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AROYL-ARYL-KETENES.

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Table 1. Crystal data and structure refinement for 22a.

Identification code	22a
Empirical formula	C30 H20 O6
Formula weight	476.46
Temperature	293(2) K
Wavelength	0.71069 A
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 17.102(8) A alpha = 90 deg. b = 12.086(6) A beta = 104.76(5) deg. c = 12.084(6) A gamma = 90 deg.
Volume	2415(2) A^3
Z	4
Density (calculated)	1.310 Mg/m^3
Absorption coefficient	0.091 mm^-1
F(000)	992
Crystal size	0.15 x 0.22 x 0.35 mm
Theta range for data collection	2.09 to 25.02 deg.
Index ranges	-20<=h<=19, 0<=k<=14, 0<=l<=14
Reflections collected	4459
Independent reflections	4253 [R(int) = 0.0255]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4253 / 0 / 405
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.0988
R indices (all data)	R1 = 0.1262, wR2 = 0.1245
Largest diff. peak and hole	0.153 and -0.170 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 22. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	4080(1)	1613(2)	156(2)	45(1)
C(2)	4908(2)	1484(3)	434(3)	40(1)
O(3)	5235(1)	1221(2)	-296(2)	55(1)
C(4)	5248(2)	1734(2)	1652(3)	40(1)
C(5)	4632(2)	2060(2)	2037(2)	38(1)
C(6)	3840(2)	1983(3)	1150(3)	40(1)
O(7)	3423(1)	3008(2)	898(2)	45(1)
C(8)	3805(2)	3927(3)	621(3)	55(1)
O(9)	4507(1)	3928(2)	626(3)	95(1)
C(10)	3244(2)	4872(3)	323(3)	47(1)
C(11)	2414(2)	4759(3)	170(3)	56(1)
C(12)	1926(2)	5675(3)	-97(4)	68(1)
C(13)	2246(3)	6692(3)	-212(4)	69(1)
C(14)	3066(3)	6799(3)	-79(3)	65(1)
C(15)	3565(2)	5894(3)	180(3)	55(1)
C(16)	3242(2)	1168(3)	1430(3)	41(1)
C(17)	2518(2)	1489(3)	1609(4)	69(1)
C(18)	2000(2)	710(4)	1859(4)	83(1)
C(19)	2200(2)	-381(4)	1928(4)	66(1)
C(20)	2915(3)	-708(3)	1750(4)	70(1)
C(21)	3441(2)	62(3)	1505(4)	63(1)
C(22)	6129(2)	1748(3)	2159(3)	42(1)
C(23)	6625(2)	929(3)	1937(3)	54(1)
C(24)	7457(2)	1022(4)	2343(4)	68(1)
C(25)	7789(2)	1929(4)	2964(3)	67(1)
C(26)	7303(2)	2741(4)	3207(4)	67(1)
C(27)	6474(2)	2656(3)	2809(3)	55(1)
O(28)	4599(1)	2479(2)	3083(2)	47(1)
C(29)	4939(2)	1888(3)	4064(3)	48(1)
O(30)	5219(2)	989(2)	4026(2)	75(1)
C(31)	4890(2)	2492(3)	5102(3)	44(1)
C(32)	4597(2)	3556(3)	5069(3)	55(1)
C(33)	4538(3)	4078(4)	6059(4)	69(1)
C(34)	4771(2)	3537(5)	7085(4)	76(1)
C(35)	5070(3)	2472(5)	7125(4)	76(1)
C(36)	5127(2)	1958(4)	6144(3)	62(1)

Table 3. Bond lengths [A] and angles [deg] for 22.

