^{1}H NMR spectra of **1b** and **2b** showed the total aromatic and aliphatic proton integrations consistent with the corresponding chemical structure containing one and two DPAF addends, respectively, using 1,4-diazabicyclo[2.2.2]octane (DABCO) as the internal reference for counting the proton integration intensity.

The number of protons per molecule was estimated by the total proton integration in the ^{1}H NMR spectrum using an internal standard of 1,4-diazabicyclo[2.2.2]octane (DABCO) with a known quantity and a formula as follows.

$$\frac{I_f}{N_{pf}}\frac{M_f}{m_f} = \frac{I_d}{N_{pd}}\frac{M_d}{m_d}$$

where I_f is total proton integration of the compound, N_{pf} is the number of protons of the compound, M_f is the molecular weight of the compound, m_f is the weight of the compound sample used, I_d is total proton integration of DABCO, N_{pd} is the number of protons of DABCO, M_d is the molecular weight of DABCO, and m_d is the weight of DABCO sample used.

For the sample 1 solution containing monoadduct C_{60}(>DPAF-C_9) **1b** (24.6 mg, 0,035 M) and DABCO (2.0 mg, 0.035 M) in $CDCl_3$ (0.5 ml), the aromatic (*d* 7.0–8.5, 18.98) and aliphatic (*d* 0.5–2.5, 42.19 in parenthesis) proton integrations in ^{1}H NMR spectrum (a) gave the following results.

$$\frac{I_f}{N_{pf}}\frac{M_f}{m_f} = \frac{I_d}{N_{pd}}\frac{M_d}{m_d} \quad ? \quad \frac{18.98\ (42.19)}{N_{pf}}\frac{1345}{24.6\ \text{mg}} = \frac{13.72}{12}\frac{112}{2.0\ \text{mg}}$$

Thus, N_{pf} = 16.2 aromatic protons for **1b** (theoretical value is 16).
N_{pf} = 35.6 aliphatic protons for **1b** (theoretical value is 38).

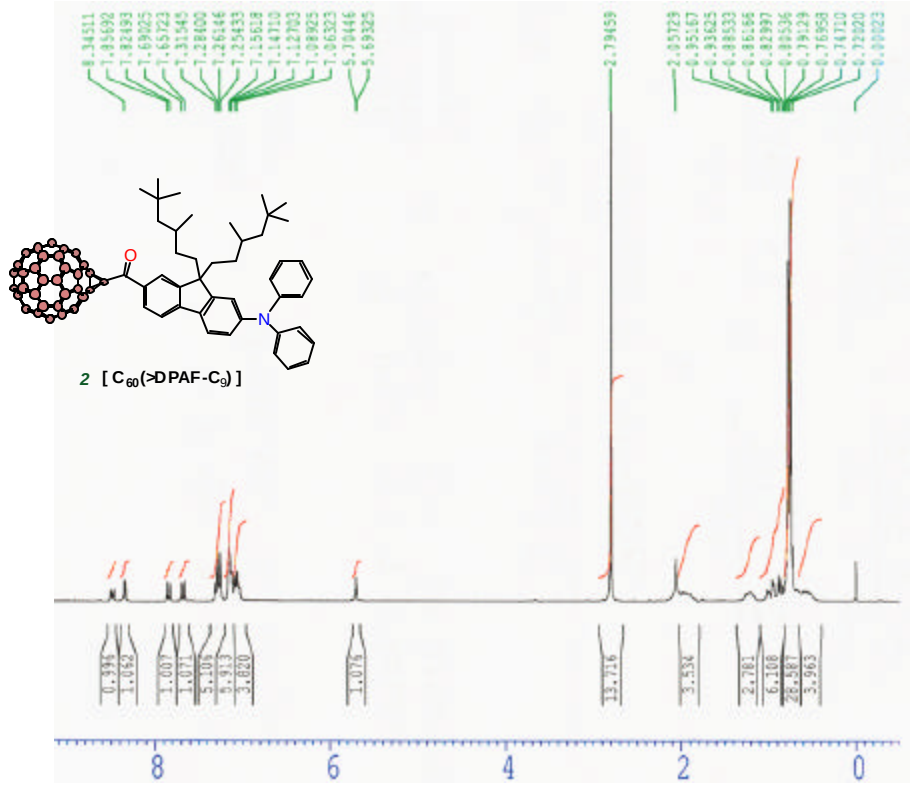
For the sample 2 solution containing bisadduct C_{60}(>DPAF-C_9)$_2$ **2b** (35.2 mg, 0.035 M) and DABCO (2.0 mg, 0.035 M) in $CDCl_3$ (0.5 ml), the aromatic (*d* 7.0–8.5, 11.67) and aliphatic (*d* 0.5–2.5, 29.13 in parenthesis) proton integrations in ^{1}H NMR spectrum (b) gave the following results.

