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X-RAY DATA FOR 6g

(5*S**,9*S**)-9-Methyl-3,6,9-triphenyl-1,8-dioxa-2,6-diazaspiro[4.4]non-2-ene-7-one **6g**

A10_08 (RN820/102/4 Paul Savage CSIRO)

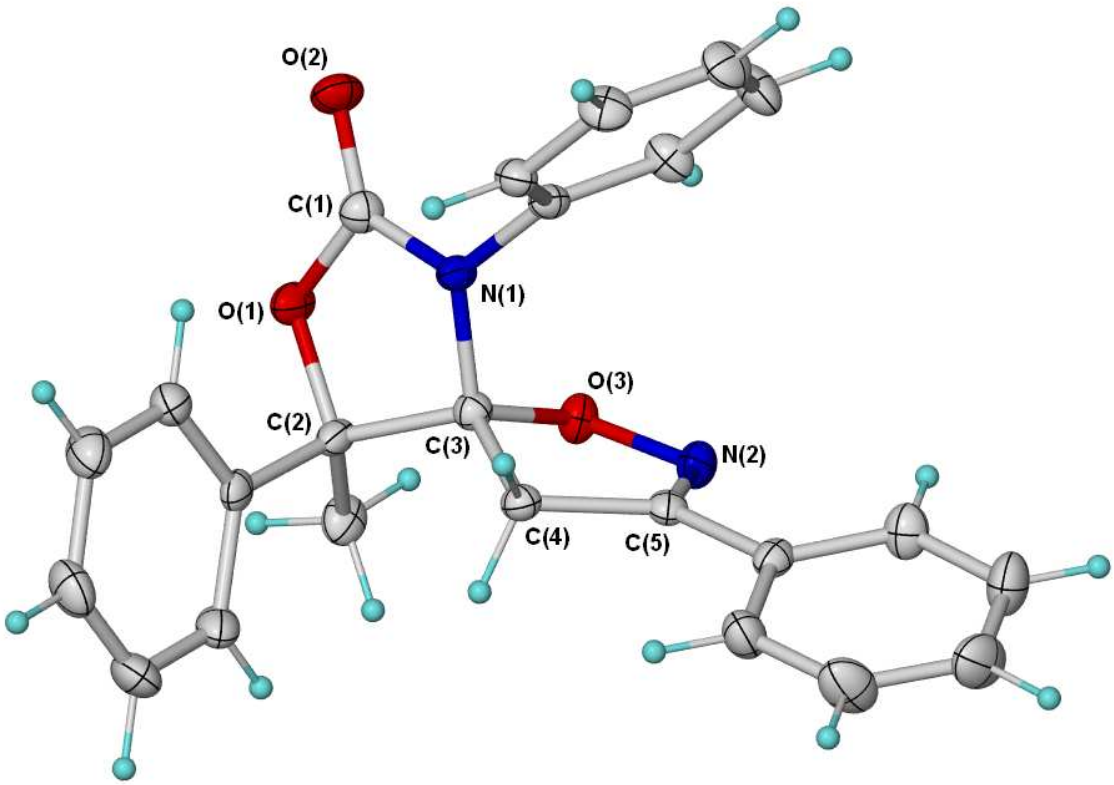

Figure 1. Molecular diagram shown with 50% thermal ellipsoids and hydrogen atoms as spheres pf arbitrary size. The molecule crystallises in a centrosymmetric space group (P21/c) which means that the inverted structure is also present in the crystal.

Table 1. Crystal data and structure refinement for A10_08.

