)-C(16B)	110.5(3)	C(2B)-C(1B)-C(16B)	114.1(3)
C(6B)-C(2B)-C(3B)	110.8(4)	C(6B)-C(2B)-C(1B)	127.7(4)
C(3B)-C(2B)-C(1B)	120.8(4)	C(2B)-C(3B)-C(4B)	104.2(5)
C(3B)-C(4B)-C(5B)	107.2(4)	C(6B)-C(5B)-C(4B)	103.7(4)
C(2B)-C(6B)-C(7B)	126.9(4)	C(2B)-C(6B)-C(5B)	112.0(5)
C(7B)-C(6B)-C(5B)	121.0(4)	O(7B)-C(7B)-C(6B)	121.6(4)
O(7B)-C(7B)-C(8B)	120.6(5)	C(6B)-C(7B)-C(8B)	117.5(4)
C(7B)-C(8B)-C(9B)	114.4(4)	C(7B)-C(8B)-C(12B)	112.0(3)
C(9B)-C(8B)-C(12B)	104.3(4)	C(10B)-C(9B)-C(8B)	105.9(4)
C(11B)-C(10B)-C(9B)	105.1(5)	O(11B)-C(11B)-C(10B)	126.4(5)
O(11B)-C(11B)-C(12B)	124.2(5)	C(10B)-C(11B)-C(12B)	109.4(4)
O(13B)-C(12B)-C(14B)	111.3(3)	O(13B)-C(12B)-C(8B)	114.0(3)
C(14B)-C(12B)-C(8B)	112.9(4)	O(13B)-C(12B)-C(11B)	103.3(3)
C(14B)-C(12B)-C(11B)	110.0(4)	C(8B)-C(12B)-C(11B)	104.6(4)
C(1B)-O(13B)-C(12B)	118.1(3)	C(15B)-C(14B)-C(12B)	110.5(4)
C(16B)-C(15B)-C(14B)	109.3(4)	C(15B)-C(16B)-C(1B)	112.4(4)
O(1D)-C(1D)-O(13D)	104.6(3)	O(1D)-C(1D)-C(2D)	109.1(3)
O(13D)-C(1D)-C(2D)	109.9(3)	O(1D)-C(1D)-C(16D)	106.8(3)
O(13D)-C(1D)-C(16D)	111.0(3)	C(2D)-C(1D)-C(16D)	114.9(3)
C(6D)-C(2D)-C(1D)	128.3(3)	C(6D)-C(2D)-C(3D)	111.0(4)
C(1D)-C(2D)-C(3D)	120.2(3)	C(4D)-C(3D)-C(2D)	104.8(4)
C(3D)-C(4D)-C(5D)	107.6(3)	C(6D)-C(5D)-C(4D)	102.8(3)
C(2D)-C(6D)-C(7D)	127.6(3)	C(2D)-C(6D)-C(5D)	112.2(3)
C(7D)-C(6D)-C(5D)	120.2(3)	O(7D)-C(7D)-C(6D)	121.5(3)
O(7D)-C(7D)-C(8D)	120.9(3)	C(6D)-C(7D)-C(8D)	117.2(3)
C(7D)-C(8D)-C(9D)	114.0(3)	C(7D)-C(8D)-C(12D)	112.4(3)
C(9D)-C(8D)-C(12D)	104.6(3)	C(10D)-C(9D)-C(8D)	105.2(3)
C(11D)-C(10D)-C(9D)	105.5(3)	O(11D)-C(11D)-C(10D)	127.1(4)
O(11D)-C(11D)-C(12D)	123.1(4)	C(10D)-C(11D)-C(12D)	109.8(3)
O(13D)-C(12D)-C(14D)	110.6(3)	O(13D)-C(12D)-C(11D)	103.5(3)
C(14D)-C(12D)-C(11D)	111.9(3)	O(13D)-C(12D)-C(8D)	114.8(3)
C(14D)-C(12D)-C(8D)	112.0(3)	C(11D)-C(12D)-C(8D)	103.4(3)
C(12D)-O(13D)-C(1D)	117.4(3)	C(15D)-C(14D)-C(12D)	110.2(3)
C(14D)-C(15D)-C(16D)	109.9(4)	C(1D)-C(16D)-C(15D)	112.6(3)
O(1H)-C(1H)-O(13H)	104.8(3)	O(1H)-C(1H)-C(2H)	109.9(3)
O(13H)-C(1H)-C(2H)	109.9(3)	O(1H)-C(1H)-C(16H)	107.0(3)
O(13H)-C(1H)-C(16H)	110.7(3)	C(2H)-C(1H)-C(16H)	114.1(4)
C(6H)-C(2H)-C(3H)	111.0(4)	C(6H)-C(2H)-C(1H)	127.2(4)
C(3H)-C(2H)-C(1H)	121.5(4)	C(2H)-C(3H)-C(4H)	103.8(5)