$$\frac{I_f}{N_{pf}}\frac{M_f}{m_f} = \frac{I_d}{N_{pd}}\frac{M_d}{m_d} \quad ? \quad \frac{11.67\ (29.13)}{N_{pf}}\frac{1970}{35.2\ \text{mg}} = \frac{4.67}{12}\frac{112}{2.0\ \text{mg}}$$

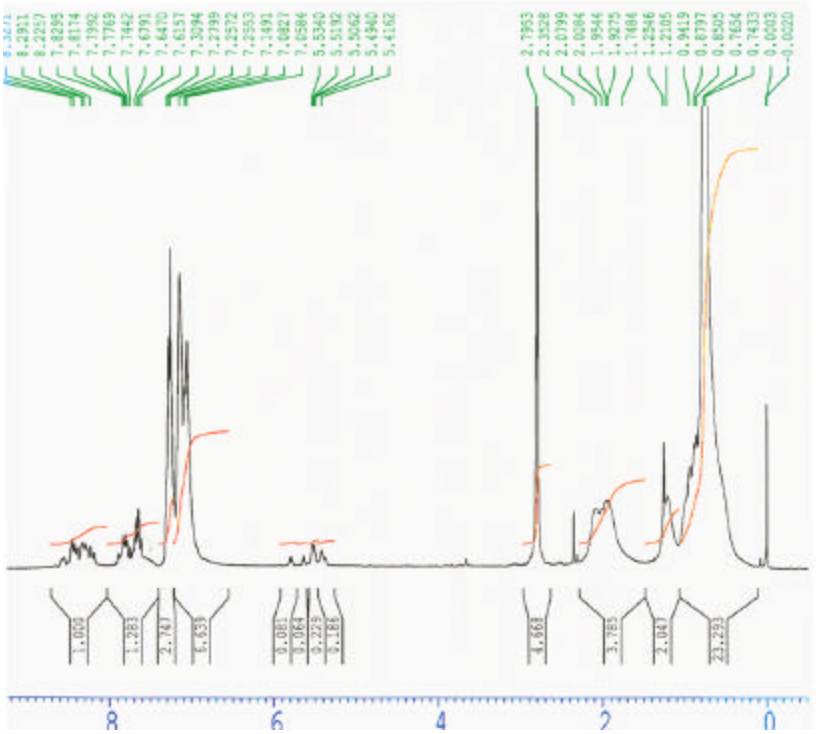
Thus, N_{pf} = 30.0 aromatic protons for **2b** (theoretical value is 32).
N_{pf} = 74.8 aliphatic protons for **2b** (theoretical value is 76).

The number of both aromatic and aliphatic protons per molecule estimated from the spectra (a) and (b) agrees well with the monoadduct and bisadduct structure of **1b** and **2b**, respectively.

