Motherwell, W. D. S. & Clegg, W. (1978). PLUTO. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

Roberts, P. & Sheldrick, G. M. (1975). XANADU. Program for crystallographic calculations. Univ. of Cambridge, England.

Sheldrick, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.

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# Structure of Dicarbonylbis-(µ-3,5dimethylpyrazolyl)-bis(4-tolyl diphenylphosphinite)diiridium(I)-Dichloromethane (1/1)

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## Abstract

In bis( $\mu$ -3,5-dimethylpyrazolyl-*N*:*N'*)-bis[carbonyl(4tolyl diphenylphosphinite-*P*)iridium(I)] dichloromethane solvate, two Ir<sup>1</sup> atoms are joined by two 3,5-dimethylpyrazolyl bridges with one carbonyl and one 4-tolyl diphenylphosphinite ligand completing the square-planar geometry about each Ir atom. The Ir···Ir distance of 3.307 (1) Å is greater than the distance of 3.22 Å found in a similar pyrazolyl-bridged iridium(I) dimer [Fox (1989). PhD dissertation, California Institute of Technology, USA].

## Comment

The title compound  $[Ir(\mu-pz^*)(CO)(Ph_2POC_6H_4CH_3)]_2$ , where pz\* is 3,5-dimethylpyrazolyl, was synthesized as a model complex for the study of electron transfer in iridium dimer/pyridinium donor-acceptor complexes (Ir<sub>2</sub>-

py<sup>+</sup>). The photophysical and electrochemical data for this compound reveal energetic and kinetic parameters  $[E_{00}(S_1) = 2.4, E_{00}(T_1) = 1.9 \text{ eV}, E_{1/2}(\text{Ir}_2/\text{Ir}_2^+) = 0.4 \text{ V}$ *versus* SSCE (sodium saturated calomel electrode),  $\tau_s =$ 125 ps,  $\tau_T = 1 \mu \text{s}$ ] used in analyzing electron-transfer rates for the series of Ir<sub>2</sub>-py<sup>+</sup> complexes. The synthesis of this compound is reported elsewhere (Farid, Chang, Winkler & Gray, 1993). Slow evaporation of a methylene chloride/acetonitrile solution produced acicular crystals.

The molecule exhibits approximate  $C_{2\nu}$  symmetry. The square-planar Ir atoms are almost identical and are coordinated to two adjacent dimethylpyrazolyl ligands with an average Ir—N distance of 2.077 [10] Å, where square brackets indicate a scatter e.s.d. A carbonyl ligand at 1.804 [9] Å and a tolyl diphenylphosphinite group with an Ir—P bond of 2.224 [0] Å complete the coordination shell about each Ir atom. The N—Ir—N angle is 84.1 [14]° and the other three angles about the Ir atom range from 91.4 [6] to 92.4 [4]°.

The bridging pyrazolyl groups retain the structure of the free ligand. The dihedral angle between the two pyrazolyl groups is  $78.8 (6)^{\circ}$ . The torsion angles Ir(1)-N(1)-N(2)-Ir(2) and Ir(1)-N(3)-N(4)-Ir(2)



 $bis(\mu-3,5-dimethylpyrazolyl-N:N')-bis[carbonyl(4-Fig. 1. An ORTEP view of the dimer with 15% probability ellipsoids. H atoms are not shown.$ 



Fig. 2. An ORTEP stereoview of the iridium complex; atoms are drawn at the 50% probability level with H atoms at one tenth scale.

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are 12.1 (4) and 4.9 (4)°, respectively. The remaining ligand geometry is as expected. Substantial overlap of the aromatic rings occurs between neighboring molecules in the crystal. The population of the dichloromethane solvate refined to near unity [0.959 (4)].