Identification code	a10_08
Empirical formula	C24 H20 N2 O3
Formula weight	384.42
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.2366(7) A alpha = 90 deg. b = 13.4923(7) A beta = 105.307(2) deg. c = 13.5806(8) A gamma = 90 deg.
Volume	1985.9(2) A^3
Z, Calculated density	4, 1.286 Mg/m^3
Absorption coefficient	0.086 mm^-1
F(000)	808
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	2.41 to 27.49 deg.
Limiting indices	-12<=h<=14, -11<=k<=17, -17<=l<=17
Reflections collected / unique	10140 / 4496 [R(int) = 0.0410]
Completeness to theta = 27.49	98.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.99 and 0.95
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4496 / 0 / 262
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0648, wR2 = 0.1202
R indices (all data)	R1 = 0.0926, wR2 = 0.1335
Largest diff. peak and hole	0.245 and -0.239 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for A10_08.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	4638(2)	2616(1)	391(1)	24(1)
O(2)	5470(2)	3543(1)	-640(1)	29(1)
O(3)	7030(1)	1984(1)	1980(1)	23(1)
N(1)	6335(2)	3469(1)	1095(1)	19(1)
N(2)	8095(2)	2136(1)	2806(1)	23(1)
C(1)	5497(2)	3242(2)	206(2)	23(1)
C(2)	4842(2)	2491(2)	1495(2)	21(1)
C(3)	6206(2)	2825(2)	1915(2)	19(1)
C(4)	6614(2)	3287(2)	2968(2)	20(1)
C(5)	7892(2)	2873(2)	3338(2)	19(1)
C(11)	7386(2)	4088(2)	1142(2)	19(1)
C(12)	7280(2)	5095(2)	1278(2)	22(1)
C(13)	8288(2)	5699(2)	1325(2)	28(1)
C(14)	9394(2)	5303(2)	1249(2)	30(1)
C(15)	9486(2)	4293(2)	1108(2)	31(1)
C(16)	8482(2)	3680(2)	1056(2)	26(1)
C(21)	3985(2)	3196(2)	1854(2)	21(1)
C(22)	3639(2)	4101(2)	1361(2)	25(1)
C(23)	2938(2)	4775(2)	1730(2)	32(1)
C(24)	2579(2)	4568(2)	2606(2)	35(1)
C(25)	2908(2)	3674(2)	3098(2)	36(1)
C(26)	3604(2)	2988(2)	2729(2)	29(1)
C(27)	4637(2)	1404(2)	1686(2)	28(1)
C(51)	8863(2)	3213(2)	4228(2)	21(1)
C(52)	10069(2)	2895(2)	4352(2)	30(1)
C(53)	10982(3)	3156(2)	5207(2)	38(1)
C(54)	10710(3)	3753(2)	5937(2)	42(1)
C(55)	9531(3)	4095(2)	5811(2)	41(1)
C(56)	8598(2)	3830(2)	4960(2)	30(1)

Table 3. Bond lengths [A] and angles [deg] for A10_08.

O(1)-C(1)	1.356(3)
O(1)-C(2)	1.466(2)
O(2)-C(1)	1.210(2)
O(3)-N(2)	1.422(2)
O(3)-C(3)	1.452(3)
N(1)-C(1)	1.356(3)
N(1)-C(11)	1.434(3)
N(1)-C(3)	1.449(3)
N(2)-C(5)	1.285(3)
C(2)-C(27)	1.517(3)
C(2)-C(21)	1.523(3)
C(2)-C(3)	1.554(3)
C(3)-C(4)	1.517(3)
C(4)-C(5)	1.498(3)
C(5)-C(51)	1.470(3)
C(11)-C(16)	1.381(3)
C(11)-C(12)	1.381(3)
C(12)-C(13)	1.382(3)
C(13)-C(14)	1.382(3)
C(14)-C(15)	1.383(3)
C(15)-C(16)	1.385(3)
C(21)-C(26)	1.392(3)
C(21)-C(22)	1.397(3)
C(22)-C(23)	1.381(3)
C(23)-C(24)	1.382(3)
C(24)-C(25)	1.382(4)
C(25)-C(26)	1.388(3)
C(51)-C(56)	1.388(3)
C(51)-C(52)	1.389(3)
C(52)-C(53)	1.377(3)
C(53)-C(54)	1.374(4)
C(54)-C(55)	1.370(4)
C(55)-C(56)	1.387(4)

C(1)-O(1)-C(2)	109.59(16)
N(2)-O(3)-C(3)	109.00(15)
C(1)-N(1)-C(11)	122.72(17)
C(1)-N(1)-C(3)	111.24(18)
C(11)-N(1)-C(3)	124.29(17)
C(5)-N(2)-O(3)	108.56(17)
O(2)-C(1)-O(1)	123.0(2)
O(2)-C(1)-N(1)	127.4(2)
O(1)-C(1)-N(1)	109.62(18)
O(1)-C(2)-C(27)	107.20(17)
O(1)-C(2)-C(21)	108.34(17)
C(27)-C(2)-C(21)	114.32(18)
O(1)-C(2)-C(3)	102.36(16)
C(27)-C(2)-C(3)	113.42(19)
C(21)-C(2)-C(3)	110.34(17)
N(1)-C(3)-O(3)	108.94(16)
N(1)-C(3)-C(4)	114.30(17)
O(3)-C(3)-C(4)	103.53(17)
N(1)-C(3)-C(2)	100.47(17)
O(3)-C(3)-C(2)	110.27(17)
C(4)-C(3)-C(2)	119.23(17)
C(5)-C(4)-C(3)	100.82(17)
N(2)-C(5)-C(51)	120.0(2)