C(5H)-C(4H)-C(3H)	108.3(5)	C(6H)-C(5H)-C(4H)	103.5(5)
C(2H)-C(6H)-C(7H)	127.4(4)	C(2H)-C(6H)-C(5H)	112.5(5)
C(7H)-C(6H)-C(5H)	120.0(5)	O(7H)-C(7H)-C(6H)	121.4(4)
O(7H)-C(7H)-C(8H)	121.6(5)	C(6H)-C(7H)-C(8H)	116.7(4)
C(7H)-C(8H)-C(9H)	113.7(4)	C(7H)-C(8H)-C(12H)	111.6(3)
C(9H)-C(8H)-C(12H)	104.4(4)	C(10H)-C(9H)-C(8H)	105.7(4)
C(11H)-C(10H)-C(9H)	104.5(4)	O(11H)-C(11H)-C(10H)	127.2(5)
O(11H)-C(11H)-C(12H)	123.1(5)	C(10H)-C(11H)-C(12H)	109.7(4)
O(13H)-C(12H)-C(14H)	112.1(4)	O(13H)-C(12H)-C(11H)	103.4(3)
C(14H)-C(12H)-C(11H)	110.7(4)	O(13H)-C(12H)-C(8H)	113.6(3)
C(14H)-C(12H)-C(8H)	112.4(3)	C(11H)-C(12H)-C(8H)	104.0(4)
C(12H)-O(13H)-C(1H)	118.0(3)	C(15H)-C(14H)-C(12H)	109.8(4)
C(16H)-C(15H)-C(14H)	110.0(4)	C(15H)-C(16H)-C(1H)	111.3(4)

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1A)	58(2)	53(2)	61(2)	-27(2)	25(2)	-15(1)
C(1A)	44(2)	43(2)	36(2)	-15(2)	10(2)	-12(2)
C(2A)	41(2)	40(2)	38(2)	-16(2)	-3(2)	-7(2)
C(3A)	73(3)	66(3)	43(3)	-9(2)	-18(2)	-1(3)
C(4A)	58(3)	48(3)	81(3)	-6(2)	-27(3)	7(2)
C(5A)	42(2)	41(2)	65(3)	-13(2)	-10(2)	2(2)
C(6A)	33(2)	34(2)	42(2)	-12(2)	-3(2)	-3(2)
C(7A)	29(2)	42(2)	42(2)	-14(2)	8(2)	-6(2)
O(7A)	76(2)	46(2)	48(2)	-22(1)	17(2)	-6(1)
C(8A)	34(2)	35(2)	35(2)	-10(2)	4(2)	-5(2)
C(9A)	54(3)	47(2)	40(2)	-7(2)	0(2)	-10(2)
C(10A)	66(3)	53(3)	45(3)	-6(2)	-13(2)	-3(2)
C(11A)	46(3)	39(2)	55(3)	-8(2)	-7(2)	-1(2)
O(11A)	46(2)	89(2)	91(3)	-13(2)	-15(2)	19(2)
C(12A)	32(2)	35(2)	41(2)	-10(2)	-1(2)	-2(2)
O(13A)	33(1)	39(1)	40(2)	-13(1)	4(1)	-6(1)
C(14A)	52(3)	39(2)	64(3)	-22(2)	6(2)	-6(2)
C(15A)	59(3)	51(3)	60(3)	-34(2)	4(2)	-12(2)
C(16A)	66(3)	57(3)	49(3)	-31(2)	5(2)	-9(2)
O(1B)	65(2)	45(2)	57(2)	-18(1)	10(2)	-8(1)
C(1B)	48(2)	51(3)	40(2)	-13(2)	2(2)	-3(2)
C(2B)	55(3)	63(3)	37(2)	-15(2)	-1(2)	11(2)
C(3B)	78(4)	135(5)	54(3)	-41(3)	-16(3)	4(3)
C(4B)	125(5)	128(5)	46(3)	-32(3)	-24(3)	52(4)
C(5B)	108(5)	120(5)	39(3)	1(3)	8(3)	28(4)
C(6B)	63(3)	63(3)	36(2)	-7(2)	8(2)	10(2)
C(7B)	65(3)	44(3)	55(3)	5(2)	23(2)	6(2)
O(7B)	76(2)	71(2)	96(3)	-21(2)	44(2)	-12(2)
C(8B)	58(3)	39(2)	58(3)	-8(2)	15(2)	3(2)
C(9B)	90(4)	47(3)	106(4)	-30(3)	24(3)	-12(3)
C(10B)	89(4)	81(4)	114(5)	-49(4)	0(4)	-6(3)
C(11B)	85(4)	59(3)	66(3)	-34(3)	-4(3)	-5(3)