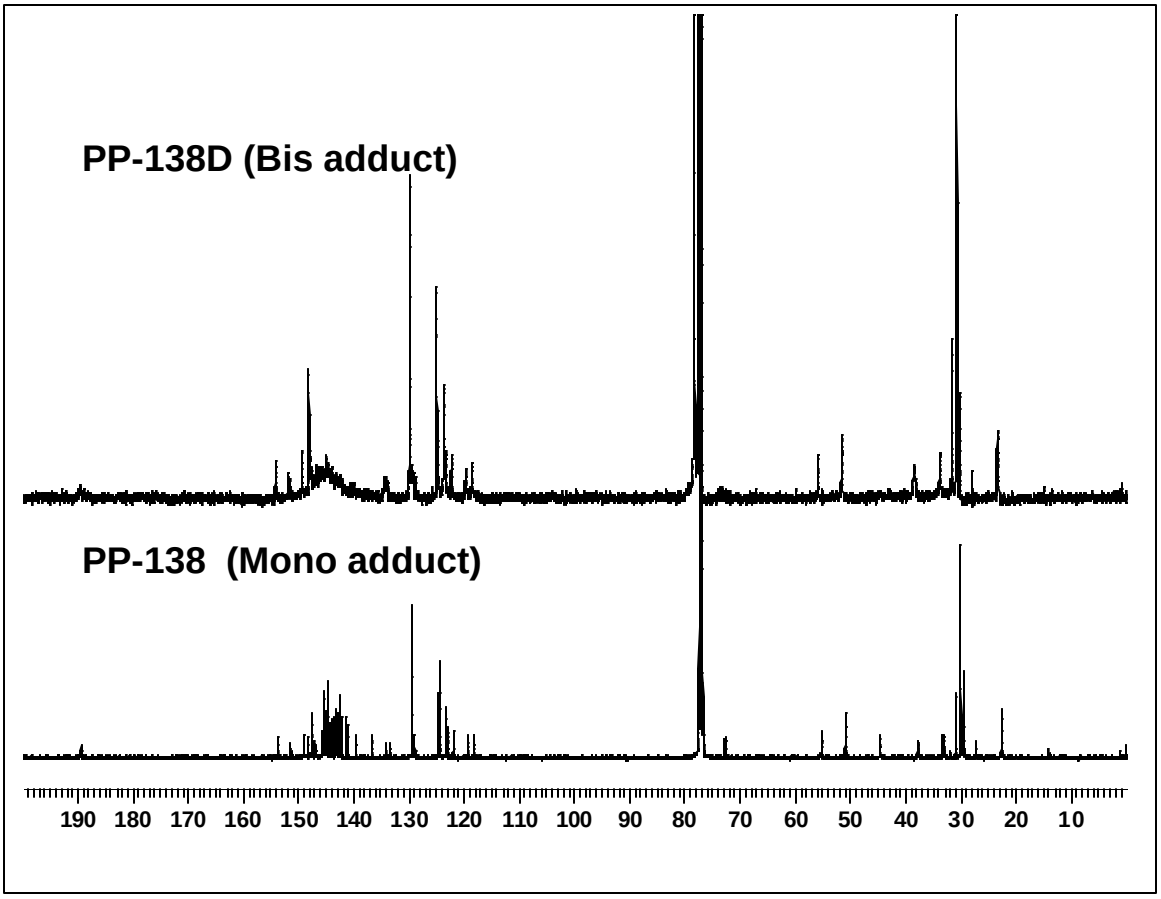
^{1}H NMR spectrum (a) of monoadduct C_{60}(>DPAF-C_9) in $CDCl_3$



^{1}H NMR spectrum (b) of bisadduct C_{60}(>DPAF-C_9)$_2$ in $CDCl_3$



^{13}C NMR spectrum of monoadduct C_{60}(>DPAF-C_9) **1b** and bisadduct C_{60}(>DPAF-C_9)$_2$ **2b**