The Ir...Ir solid-state non-bonding separation of 3.307 (1) Å is similar to the M 
dots M separations in analogous bispyrazolyl-bridged Ir and Rh  $d^8-d^8$  dimers. For six iridium compounds (Nussbaum, Rettig, Storr & Trotter, 1985; Beveridge, Bushnell & Stobart, 1983; Coleman, Eadie, Stobart, Zaworotko & Atwood, 1982; Beveridge, Bushnell, Dixon, Eadie, Stobart, Atwood & Zaworotko, 1982; Fox, 1989), the average Ir...Ir separation is 3.28 [12] Å (ranging from 3.162 to 3.506 Å); and for four rhodium compounds (Beveridge, Bushnell & Stobart, 1983; Louie, Rettig, Storr & Trotter, 1984; Uson, Oro, Ciriano, Pinillos, Tiripicchio & Carmellini, 1981), the average Rh...Rh separation is 3.31 [18] Å (ranging from 3.154 to 3.568 Å).

# **Experimental**

Crystal data		C(4)	
$\Pi r_2(C_5H_7N_2)_2(C_{10}H_{17}OP)_2$ -	$D_r = 1.69 \text{ Mg m}^{-3}$	C(5)	
$(CO)_2 CH_2 Cl_2$	Mo $K\alpha$ radiation	C(6)	
$M_{\rm c} = 1300.28$	$\lambda = 0.71073$ Å	C(7)	
Monoclinia	A = 0.71075  A	C(9)	
	Cell parameters from 24	C(10)	
$P_{2_1/c}$	reflections	C(11)	
a = 18.677 (2) Å	$\theta = 15 - 16.5^{\circ}$	C(12)	
<i>b</i> = 13.817 (1) Å	$\mu = 5.391 \text{ mm}^{-1}$	C(13)	
c = 20.225 (3) Å	T = 293  K	C(14)	1
$\beta = 101.37(1)^{\circ}$	Irregular	C(15)	
$V = 5116.8 (10) Å^3$	$0.6 \times 0.6 \times 0.4 \text{ mm}$	C(10)	
7 = 3110.8 (10)  A	Orange_red	C(18)	
L = 4	olunge lea	C(19)	(
Data collection		C(20)	
Data concention		C(21)	(
Enrat-Nonius CAD-4	6662 observed reflections	C(22)	(
diffractometer	$\theta_{\rm max} = 22.5^{\circ}$	C(23)	
$\theta$ scans	$h = -20 \rightarrow 20$	C(24)	
Absorption correction:	$k = 0 \rightarrow 14$	C(26)	č
by integration from crystal	$l = -21 \rightarrow 21$	C(27)	Ċ
shape	3 standard reflections	C(28)	(
$T_{\rm min} = 0.39$ $T_{\rm max} = 0.54$	frequency: 180 min	C(29)	(
1/173 measured reflections	intensity variation, 2%	C(30)	(
14175 measured reflections	intensity variation, 2%	C(31)	(
0002 independent reflections		C(32)	
Defer and		C(33)	
Kejinement		C(35)	Č
Refinement on $F^2$	$\Delta \rho_{\rm min} = -0.64 \ {\rm e} \ {\rm \AA}^{-3}$	C(36)	Č
Final $R = 0.0316$	Extinction correction:	C(37)	C
wR = 0.0025	Becket-Coppens type 1	C(38)	C
S = 1.46	isotropic	C(39)	0
6662 reflections	Extinction coofficients	C(40)	0
590 managementants	Extinction coefficient:	C(41)	0
Joo parameters	0.092 (3)×10	C(42)	ő
H-atom parameters not re-	Atomic scattering factors	C(44)	Ő
fined	from International Tables	C(45)	0
Weighting scheme based on	for X-ray Crystallogra-	C(46)	0
measured e.s.d.'s	phy (1974, Vol. IV, Table	C(47)	0
$(\Delta/\sigma)_{\rm max} = 0.04$	2.2 <i>B</i> )	C(48) C(49)	0
$\Delta \rho_{\rm max} = 0.78 \ {\rm e} \ {\rm \AA}^{-3}$		C(50)	0

Data collection: CAD-4 software (Schagen, Straver, van Meurs & Williams, 1989). Cell refinement: CAD-4 software. Data reduction: CRYM (Duchamp, 1964). Program(s) used to solve structure: CRYM. Program(s) used to refine structure: CRYM. Molecular graphics: ORTEPII (Johnson, 1976). Software used to prepare material for publication: CRYM.

# Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å<sup>2</sup>)

$$U_{\rm eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_i^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	/ea
	370 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	384 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	438 (̀3)
N(1) $0.2567$ (2) $0.1699$ (3) $0.7636$ (2) $0.00$ N(2) $0.2361$ (2) $0.2607$ (3) $0.7798$ (2) $0.00$ N(3) $0.1438$ (2) $0.1024$ (3) $0.8281$ (2) $0.00$ N(4) $0.1346$ (2) $0.1941$ (3) $0.8505$ (2) $0.00$ O(1) $0.4071$ (2) $0.0045$ (3) $0.8293$ (2) $0.007$ O(2) $0.1913$ (3) $0.3201$ (3) $1.0135$ (2) $0.007$ O(3) $0.2176$ (2) $-0.1645$ (3) $0.8786$ (2) $0.007$ O(4) $0.3235$ (2) $0.4862$ (2) $0.9104$ (2) $0.007$ O(4) $0.3235$ (2) $0.4862$ (2) $0.9104$ (2) $0.077$ O(2) $0.2050$ (3) $0.3056$ (4) $0.9610$ (3) $0.077$ C(1) $0.23934$ (4) $0.0880$ (5) $0.6668$ (3) $0.067$ O(7) $0.2126$ (4) $0.4232$ (4) $0.7771$ (3) $0.2631$ (3) $0.077$ C(10) $0.02811$ (3) $0.02442$ (5) $0.8731$ (4) $0.056$	<b>1</b> 44 (3)
N(2)         0.2361 (2)         0.2607 (3)         0.778 (2)         0.0           N(3)         0.1458 (2)         0.1024 (3)         0.8281 (2)         0.0           N(4)         0.1346 (2)         0.1941 (3)         0.8505 (2)         0.0           O(1)         0.4071 (2)         0.0045 (3)         0.8293 (2)         0.07           O(2)         0.1901 (3)         0.3201 (3)         1.0135 (2)         0.06           O(3)         0.2176 (2)         -0.1645 (3)         0.8786 (2)         0.07           O(4)         0.3325 (2)         0.4862 (2)         0.9104 (2)         0.07           C(1)         0.3465 (3)         0.0257 (4)         0.8308 (3)         0.05           C(3)         0.2703 (3)         0.1753 (4)         0.7005 (3)         0.05           C(4)         0.2360 (3)         0.3206 (4)         0.7278 (3)         0.05           C(5)         0.2577 (3)         0.2681 (4)         0.6771 (3)         0.05           C(6)         0.931 (3)         0.0244 (5)         0.8421 (3)         0.05           C(10)         0.0281 (3)         0.1204 (5)         0.821 (3)         0.05           C(10)         0.0281 (3)         0.0244 (5)         0.8487 (4)         0.055 <td>41 m</td>	41 m
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	+3 (1)
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	/8 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	33 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<b>98 (1)</b>
$\begin{array}{ccccccc} C(1) & 0.3465 (3) & 0.0257 (4) & 0.8308 (3) & 0.0257 (2) & 0.2050 (3) & 0.3056 (4) & 0.9610 (3) & 0.0257 (4) & 0.2050 (3) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.2257 (3) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.2257 (3) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.2257 (4) & 0.2257 (4) & 0.0257 (4) & 0.7278 (3) & 0.0257 (4) & 0.2257 (4) & 0.0257 (4) & 0.0257 (4) & 0.0257 (3) & 0.0257 (4) & 0.0257 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0253 (3) & 0.0257 (4) & 0.0753 (4) & 0.0557 (4) & 0.0755 (4) & 0.0757 (4) & 0.7834 (4) & 0.0257 (1) & 0.02561 (3) & -0.2126 (4) & 0.8231 (3) & 0.0557 (1) & 0.1987 (3) & -0.2164 (4) & 0.7831 (3) & 0.0557 (1) & 