O(11B)	159(4)	93(3)	70(3)	-16(2)	-48(3)	-13(3)
C(12B)	63(3)	42(2)	44(2)	-14(2)	5(2)	4(2)
O(13B)	51(2)	40(2)	37(2)	-12(1)	-1(1)	3(1)
C(14B)	87(4)	59(3)	58(3)	-24(2)	26(3)	1(3)
C(15B)	60(3)	69(3)	75(3)	-11(3)	29(3)	13(3)
C(16B)	54(3)	67(3)	55(3)	-14(2)	14(2)	-2(2)
O(1D)	41(2)	49(2)	66(2)	-22(1)	-20(1)	7(1)
C(1D)	37(2)	44(2)	43(2)	-16(2)	-10(2)	6(2)
C(2D)	38(2)	45(2)	38(2)	-12(2)	0(2)	7(2)
C(3D)	73(3)	87(4)	45(3)	-7(3)	6(2)	-3(3)
C(4D)	68(3)	64(3)	69(3)	12(3)	16(3)	-2(3)
C(5D)	41(2)	43(2)	69(3)	-7(2)	9(2)	-9(2)
C(6D)	29(2)	37(2)	47(2)	-9(2)	-3(2)	1(2)
C(7D)	26(2)	40(2)	49(2)	-17(2)	-6(2)	3(2)
O(7D)	72(2)	51(2)	62(2)	-23(2)	-26(2)	4(2)
C(8D)	30(2)	40(2)	41(2)	-10(2)	0(2)	3(2)

C(9D)	47(2)	52(3)	48(3)	-4(2)	-5(2)	5(2)
C(10D)	62(3)	68(3)	46(3)	-6(2)	6(2)	5(2)
C(11D)	44(3)	45(2)	61(3)	-5(2)	8(2)	0(2)
O(11D)	50(2)	105(3)	86(3)	-3(2)	21(2)	-17(2)
C(12D)	33(2)	35(2)	48(2)	-11(2)	0(2)	-3(2)
O(13D)	30(1)	37(1)	49(2)	-13(1)	-1(1)	2(1)
C(14D)	49(3)	39(2)	77(3)	-19(2)	-3(2)	-3(2)
C(15D)	58(3)	47(3)	70(3)	-34(2)	-11(2)	10(2)
C(16D)	52(3)	57(3)	63(3)	-33(2)	-9(2)	5(2)
O(1H)	72(2)	48(2)	60(2)	-21(1)	-16(2)	6(2)
C(1H)	57(3)	43(2)	44(2)	-12(2)	-8(2)	-2(2)
C(2H)	59(3)	64(3)	45(3)	-22(2)	-1(2)	-15(2)
C(3H)	85(4)	129(5)	77(4)	-48(4)	18(3)	-17(4)
C(4H)	148(6)	129(6)	55(4)	-33(4)	25(4)	-48(5)
C(5H)	122(5)	127(5)	43(3)	-12(3)	-8(3)	-19(4)
C(6H)	80(3)	62(3)	37(2)	-9(2)	-11(2)	-21(3)
C(7H)	79(3)	41(2)	49(3)	2(2)	-25(3)	-6(2)
O(7H)	90(3)	62(2)	82(2)	-21(2)	-46(2)	12(2)
C(8H)	71(3)	39(2)	49(3)	-11(2)	-18(2)	-6(2)
C(9H)	97(4)	49(3)	88(4)	-28(3)	-28(3)	9(3)
C(10H)	88(4)	69(3)	87(4)	-36(3)	-3(3)	1(3)
C(11H)	97(4)	53(3)	52(3)	-29(2)	-3(3)	-4(3)
O(11H)	156(4)	75(3)	63(2)	-16(2)	30(2)	8(2)
C(12H)	76(3)	37(2)	42(2)	-14(2)	-16(2)	-3(2)
O(13H)	61(2)	38(2)	42(2)	-14(1)	-8(1)	-2(1)
C(14H)	94(4)	55(3)	58(3)	-21(2)	-31(3)	-5(3)
C(15H)	81(4)	65(3)	69(3)	-12(3)	-38(3)	-12(3)
C(16H)	62(3)	68(3)	65(3)	-18(3)	-22(2)	0(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1AA)	6109	4620	3715	80
H(3AA)	3536(4)	4679(3)	2887(3)	80
H(3AB)	4360(4)	5460(3)	3069(3)	80
H(4AA)	2011(4)	5226(3)	3417(3)	80
H(4AB)	2745(4)	6176(3)	3317(3)	80
H(5AA)	2069(3)	5058(3)	4748(3)	80
H(5AB)	3137(3)	5764(3)	4646(3)	80
H(8AA)	3227(3)	2416(2)	5449(2)	80