N(2)-C(5)-C(4)	113.34(19)
C(51)-C(5)-C(4)	126.62(19)
C(16)-C(11)-C(12)	120.9(2)
C(16)-C(11)-N(1)	120.46(19)
C(12)-C(11)-N(1)	118.6(2)
C(11)-C(12)-C(13)	119.2(2)
C(14)-C(13)-C(12)	120.7(2)
C(13)-C(14)-C(15)	119.5(2)
C(14)-C(15)-C(16)	120.3(2)
C(11)-C(16)-C(15)	119.4(2)
C(26)-C(21)-C(22)	118.4(2)
C(26)-C(21)-C(2)	120.7(2)
C(22)-C(21)-C(2)	120.79(19)
C(23)-C(22)-C(21)	121.0(2)
C(22)-C(23)-C(24)	120.2(2)
C(25)-C(24)-C(23)	119.5(2)
C(24)-C(25)-C(26)	120.7(2)
C(25)-C(26)-C(21)	120.3(2)
C(56)-C(51)-C(52)	119.0(2)
C(56)-C(51)-C(5)	121.5(2)
C(52)-C(51)-C(5)	119.5(2)
C(53)-C(52)-C(51)	120.6(2)
C(54)-C(53)-C(52)	120.0(3)
C(55)-C(54)-C(53)	120.0(3)
C(54)-C(55)-C(56)	120.7(2)
C(55)-C(56)-C(51)	119.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for A10_08.
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)	24(1)	26(1)	21(1)	-1(1)	2(1)	-7(1)
O(2)	34(1)	35(1)	17(1)	0(1)	6(1)	-5(1)
O(3)	21(1)	20(1)	26(1)	-3(1)	1(1)	1(1)
N(1)	20(1)	20(1)	16(1)	1(1)	4(1)	-4(1)
N(2)	20(1)	23(1)	24(1)	-1(1)	1(1)	-2(1)
C(1)	24(1)	23(1)	21(1)	-2(1)	5(1)	-2(1)
C(2)	19(1)	23(1)	17(1)	4(1)	1(1)	-3(1)
C(3)	20(1)	18(1)	19(1)	1(1)	4(1)	0(1)
C(4)	21(1)	20(1)	18(1)	2(1)	6(1)	1(1)
C(5)	19(1)	18(1)	20(1)	4(1)	6(1)	-2(1)
C(11)	21(1)	21(1)	15(1)	0(1)	5(1)	-4(1)
C(12)	23(1)	22(1)	22(1)	3(1)	9(1)	2(1)
C(13)	35(2)	19(1)	32(1)	2(1)	12(1)	-4(1)
C(14)	26(1)	29(1)	35(1)	1(1)	9(1)	-10(1)
C(15)	25(1)	31(1)	43(2)	-1(1)	18(1)	-2(1)
C(16)	28(1)	22(1)	31(1)	-5(1)	12(1)	-1(1)
C(21)	13(1)	24(1)	21(1)	2(1)	-1(1)	-3(1)
C(22)	22(1)	28(1)	26(1)	3(1)	6(1)	0(1)
C(23)	27(1)	29(1)	40(1)	7(1)	9(1)	4(1)
C(24)	25(1)	36(2)	48(2)	0(1)	16(1)	5(1)
C(25)	30(2)	46(2)	36(1)	7(1)	18(1)	2(1)
C(26)	23(1)	31(1)	33(1)	12(1)	9(1)	0(1)
C(27)	25(1)	24(1)	31(1)	0(1)	2(1)	-5(1)
C(51)	21(1)	20(1)	20(1)	3(1)	2(1)	-4(1)
C(52)	26(1)	27(1)	33(1)	-5(1)	4(1)	2(1)
C(53)	24(1)	45(2)	39(2)	-2(1)	-3(1)	3(1)
C(54)	33(2)	61(2)	26(1)	-5(1)	-2(1)	-14(1)
C(55)	38(2)	59(2)	29(1)	-16(1)	13(1)	-10(1)
C(56)	23(1)	41(2)	28(1)	-3(1)	8(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for A10_08.