0.1987 (3) & -0.2164 (4) & 0.7831 (3) & 0.0557 (15) & 0.1987 (3) & -0.2108 (4) & 0.8100 (3) & 0.0256 (5) & 0.75550 (4) & 0.0755 (21) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.0257 (21) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.0557 (21) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.0557 (21) & 0.3057 (4) & -0.3556 (5) & 0.6525 (4) & 0.0957 (22) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.0557 (21) & 0.3087 (4) & 0.5387 (6) & 0.9652 (5) & 0.1005 (22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.088 (223) & 0.0387 (4) & 0.3587 (6) & 0.9652 (5) & 0.1005 (22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.088 (23) & 0.3350 (4) & 0.9793 (3) & 0.044 (228) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.066 (23) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.066 (23) & 0.3703 (3) & -0.2928 (6) & 1.0445 (4) & 0.088 (231) & 0.3350 (4) & 0.9793 (3) & 0.044 (234) & 0.4355 (3) & 0.3381 (5) & 0.9947 (3) & 0.066 (233) & 0.3718 (3) & 0.2584 (4) & 0.8237 (3) & 0.0525 (4) & 0.9904 (3) & 0.066 (233) & 0.3718 (3) & 0.2792 (5) & 0.7773 (4) & 0.8405 (2) & 0.0771 (3) & 0.088 (4) & -0.1290 (7) & 1.04666 (4) & 0.088 (731) & 0.4355 (4) & 0.4355 (5) & 0.7573 (4) & 0.0808 (741) & 0.455$	56 (1)
$\begin{array}{ccccccc} C(2) & 0.2050 (3) & 0.3056 (4) & 0.9610 (3) & 0.02 \\ C(3) & 0.2700 (3) & 0.1753 (4) & 0.7005 (3) & 0.03 \\ C(4) & 0.2360 (3) & 0.3200 (4) & 0.7278 (3) & 0.05 \\ C(5) & 0.2577 (3) & 0.2681 (4) & 0.6771 (3) & 0.05 \\ C(6) & 0.2934 (4) & 0.0880 (5) & 0.6668 (3) & 0.06 \\ C(7) & 0.2126 (4) & 0.4232 (4) & 0.7305 (3) & 0.07 \\ C(8) & 0.0811 (3) & 0.0579 (4) & 0.8120 (3) & 0.05 \\ C(9) & 0.0631 (3) & 0.2048 (5) & 0.8470 (3) & 0.05 \\ C(10) & 0.0281 (3) & 0.1204 (5) & 0.8231 (3) & 0.07 \\ C(11) & 0.0745 (4) & -0.0424 (5) & 0.8873 (4) & 0.08 \\ C(12) & 0.0318 (4) & 0.2971 (5) & 0.8673 (4) & 0.05 \\ C(13) & 0.2366 (3) & -0.2126 (4) & 0.8231 (3) & 0.05 \\ C(14) & 0.1824 (3) & -0.2647 (4) & 0.7831 (3) & 0.05 \\ C(15) & 0.1987 (3) & -0.3147 (4) & 0.7288 (3) & 0.06 \\ C(16) & 0.2668 (3) & -0.3135 (4) & 0.7135 (3) & 0.06 \\ C(17) & 0.3199 (3) & -0.2608 (5) & 0.7550 (4) & 0.07 \\ C(18) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.06 \\ C(20) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.05 \\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06 \\ C(22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.08 \\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.99 \\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(25) & 0.2078 (4) & 0.5487 (6) & 0.9650 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1299 (7) & 1.0666 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9753 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0474 (6) & 0.16 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9773 (3) & 0.06 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(44) & 0.4535 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(35) & 0.3689 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(44) & 0.4555 (4) & 0.4555 (4) & 0.8117 (3) & 0.06 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.06 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.06 \\ C(44) & 0.4082 (3) & -0.0055 (6) & 1.0341 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5$	55 (2)