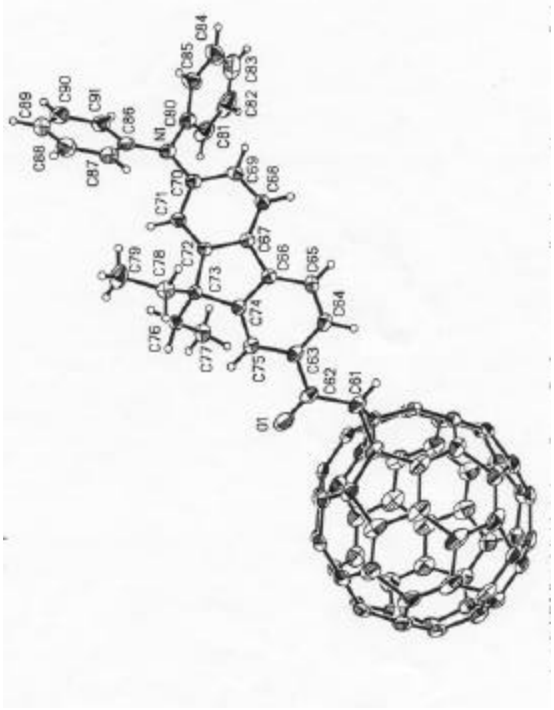


X-ray crystal structural data of 7-(1,2-dihydro-1,2-methanofullerene[60]-61-carbonyl)-9,9-diethyl-2-diphenylaminofluorene, C_{60}(>DPAF-C_2) 1a.

Table 1. Crystal data and structure refinement for IC8386.

Identification code	ic8386
Diffractometer used	Nonius KappaCCD
Empirical formula	$C_{91}H_{27}NO$
Formula weight	1150.14
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 10.00100(10) Å alpha = 90° b = 19.5790(2) Å beta = 93.0510(10)° c = 25.7150(3) Å gamma = 90°
Volume, Z	5028.11(9) $Å^3$, 4
Density (calculated)	1.519 Mg/m^3
Absorption coefficient	0.089 mm^{-1}
F(000)	2352
Crystal size	0.30 x 0.25 x 0.20 mm
θ range for data collection	1.90 to 25.00°
Limiting indices	$-12 \le h \le 12$, $-23 \le k \le 25$, $-33 \le l \le 33$
Reflections collected	31355
Independent reflections	8838 (R_{int} = 0.0396)
Absorption correction	Multi-scan
Max. and min. transmission	0.994 and 0.900
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8800 / 0 / 839
Goodness-of-fit on F^2	1.126
Final R indices [I>2σ(I)]	R1 = 0.0524, wR2 = 0.1279
R indices (all data)	R1 = 0.0786, wR2 = 0.1510
Extinction coefficient	0.0194(12)
Largest diff. peak and hole	0.448 and -0.401 $eÅ^{-3}$

Unit cell packing of 7-(1,2-dihydro-1,2-methanofullerene[60]-61-carbonyl)-9,9-diethyl-2-diphenyl-aminofluorene crystal, C_{60}(>DPAF-C_2) 1a.