	x	y	z	U(eq)
H(4A)	6623	4020	2933	24
H(4B)	6082	3076	3406	24
H(12)	6523	5370	1337	26
H(13)	8219	6394	1412	34
H(14)	10086	5721	1293	36
H(15)	10242	4018	1047	37
H(16)	8546	2987	961	32
H(22)	3889	4254	763	30
H(23)	2702	5383	1380	38
H(24)	2110	5037	2868	42
H(25)	2655	3527	3696	43
H(26)	3822	2375	3073	34
H(27A)	5218	1000	1432	41
H(27B)	3790	1219	1328	41
H(27C)	4771	1292	2420	41
H(52)	10266	2495	3841	35
H(53)	11800	2922	5292	46
H(54)	11339	3928	6530	50
H(55)	9351	4519	6312	50
H(56)	7783	4069	4879	36

X-RAY DATA FOR 6b

(5*S**,9*S**)-9-Ethyl-3,6-diphenyl-1,8-dioxa-2,6-diazaspiro[4.4]non-2-en-7-one **6b**

A8_08 (RN810/107/2 Paul Savage CSIRO)

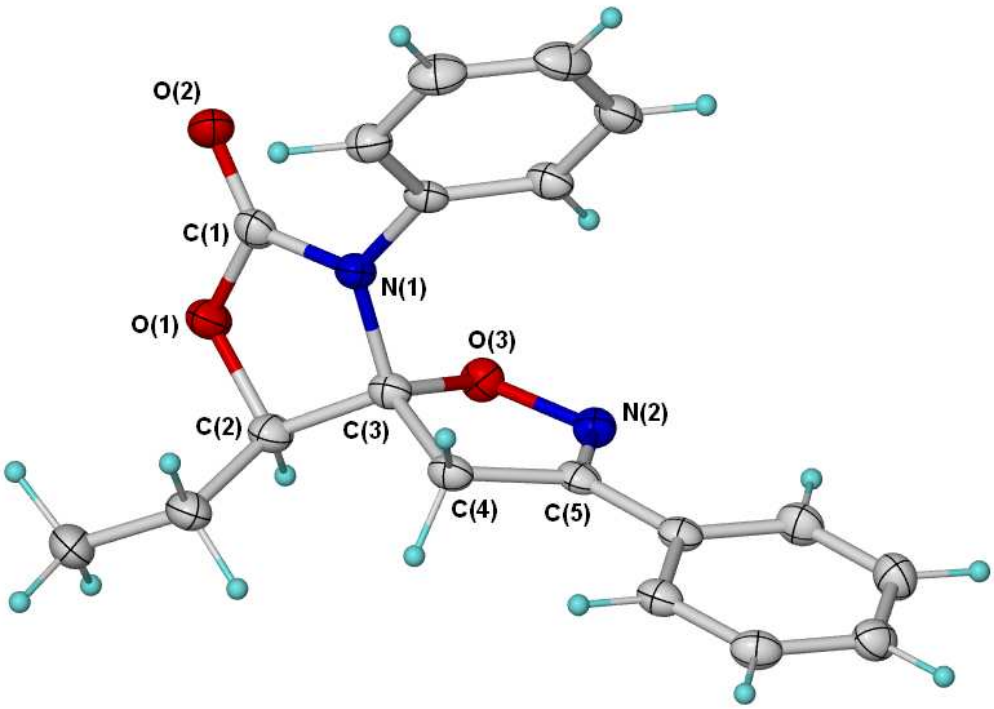

Figure 1. Molecular diagram shown with 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size. The molecule crystallises in a centrosymmetric space group (P21/c) which means that the inverted structure is also present in the crystal.

Table 1. Crystal data and structure refinement for A8_08m.