O(1)-C(2)	1.379(3)
O(1)-C(6)	1.437(3)
C(2)-O(3)	1.202(3)
C(2)-C(4)	1.469(4)
C(4)-C(5)	1.317(4)
C(4)-C(22)	1.474(4)
C(5)-O(28)	1.376(3)
C(5)-C(6)	1.501(4)
C(6)-O(7)	1.423(3)
C(6)-C(16)	1.518(4)
O(7)-C(8)	1.374(4)
C(8)-O(9)	1.198(4)
C(8)-C(10)	1.476(4)
C(10)-C(15)	1.379(5)
C(10)-C(11)	1.391(4)
C(11)-C(12)	1.375(5)
C(12)-C(13)	1.367(5)
C(13)-C(14)	1.376(5)
C(14)-C(15)	1.374(5)
C(16)-C(17)	1.367(4)
C(16)-C(21)	1.377(5)
C(17)-C(18)	1.379(5)
C(18)-C(19)	1.358(6)
C(19)-C(20)	1.354(5)
C(20)-C(21)	1.378(5)
C(22)-C(23)	1.374(4)
C(22)-C(27)	1.391(5)
C(23)-C(24)	1.388(5)
C(24)-C(25)	1.367(6)
C(25)-C(26)	1.365(5)
C(26)-C(27)	1.380(5)
O(28)-C(29)	1.379(4)
C(29)-O(30)	1.193(4)
C(29)-C(31)	1.473(4)
C(31)-C(32)	1.377(5)
C(31)-C(36)	1.381(5)
C(32)-C(33)	1.379(5)
C(33)-C(34)	1.368(6)
C(34)-C(35)	1.382(6)
C(35)-C(36)	1.364(6)

C(2)-O(1)-C(6)	109.0(2)
O(3)-C(2)-O(1)	119.5(3)
O(3)-C(2)-C(4)	130.6(3)
O(1)-C(2)-C(4)	109.9(3)
C(5)-C(4)-C(2)	105.5(3)
C(5)-C(4)-C(22)	132.4(3)
C(2)-C(4)-C(22)	121.4(3)
C(4)-C(5)-O(28)	131.2(3)
C(4)-C(5)-C(6)	112.8(3)
O(28)-C(5)-C(6)	116.0(2)
O(7)-C(6)-O(1)	109.1(2)
O(7)-C(6)-C(5)	114.3(2)
O(1)-C(6)-C(5)	102.6(2)
O(7)-C(6)-C(16)	106.5(2)
O(1)-C(6)-C(16)	109.6(2)
C(5)-C(6)-C(16)	114.6(2)
C(8)-O(7)-C(6)	120.8(2)
O(9)-C(8)-O(7)	122.5(3)
O(9)-C(8)-C(10)	126.1(3)
O(7)-C(8)-C(10)	111.4(3)
C(15)-C(10)-C(11)	119.8(3)
C(15)-C(10)-C(8)	117.9(3)
C(11)-C(10)-C(8)	122.3(3)
C(12)-C(11)-C(10)	119.3(4)