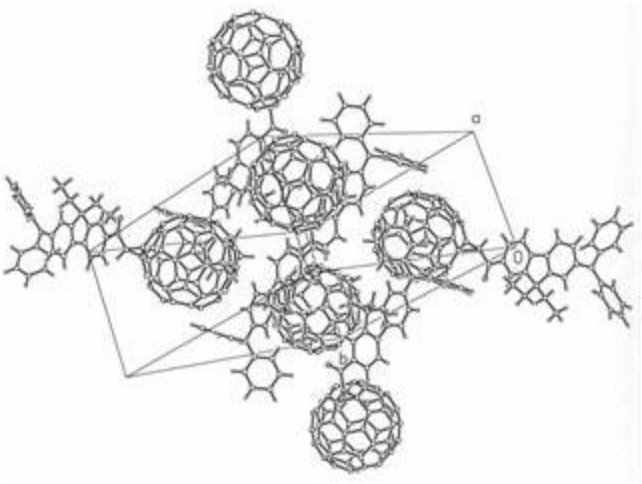


Table 1. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	-1420(2)	1441(1)	570(1)	67(1)
N(1)	-4555(2)	-3510(1)	882(1)	51(1)
C(1)	1391(2)	1877(1)	771(1)	49(1)
C(2)	1636(2)	1208(1)	1139(1)	42(1)
C(3)	3048(2)	1001(1)	1256(1)	48(1)
C(4)	4104(2)	1306(1)	1023(1)	56(1)
C(5)	3901(2)	1908(1)	692(1)	60(1)
C(6)	2650(3)	2198(1)	598(1)	58(1)
C(7)	2491(3)	2922(1)	624(1)	64(1)
C(8)	3598(3)	3352(1)	707(1)	70(1)
C(9)	4907(3)	3053(2)	791(1)	68(1)
C(10)	5062(3)	2348(2)	790(1)	69(1)
C(11)	5955(2)	2026(1)	1170(1)	69(1)
C(12)	6666(2)	2419(1)	1541(1)	70(1)
C(13)	6500(2)	3154(1)	1542(1)	63(1)
C(14)	5643(3)	3466(1)	1179(1)	66(1)
C(15)	4775(3)	4014(1)	1329(1)	64(1)
C(16)	4810(2)	4230(1)	1846(1)	59(1)
C(17)	5709(2)	3905(1)	2228(1)	55(1)
C(18)	6541(2)	3378(1)	2078(1)	58(1)
C(19)	6732(2)	2784(1)	2407(1)	62(1)
C(20)	6096(2)	2733(1)	2867(1)	65(1)
C(21)	5235(3)	3277(1)	3021(1)	62(1)
C(22)	5046(2)	3849(1)	2709(1)	57(1)
C(23)	3720(2)	4145(1)	2626(1)	62(1)
C(24)	2645(3)	3852(1)	2859(1)	71(1)
C(25)	2838(3)	3257(2)	3184(1)	72(1)
C(26)	4098(3)	2972(2)	3264(1)	70(1)
C(27)	4277(3)	2244(2)	3263(1)	75(1)
C(28)	3174(3)	1815(2)	3176(1)	76(1)
C(29)	1855(3)	2108(2)	3092(1)	72(1)
C(30)	1686(3)	2810(2)	3092(1)	76(1)
C(31)	799(3)	3129(2)	2712(1)	73(1)
C(32)	96(2)	2734(1)	2334(1)	66(1)
C(33)	265(2)	2001(1)	2333(1)	58(1)
C(34)	1117(3)	1694(1)	2704(1)	64(1)
C(35)	1986(3)	1153(1)	2553(1)	60(1)
C(36)	1954(2)	944(1)	2034(1)	47(1)
C(37)	1029(2)	1243(1)	1651(1)	41(1)
C(38)	216(2)	1772(1)	1797(1)	46(1)
C(39)	15(2)	2379(1)	1465(1)	52(1)
C(40)	627(2)	2437(1)	1001(1)	52(1)
C(41)	1258(3)	3076(1)	868(1)	64(1)
C(42)	1168(3)	3644(1)	1187(1)	68(1)
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C(54)	4436(3)	1080(1)	2612(1)	70(1)
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C(58)	5503(3)	2089(1)	3018(1)	74(1)
C(59)	3268(3)	1223(1)	2843(1)	69(1)
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C(61)	905(2)	1185(1)	616(1)	51(1)
C(62)	-564(2)	1004(1)	615(1)	48(1)
C(63)	-881(2)	274(1)	678(1)	42(1)
C(64)	112(2)	-227(1)	661(1)	47(1)
C(65)	-196(2)	-911(1)	688(1)	44(1)
C(66)	-1519(2)	-1099(1)	744(1)	38(1)
C(67)	-2133(2)	-1770(1)	774(1)	37(1)
C(68)	-1589(2)	-2413(1)	711(1)	43(1)
C(69)	-2407(2)	-2978(1)	740(1)	46(1)
C(70)	-3758(2)	-2914(1)	845(1)	43(1)
C(71)	-4288(2)	-2264(1)	922(1)	43(1)
C(72)	-3491(2)	-1692(1)	868(1)	37(1)
C(73)	-3868(2)	-935(1)	880(1)	37(1)
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C(76)	-4405(2)	-695(1)	1400(1)	40(1)
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C(79)	-6303(2)	-1008(1)	461(1)	71(1)
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C(91)	-6709(2)	-4071(1)	899(1)	58(1)

CIF file of 7-(1,2-dihydro-1,2-methanofullerene[60]-61-carbonyl)-9,9-diethyl-2-diphenyl-aminofluorene, C_{60}(>DPAF-C_2) 1a.