Identification code	a8_08m
Empirical formula	C19 H18 N2 O3
Formula weight	322.35
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 12.2721(8) A alpha = 90 deg. b = 16.3999(9) A beta = 105.518(2) deg. c = 8.2479(5) A gamma = 90 deg.
Volume	1599.47(17) A^3
Z, Calculated density	4, 1.339 Mg/m^3
Absorption coefficient	0.092 mm^-1
F(000)	680
Crystal size	0.25 x 0.25 x 0.13 mm
Theta range for data collection	2.48 to 27.50 deg.
Limiting indices	-15<=h<=15, -21<=k<=20, -10<=l<=8
Reflections collected / unique	13111 / 3681 [R(int) = 0.0295]
Completeness to theta = 27.50	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.99 and 0.94
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3681 / 0 / 289
Goodness-of-fit on F^2	1.266
Final R indices [I>2sigma(I)]	R1 = 0.0661, wR2 = 0.1214
R indices (all data)	R1 = 0.0716, wR2 = 0.1236
Largest diff. peak and hole	0.248 and -0.197 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for A8_08m.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	9742(1)	1483(1)	5985(2)	30(1)
O(2)	10098(1)	762(1)	3864(2)	30(1)
O(3)	7501(1)	2325(1)	4209(2)	27(1)
N(1)	8274(2)	1009(1)	4017(2)	24(1)
N(2)	6317(2)	2436(1)	3665(2)	25(1)
C(1)	9426(2)	1049(1)	4532(3)	26(1)
C(2)	8754(2)	1641(2)	6598(3)	28(1)
C(3)	7763(2)	1526(1)	5023(3)	24(1)
C(4)	6631(2)	1237(1)	5232(3)	25(1)
C(5)	5830(2)	1843(1)	4201(3)	22(1)
C(11)	7673(2)	593(1)	2509(3)	22(1)
C(12)	7889(2)	-226(1)	2338(3)	29(1)
C(13)	7285(2)	-635(2)	914(3)	35(1)
C(14)	6459(2)	-240(2)	-310(3)	34(1)
C(15)	6261(2)	582(2)	-130(3)	31(1)
C(16)	6878(2)	1004(1)	1277(3)	27(1)
C(21)	8771(2)	1069(2)	8042(3)	32(1)
C(22)	9794(2)	1217(2)	9536(3)	40(1)
C(51)	4599(2)	1789(1)	3815(3)	23(1)
C(52)	3907(2)	2338(2)	2705(3)	29(1)
C(53)	2752(2)	2280(2)	2339(3)	32(1)
C(54)	2246(2)	1672(2)	3055(3)	30(1)
C(55)	2920(2)	1122(1)	4150(3)	29(1)
C(56)	4086(2)	1177(1)	4532(3)	26(1)

Table 3. Bond lengths [A] and angles [deg] for A8_08m.

O(1)-C(1)	1.358(3)
O(1)-C(2)	1.456(3)
O(2)-C(1)	1.203(3)
O(3)-N(2)	1.413(2)
O(3)-C(3)	1.468(3)
N(1)-C(1)	1.364(3)
N(1)-C(11)	1.437(3)
N(1)-C(3)	1.442(3)
N(2)-C(5)	1.281(3)
C(2)-C(21)	1.512(3)
C(2)-C(3)	1.535(3)
C(3)-C(4)	1.521(3)
C(4)-C(5)	1.493(3)
C(5)-C(51)	1.461(3)
C(11)-C(16)	1.382(3)
C(11)-C(12)	1.383(3)
C(12)-C(13)	1.384(3)
C(13)-C(14)	1.385(4)
C(14)-C(15)	1.385(4)
C(15)-C(16)	1.388(3)
C(21)-C(22)	1.525(4)
C(51)-C(52)	1.397(3)
C(51)-C(56)	1.397(3)
C(52)-C(53)	1.371(3)
C(53)-C(54)	1.389(3)
C(54)-C(55)	1.383(3)
C(55)-C(56)	1.384(3)

C(1)-O(1)-C(2)	109.39(17)
N(2)-O(3)-C(3)	109.94(15)
C(1)-N(1)-C(11)	122.73(18)
C(1)-N(1)-C(3)	111.53(18)
C(11)-N(1)-C(3)	125.17(18)
C(5)-N(2)-O(3)	109.11(17)
O(2)-C(1)-O(1)	122.7(2)
O(2)-C(1)-N(1)	128.3(2)
O(1)-C(1)-N(1)	109.09(19)
O(1)-C(2)-C(21)	109.07(19)
O(1)-C(2)-C(3)	103.22(17)
C(21)-C(2)-C(3)	115.5(2)
N(1)-C(3)-O(3)	109.69(17)
N(1)-C(3)-C(4)	115.63(18)
O(3)-C(3)-C(4)	103.63(17)
N(1)-C(3)-C(2)	101.01(18)
O(3)-C(3)-C(2)	107.75(18)
C(4)-C(3)-C(2)	118.91(19)
C(5)-C(4)-C(3)	102.13(18)
N(2)-C(5)-C(51)	121.4(2)
N(2)-C(5)-C(4)	113.9(2)
C(51)-C(5)-C(4)	124.69(19)
C(16)-C(11)-C(12)	121.0(2)
C(16)-C(11)-N(1)	120.2(2)
C(12)-C(11)-N(1)	118.8(2)
C(11)-C(12)-C(13)	118.9(2)
C(12)-C(13)-C(14)	120.9(2)
C(13)-C(14)-C(15)	119.5(2)
C(14)-C(15)-C(16)	120.1(2)