C(12)-C(13)-C(14)	119.7(4)
C(15)-C(14)-C(13)	120.5(4)
C(14)-C(15)-C(10)	119.8(3)
C(17)-C(16)-C(21)	118.9(3)
C(17)-C(16)-C(6)	122.6(3)
C(21)-C(16)-C(6)	118.4(3)
C(16)-C(17)-C(18)	119.9(4)
C(19)-C(18)-C(17)	120.7(4)
C(20)-C(19)-C(18)	119.8(4)
C(19)-C(20)-C(21)	120.1(4)
C(16)-C(21)-C(20)	120.5(4)
C(23)-C(22)-C(27)	118.9(3)
C(23)-C(22)-C(4)	121.8(3)
C(27)-C(22)-C(4)	119.1(3)
C(22)-C(23)-C(24)	120.1(4)
C(25)-C(24)-C(23)	120.3(4)
C(26)-C(25)-C(24)	120.3(4)
C(25)-C(26)-C(27)	120.0(4)
C(26)-C(27)-C(22)	120.4(4)
C(5)-O(28)-C(29)	119.4(2)
O(30)-C(29)-O(28)	121.6(3)
O(30)-C(29)-C(31)	126.5(3)
O(28)-C(29)-C(31)	111.8(3)
C(32)-C(31)-C(36)	118.9(4)
C(32)-C(31)-C(29)	122.6(3)
C(36)-C(31)-C(29)	118.5(3)
C(31)-C(32)-C(33)	120.6(4)
C(34)-C(33)-C(32)	119.9(4)
C(33)-C(34)-C(35)	119.8(4)
C(36)-C(35)-C(34)	120.1(5)
C(35)-C(36)-C(31)	120.7(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 22. 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
O(1)	36(1)	62(1)	38(1)	-1(1)	10(1)	3(1)
C(2)	35(2)	43(2)	45(2)	7(2)	14(2)	2(1)
O(3)	51(1)	74(2)	44(1)	1(1)	20(1)	6(1)
C(4)	35(2)	38(2)	45(2)	2(2)	9(1)	2(1)
C(5)	38(2)	43(2)	34(2)	0(2)	12(1)	1(1)
C(6)	37(2)	44(2)	39(2)	2(2)	11(1)	7(1)
O(7)	36(1)	40(1)	59(1)	8(1)	12(1)	8(1)
C(8)	44(2)	52(2)	68(2)	12(2)	12(2)	3(2)
O(9)	40(1)	71(2)	175(3)	51(2)	32(2)	10(1)
C(10)	42(2)	44(2)	52(2)	5(2)	9(2)	2(2)
C(11)	50(2)	45(2)	72(3)	7(2)	14(2)	2(2)
C(12)	46(2)	59(3)	97(3)	7(2)	12(2)	19(2)
C(13)	73(3)	52(3)	84(3)	13(2)	26(2)	20(2)
C(14)	74(3)	49(2)	74(3)	14(2)	26(2)	3(2)
C(15)	47(2)	57(2)	58(2)	7(2)	9(2)	2(2)
C(16)	39(2)	45(2)	39(2)	-1(2)	11(1)	1(2)
C(17)	60(2)	46(2)	113(4)	8(2)	43(2)	9(2)
C(18)	48(2)	81(3)	132(4)	23(3)	46(3)	5(2)
C(19)	56(2)	70(3)	73(3)	2(2)	18(2)	-16(2)
C(20)	82(3)	47(2)	91(3)	2(2)	42(3)	-3(2)
C(21)	61(2)	49(2)	90(3)	-1(2)	39(2)	0(2)
C(22)	36(2)	46(2)	44(2)	7(2)	8(1)	3(2)
C(23)	44(2)	50(2)	65(3)	-4(2)	8(2)	4(2)
C(24)	46(2)	83(3)	71(3)	1(2)	9(2)	22(2)
C(25)	41(2)	95(3)	61(3)	9(3)	7(2)	4(2)
C(26)	49(2)	82(3)	64(3)	-3(2)	1(2)	-9(2)
C(27)	45(2)	57(2)	60(2)	2(2)	10(2)	3(2)
O(28)	50(1)	50(1)	39(1)	1(1)	9(1)	11(1)
C(29)	46(2)	49(2)	49(2)	12(2)	14(2)	3(2)
O(30)	111(2)	57(2)	59(2)	14(1)	27(2)	25(2)
C(31)	42(2)	52(2)	39(2)	3(2)	11(2)	-8(2)
C(32)	62(2)	55(2)	48(2)	-1(2)	15(2)	2(2)
C(33)	76(3)	71(3)	65(3)	-15(2)	28(2)	2(2)
C(34)	69(3)	116(4)	49(3)	-31(3)	27(2)	-19(3)
C(35)	77(3)	103(4)	49(3)	4(3)	20(2)	-11(3)
C(36)	70(3)	68(3)	47(2)	0(2)	15(2)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 22.

	x	y	z	U(eq)
H(11)	2189(17)	4040(25)	307(25)	46(9)
H(12)	1362(22)	5579(30)	-173(31)	82(12)
H(13)	1923(23)	7374(33)	-335(33)	92(13)
H(14)	3293(20)	7536(30)	-149(30)	75(11)
H(15)	4126(21)	5947(27)	298(29)	71(11)
H(17)	2388(19)	2241(28)	1600(27)	60(10)
H(18)	1510(22)	932(30)	2002(31)	85(12)
H(19)	1835(21)	-928(29)	2087(30)	75(11)
H(20)	3116(19)	-1477(31)	1809(28)	70(11)
H(21)	3940(23)	-136(32)	1358(33)	94(13)
H(23)	6424(16)	289(24)	1541(25)	41(9)
H(24)	7791(21)	459(30)	2186(30)	75(12)
H(25)	8379(22)	1997(28)	3190(30)	76(11)
H(26)	7527(20)	3367(30)	3636(29)	66(11)
H(27)	6139(19)	3269(29)	2933(28)	69(11)
H(32)	4449(17)	3964(24)	4382(27)	49(10)
H(33)	4320(21)	4804(33)	6007(32)	80(13)
H(34)	4733(20)	3858(28)	7766(32)	71(12)
H(35)	5206(23)	2095(34)	7833(37)	94(15)
H(36)	5314(19)	1222(29)	6132(29)	62(11)