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C19 C 0.6732(2) 0.27841(13) 0.24067(11) 0.0624(7) Uani 1 d . .
C20 C 0.6096(2) 0.27332(13) 0.28673(11) 0.0651(7) Uani 1 d . .
C21 C 0.5235(3) 0.32766(13) 0.30208(9) 0.0625(7) Uani 1 d . .
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C22 C 0.5046(2) 0.38486(12) 0.27088(9) 0.0573(6) Uani 1 d . .
C23 C 0.3720(2) 0.41448(12) 0.26258(11) 0.0621(7) Uani 1 d . .
C24 C 0.2645(3) 0.38516(14) 0.28592(11) 0.0711(8) Uani 1 d . .
C25 C 0.2838(3) 0.3257(2) 0.31837(10) 0.0723(8) Uani 1 d . .
C26 C 0.4098(3) 0.29723(15) 0.32644(9) 0.0703(7) Uani 1 d . .
C27 C 0.4277(3) 0.2244(2) 0.32634(9) 0.0753(8) Uani 1 d . .
C28 C 0.3174(3) 0.1815(2) 0.31759(9) 0.0764(8) Uani 1 d . .
C29 C 0.1855(3) 0.2108(2) 0.30916(9) 0.0722(8) Uani 1 d . .
C30 C 0.1686(3) 0.2810(2) 0.30922(10) 0.0761(8) Uani 1 d . .
C31 C 0.0799(3) 0.3129(2) 0.27117(12) 0.0728(8) Uani 1 d . .
C32 C 0.0096(2) 0.27336(14) 0.23342(12) 0.0658(7) Uani 1 d . .
C33 C 0.0265(2) 0.20013(13) 0.23332(10) 0.0583(6) Uani 1 d . .
C34 C 0.1117(3) 0.16937(14) 0.27044(9) 0.0638(7) Uani 1 d . .
C35 C 0.1986(3) 0.11527(12) 0.25526(9) 0.0598(6) Uani 1 d . .
C36 C 0.1954(2) 0.09443(10) 0.20339(8) 0.0473(5) Uani 1 d . .
C37 C 0.1029(2) 0.12433(10) 0.16512(8) 0.0412(5) Uani 1 d . .
C38 C 0.0216(2) 0.17722(11) 0.17969(9) 0.0465(5) Uani 1 d . .
C39 C 0.0015(2) 0.23790(11) 0.14647(10) 0.0518(6) Uani 1 d . .
C40 C 0.0627(2) 0.24370(11) 0.10011(9) 0.0518(6) Uani 1 d . .
C41 C 0.1258(3) 0.30756(12) 0.08680(10) 0.0637(7) Uani 1 d . .
C42 C 0.1168(3) 0.36444(12) 0.11867(12) 0.0684(8) Uani 1 d . .
C43 C 0.0502(2) 0.35902(12) 0.16654(13) 0.0708(8) Uani 1 d . .
C44 C -0.0047(2) 0.29675(12) 0.18057(12) 0.0644(7) Uani 1 d . .
C45 C 0.3503(3) 0.39466(12) 0.10391(11) 0.0701(8) Uani 1 d . .
C46 C 0.2328(3) 0.40920(11) 0.12759(12) 0.0703(8) Uani 1 d . .
C47 C 0.2354(3) 0.43122(11) 0.18088(12) 0.0688(7) Uani 1 d . .
C48 C 0.1232(2) 0.40036(12) 0.20539(14) 0.0720(8) Uani 1 d . .
C49 C 0.1371(2) 0.37792(14) 0.25598(13) 0.0725(8) Uani 1 d . .
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C56 C 0.5374(2) 0.13821(13) 0.13219(12) 0.0654(7) Uani 1 d . .
C57 C 0.6815(2) 0.21918(14) 0.20724(13) 0.0703(8) Uani 1 d . .
C58 C 0.5503(3) 0.20887(14) 0.30185(11) 0.0736(8) Uani 1 d . .
C59 C 0.3268(3) 0.12229(13) 0.28429(10) 0.0687(8) Uani 1 d . .
C60 C 0.3187(2) 0.07974(10) 0.17911(9) 0.0500(5) Uani 1 d . .
C61 C 0.0905(2) 0.11853(11) 0.06157(8) 0.0507(5) Uani 1 d . .
H61A H 0.1396(2) 0.09672(11) 0.03408(8) 0.061 Uiso 1 calc R .
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H64A H 0.0999(2) -0.00953(11) 0.06316(8) 0.056 Uiso 1 calc R .
C65 C -0.0196(2) -0.09114(11) 0.06877(8) 0.0443(5) Uani 1 d . .