C(11)-C(16)-C(15)	119.5(2)
C(2)-C(21)-C(22)	111.8(2)
C(52)-C(51)-C(56)	118.4(2)
C(52)-C(51)-C(5)	121.0(2)
C(56)-C(51)-C(5)	120.5(2)
C(53)-C(52)-C(51)	120.7(2)
C(52)-C(53)-C(54)	120.6(2)
C(55)-C(54)-C(53)	119.3(2)
C(54)-C(55)-C(56)	120.5(2)
C(55)-C(56)-C(51)	120.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for A8_08m.
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)	29(1)	39(1)	23(1)	-2(1)	8(1)	-2(1)
O(2)	29(1)	37(1)	28(1)	3(1)	14(1)	2(1)
O(3)	29(1)	22(1)	30(1)	3(1)	9(1)	-1(1)
N(1)	26(1)	26(1)	21(1)	-1(1)	8(1)	1(1)
N(2)	27(1)	22(1)	25(1)	-3(1)	8(1)	-1(1)
C(1)	29(1)	29(1)	21(1)	5(1)	9(1)	0(1)
C(2)	31(1)	31(1)	23(1)	-4(1)	9(1)	0(1)
C(3)	29(1)	22(1)	22(1)	0(1)	10(1)	0(1)
C(4)	31(1)	23(1)	22(1)	1(1)	12(1)	-1(1)
C(5)	32(1)	19(1)	17(1)	-4(1)	9(1)	-1(1)
C(11)	27(1)	24(1)	20(1)	-1(1)	12(1)	-3(1)
C(12)	34(1)	27(1)	29(1)	0(1)	14(1)	3(1)
C(13)	45(2)	27(1)	40(1)	-8(1)	21(1)	-3(1)
C(14)	38(1)	40(1)	28(1)	-13(1)	14(1)	-12(1)
C(15)	35(1)	38(1)	22(1)	-1(1)	11(1)	-2(1)
C(16)	36(1)	24(1)	23(1)	1(1)	12(1)	0(1)
C(21)	37(1)	36(1)	23(1)	-1(1)	10(1)	5(1)
C(22)	39(2)	56(2)	25(1)	0(1)	6(1)	11(1)
C(51)	30(1)	20(1)	19(1)	-4(1)	9(1)	-2(1)
C(52)	35(1)	27(1)	27(1)	3(1)	11(1)	-2(1)
C(53)	34(1)	34(1)	28(1)	5(1)	7(1)	2(1)
C(54)	27(1)	36(1)	26(1)	-3(1)	7(1)	-3(1)
C(55)	35(1)	27(1)	28(1)	-3(1)	15(1)	-6(1)
C(56)	35(1)	23(1)	21(1)	-1(1)	11(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for A8_08m.

	x	y	z	U(eq)
H(2)	8820(20)	2215(16)	7010(30)	31(7)
H(2A)	8760(20)	482(16)	7610(30)	28(7)
H(2B)	8030(20)	1166(17)	8400(30)	38(7)
H(2C)	10570(30)	1087(19)	9280(40)	54(9)
H(2D)	9850(30)	1810(20)	9880(40)	52(9)
H(2E)	9760(30)	840(20)	10510(40)	59(10)
H(4A)	6450(20)	665(16)	4810(30)	26(6)
H(4B)	6610(20)	1265(17)	6430(40)	43(8)
H(12)	8500(20)	-496(15)	3220(30)	29(7)
H(13)	7420(20)	-1205(18)	760(30)	42(8)
H(14)	6020(20)	-518(16)	-1260(30)	29(7)
H(15)	5690(20)	869(16)	-990(30)	35(7)
H(16)	6740(20)	1580(16)	1420(30)	30(7)
H(52)	4290(20)	2759(15)	2220(30)	28(7)
H(53)	2270(20)	2688(15)	1580(30)	29(7)
H(54)	1400(20)	1615(17)	2770(30)	41(8)
H(55)	2540(20)	695(16)	4620(30)	30(7)
H(56)	4550(20)	797(15)	5290(30)	27(6)

Table 6. Hydrogen bonds for A8_08m [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)