H(9AA)	3546(3)	1397(3)	6696(2)	80
H(9AB)	3372(3)	2378(3)	6927(2)	80
H(10A)	5286(4)	1401(3)	7305(2)	80
H(10B)	5309(4)	2553(3)	7080(2)	80
H(14A)	4425(4)	977(3)	5379(3)	80
H(14B)	5619(4)	1222(3)	4925(3)	80
H(15A)	3483(4)	2081(3)	4289(2)	80
H(15B)	4186(4)	1342(3)	3946(2)	80
H(16A)	5640(4)	2483(3)	3466(2)	80
H(16B)	4469(4)	3004(3)	3145(2)	80
H(1BA)	1579(2)	6394(2)	-882(2)	80
H(3BA)	2631(5)	5827(5)	414(3)	80
H(3BB)	3686(5)	5135(5)	370(3)	80
H(4BA)	2315(6)	4851(5)	1654(3)	80
H(4BB)	3161(6)	4048(5)	1513(3)	80
H(5BA)	780(6)	4118(5)	1349(3)	80
H(5BB)	1593(6)	3200(5)	1445(3)	80
H(8BA)	1830(4)	2781(3)	-633(3)	80
H(9BA)	-229(5)	2151(4)	-663(3)	80
H(9BB)	680(5)	2043(4)	-1318(3)	80
H(10C)	-1092(5)	3456(4)	-1543(4)	80
H(10D)	-690(5)	2898(4)	-2165(4)	80
H(14C)	2585(4)	4303(3)	-2529(3)	80
H(14D)	2606(4)	3203(3)	-2001(3)	80
H(15C)	4296(4)	4028(4)	-1775(3)	80
H(15D)	3584(4)	3624(4)	-969(3)	80
H(16C)	4065(4)	5247(3)	-1100(3)	80
H(16D)	3502(4)	5585(3)	-1959(3)	80
H(1DA)	1553(2)	476(2)	6025(2)	80
H(3DA)	-747(4)	587(4)	7198(3)	80
H(3DB)	3(4)	-226(4)	6973(3)	80
H(4DA)	-2367(4)	-111(4)	7022(3)	80
H(4DB)	-1620(4)	-1028(4)	7001(3)	80
H(5DA)	-2803(3)	49(3)	5736(3)	80
H(5DB)	-1820(3)	-695(3)	5663(3)	80
H(8DA)	-1748(3)	2619(3)	4668(2)	80
H(9DA)	-1786(3)	3537(3)	3368(2)	80
H(9DB)	-2057(3)	2514(3)	3240(2)	80
H(10E)	-300(4)	3484(4)	2516(3)	80
H(10F)	-228(4)	2332(4)	2816(3)	80
H(14E)	-522(4)	4072(3)	4497(3)	80

H(14F)	782(4)	3877(3)	4734(3)	80
H(15E)	-1092(4)	3010(3)	5751(3)	80
H(15F)	-273(4)	3799(3)	5915(3)	80
H(16E)	1281(4)	2704(3)	6149(3)	80
H(16F)	260(4)	2186(3)	6711(3)	80
H(1HA)	6580(3)	-1316(2)	893(2)	80
H(3HA)	7724(5)	-652(5)	-356(3)	80
H(3HB)	8681(5)	88(5)	-265(3)	80
H(4HA)	7386(7)	340(5)	-1591(3)	80
H(4HB)	8143(7)	1162(5)	-1419(3)	80
H(5HA)	5792(6)	1045(5)	-1313(3)	80
H(5HB)	6539(6)	1974(5)	-1345(3)	80
H(8HA)	6486(4)	2301(3)	729(2)	80
H(9HA)	4381(5)	2843(3)	726(3)	80
H(9HB)	5196(5)	2967(3)	1412(3)	80
H(10G)	3541(5)	1485(4)	1552(3)	80
H(10H)	3799(5)	2045(4)	2193(3)	80
H(14G)	7196(4)	759(3)	2626(3)	80
H(14H)	7171(4)	1869(3)	2122(3)	80
H(15G)	8943(5)	1130(3)	1890(3)	80
H(15H)	8253(5)	1496(3)	1080(3)	80
H(16G)	8897(4)	-112(3)	1220(3)	80
H(16H)	8266(4)	-474(3)	2063(3)	80