H65A H 0.0469(2) -0.12411(11) 0.06680(8) 0.053 Uiso 1 calc R .
C66 C -0.1519(2) -0.10992(9) 0.07444(7) 0.0378(4) Uani 1 d . .
C67 C -0.2133(2) -0.17699(9) 0.07738(7) 0.0372(4) Uani 1 d . .
C68 C -0.1589(2) -0.24131(10) 0.07111(8) 0.0431(5) Uani 1 d . .
H68A H -0.0686(2) -0.24637(10) 0.06505(8) 0.052 Uiso 1 calc R .
C69 C -0.2407(2) -0.29775(10) 0.07399(8) 0.0459(5) Uani 1 d . .
H69A H -0.2052(2) -0.34097(10) 0.06881(8) 0.055 Uiso 1 calc R .
C70 C -0.3758(2) -0.29142(10) 0.08452(8) 0.0429(5) Uani 1 d . .
C71 C -0.4288(2) -0.22637(10) 0.09225(8) 0.0426(5) Uani 1 d . .
H71A H -0.5173(2) -0.22148(10) 0.10099(8) 0.051 Uiso 1 calc R .
C72 C -0.3491(2) -0.16917(9) 0.08685(7) 0.0370(4) Uani 1 d . .
C73 C -0.3868(2) -0.09347(9) 0.08803(7) 0.0366(4) Uani 1 d . .
C74 C -0.2519(2) -0.06037(10) 0.07891(7) 0.0375(4) Uani 1 d . .
C75 C -0.2205(2) 0.00795(10) 0.07500(7) 0.0407(5) Uani 1 d . .
H75A H -0.2870(2) 0.04092(10) 0.07713(7) 0.049 Uiso 1 calc R .
C76 C -0.4405(2) -0.06954(10) 0.14000(7) 0.0396(4) Uani 1 d . .
H76A H -0.4693(2) -0.02243(10) 0.13612(7) 0.048 Uiso 1 calc R .
H76B H -0.5188(2) -0.09661(10) 0.14694(7) 0.048 Uiso 1 calc R .
C77 C -0.3429(2) -0.07419(12) 0.18659(8) 0.0537(6) Uani 1 d . .
H77A H -0.3851(2) -0.05825(12) 0.21698(8) 0.081 Uiso 1 calc R .
H77B H -0.2659(2) -0.04646(12) 0.18081(8) 0.081 Uiso 1 calc R .
H77C H -0.3155(2) -0.12081(12) 0.19166(8) 0.081 Uiso 1 calc R .
C78 C -0.4876(2) -0.07402(11) 0.04293(8) 0.0471(5) Uani 1 d . .
H78A H -0.4916(2) -0.02458(11) 0.04084(8) 0.057 Uiso 1 calc R .
H78B H -0.4529(2) -0.09038(11) 0.01071(8) 0.057 Uiso 1 calc R .
C79 C -0.6303(2) -0.10083(14) 0.04611(11) 0.0707(7) Uani 1 d . .
H79A H -0.6838(2) -0.08565(14) 0.01622(11) 0.106 Uiso 1 calc R .
H79B H -0.6679(2) -0.08384(14) 0.07718(11) 0.106 Uiso 1 calc R .
H79C H -0.6290(2) -0.14984(14) 0.04694(11) 0.106 Uiso 1 calc R .
C80 C -0.3831(2) -0.41393(10) 0.09553(10) 0.0541(6) Uani 1 d . .
C81 C -0.3165(3) -0.42669(14) 0.14248(12) 0.0777(8) Uani 1 d . .
H81A H -0.3271(3) -0.39780(14) 0.17067(12) 0.093 Uiso 1 calc R .
C82 C -0.2320(3) -0.4838(2) 0.1476(2) 0.1095(14) Uani 1 d . .
H82A H -0.1843(3) -0.4925(2) 0.1789(2) 0.131 Uiso 1 calc R .
C83 C -0.2205(3) -0.5267(2) 0.1057(2) 0.115(2) Uani 1 d . .
H83A H -0.1642(3) -0.5644(2) 0.1088(2) 0.138 Uiso 1 calc R .
C84 C -0.2907(3) -0.51462(14) 0.0594(2) 0.0945(11) Uani 1 d . .
H84A H -0.2831(3) -0.54454(14) 0.0316(2) 0.113 Uiso 1 calc R .
C85 C -0.3720(3) -0.45854(12) 0.05403(11) 0.0682(7) Uani 1 d . .
H85A H -0.4196(3) -0.45034(12) 0.02262(11) 0.082 Uiso 1 calc R .
C86 C -0.5925(2) -0.35462(10) 0.07132(8) 0.0461(5) Uani 1 d . .
C87 C -0.6517(2) -0.30882(11) 0.03568(9) 0.0537(6) Uani 1 d . .
H87A H -0.6005(2) -0.27401(11) 0.02224(9) 0.064 Uiso 1 calc R .
C88 C -0.7864(3) -0.31439(13) 0.01989(11) 0.0679(7) Uani 1 d . .
H88A H -0.8250(3) -0.28307(13) -0.00359(11) 0.081 Uiso 1 calc R .
C89 C -0.8627(3) -0.36633(15) 0.03904(12) 0.0747(8) Uani 1 d . .

H89A H -0.9528(3) -0.37021(15) 0.02864(12) 0.090 Uiso 1 calc R .
C90 C -0.8043(3) -0.41234(13) 0.07363(12) 0.0699(7) Uani 1 d . .
H90A H -0.8556(3) -0.44766(13) 0.08629(12) 0.084 Uiso 1 calc R .
C91 C -0.6709(2) -0.40705(11) 0.08992(10) 0.0580(6) Uani 1 d . .
H91A H -0.6333(2) -0.43865(11) 0.11342(10) 0.070 Uiso 1 calc R .

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C87 0.0609(14) 0.0476(12) 0.0529(13) -0.0031(10) 0.0065(11) -0.0032(10)
C88 0.066(2) 0.063(2) 0.073(2) -0.0083(13) -0.0024(13) 0.0071(13)
C89 0.0497(14) 0.070(2) 0.105(2) -0.020(2) 0.0052(14) -0.0004(13)
C90 0.062(2) 0.0560(15) 0.094(2) -0.0116(14) 0.0207(14) -0.0123(13)
C91 0.065(2) 0.0421(12) 0.068(2) -0.0007(11) 0.0124(12) -0.0061(11)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C1 C6 1.496(3) . ?
C1 C2 1.628(3) . ?
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C2 C3 1.484(3) . ?
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C4 C56 1.456(3) . ?

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C5 C6 1.383(4) . ?
C5 C10 1.457(3) . ?
C6 C7 1.430(4) . ?
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C7 C41 1.444(4) . ?
C8 C9 1.440(4) . ?
C8 C45 1.450(4) . ?
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