$\begin{array}{cccccc} C(3) & 0.2700 (3) & 0.1753 (4) & 0.7005 (3) & 0.02 \\ C(4) & 0.2360 (3) & 0.3200 (4) & 0.7728 (3) & 0.05 \\ C(5) & 0.2577 (3) & 0.2681 (4) & 0.6771 (3) & 0.05 \\ C(6) & 0.2934 (4) & 0.0880 (5) & 0.6668 (3) & 0.06 \\ C(7) & 0.2126 (4) & 0.4232 (4) & 0.7305 (3) & 0.07 \\ C(8) & 0.0811 (3) & 0.0579 (4) & 0.8120 (3) & 0.05 \\ C(9) & 0.0631 (3) & 0.2048 (5) & 0.8470 (3) & 0.05 \\ C(10) & 0.0281 (3) & 0.1204 (5) & 0.8470 (3) & 0.05 \\ C(11) & 0.0745 (4) & -0.0424 (5) & 0.7848 (4) & 0.08 \\ C(12) & 0.0318 (4) & 0.2971 (5) & 0.8673 (4) & 0.09 \\ C(13) & 0.2366 (3) & -0.2126 (4) & 0.8231 (3) & 0.05 \\ C(14) & 0.1824 (3) & -0.2647 (4) & 0.7831 (3) & 0.05 \\ C(15) & 0.1987 (3) & -0.3147 (4) & 0.7288 (3) & 0.06 \\ C(16) & 0.2668 (3) & -0.3135 (4) & 0.7135 (3) & 0.06 \\ C(17) & 0.3199 (3) & -0.2608 (5) & 0.7550 (4) & 0.07 \\ C(18) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.06 \\ C(19) & 0.2830 (4) & -0.3656 (5) & 0.6525 (4) & 0.09 \\ C(20) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.05 \\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06 \\ C(22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.08 \\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09 \\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(25) & 0.2078 (4) & 0.5454 (6) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1795 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1299 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.3455 (4) & -0.0111 (5) & 0.9947 (3) & 0.04 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9773 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(33) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.66 \\ C(44) & 0.4623 (3) & 0.3707 (4) & 0.8405 (2) & 0.047 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.055 \\ C(41) & 0.4625 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.077 \\ C(43) & 0.4531 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(44) & 0.0882 (3) & -0.0$	58 (2)
$\begin{array}{cccccc} C(4) & 0.2360 (3) & 0.3200 (4) & 0.7278 (3) & 0.02\\ C(5) & 0.2577 (3) & 0.2681 (4) & 0.6771 (3) & 0.02\\ C(6) & 0.2934 (4) & 0.0880 (5) & 0.6668 (3) & 0.08\\ C(7) & 0.2126 (4) & 0.4232 (4) & 0.7305 (3) & 0.05\\ C(9) & 0.0631 (3) & 0.2048 (5) & 0.8470 (3) & 0.02\\ C(10) & 0.0281 (3) & 0.1204 (5) & 0.8231 (3) & 0.07\\ C(11) & 0.0745 (4) & -0.0424 (5) & 0.7848 (4) & 0.08\\ C(12) & 0.0318 (4) & 0.2971 (5) & 0.8673 (4) & 0.09\\ C(13) & 0.2366 (3) & -0.2126 (4) & 0.8231 (3) & 0.05\\ C(14) & 0.1824 (3) & -0.2647 (4) & 0.7831 (3) & 0.05\\ C(15) & 0.1987 (3) & -0.3147 (4) & 0.7288 (3) & 0.06\\ C(16) & 0.2668 (3) & -0.3135 (4) & 0.7135 (3) & 0.06\\ C(17) & 0.3199 (3) & -0.2608 (5) & 0.7550 (4) & 0.07\\ C(18) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.06\\ C(20) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.05\\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06\\ C(22) & 0.2673 (5) & 0.6532 (4) & 0.07\\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09\\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & 0.5487 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & 0.5487 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & 0.5487 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & -0.1951 (5) & 1.0400 (4) & 0.08\\ C(30) & 0.4508 (4) & -0.1792 (4) & 0.9904 (3) & 0.06\\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08\\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9773 (3) & 0.04\\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.3506 (4) & 0.9791 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.3506 (4) & 0.9771 (3) & 0.08\\ C(31) & 0.4435 (4) & -0.0292 (6) & 1.0445 (4) & 0.08\\ C(33) & 0.3914 (3) & 0.3506 (4) & 0.9791 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.3506 (5) & 0.7520 (3) & 0.077\\ C(43) & 0.4531 (4) & 0.4555 (4) & 0.8117 (3) & 0.06\\ C(44) & 0.4082 (3) & 0.2792 (5) & 0.7793 (3) & 0.04\\ C(44) & 0.4055 (4) & 0.4355 (4) & 0.9906 (3) & 0.045\\ C(44) & 0.4082 (3) & 0.0707 (4) & 0.8405 (2) & 0.7673 (4) & 0.08\\ C(44) & 0.4082 (3) & -0.0385 (4) & 0.900 (3) & 0.04\\ C(44) & 0.4082 (3) & -0.00355 (4) & 0.9900 (3) & 0.04\\ C(44) & 0$	53 (2)
$\begin{array}{cccccc} C(5) & 0.2577 (3) & 0.2681 (4) & 0.6771 (3) & 0.05 \\ C(6) & 0.2934 (4) & 0.0880 (5) & 0.6668 (3) & 0.06 \\ C(7) & 0.2126 (4) & 0.4232 (4) & 0.7305 (3) & 0.07 \\ C(8) & 0.0811 (3) & 0.0579 (4) & 0.8120 (3) & 0.05 \\ C(9) & 0.0631 (3) & 0.2048 (5) & 0.8470 (3) & 0.05 \\ C(10) & 0.0281 (3) & 0.1204 (5) & 0.8231 (3) & 0.07 \\ C(11) & 0.0745 (4) & -0.0424 (5) & 0.7848 (4) & 0.08 \\ C(12) & 0.0318 (4) & 0.2971 (5) & 0.8673 (4) & 0.09 \\ C(13) & 0.2366 (3) & -0.2126 (4) & 0.8231 (3) & 0.05 \\ C(14) & 0.1824 (3) & -0.2647 (4) & 0.7831 (3) & 0.05 \\ C(15) & 0.1987 (3) & -0.3147 (4) & 0.7288 (3) & 0.06 \\ C(16) & 0.2668 (3) & -0.2108 (4) & 0.8100 (3) & 0.06 \\ C(17) & 0.3199 (3) & -0.2608 (5) & 0.7550 (4) & 0.07 \\ C(18) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.06 \\ C(21) & 0.2830 (4) & -0.3656 (5) & 0.6525 (4) & 0.09 \\ C(20) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.05 \\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06 \\ C(22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.08 \\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09 \\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(25) & 0.2078 (4) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.970 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(23) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(34) & 0.4586 (3) & 0.33813 (5) & 0.9961 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(43) & 0.4586 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(44) & 0.4586 (3) & 0.3707 (4) & 0.8405 (2) & 0.044 \\ C(44) & 0.4653 (4) & 0.2792 (5) & 0.7798 (3) & 0.066 \\ C(33) & 0.3914 (3) & 0.2521 (4) & 0.8237 (3) & 0.056 \\ C(43) & 0.1804 (3) & -0.0385 (4) & 0.9909 (3) & 0.066 \\ C(44) & 0.4653 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(44) & 0.4653 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0$	52 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	57 (2)
$\begin{array}{ccccccc} C(7) & 0.2126 (4) & 0.4232 (4) & 0.7305 (3) & 0.07\\ C(8) & 0.0811 (3) & 0.0579 (4) & 0.8120 (3) & 0.05\\ C(9) & 0.0631 (3) & 0.2048 (5) & 0.8470 (3) & 0.05\\ C(10) & 0.0281 (3) & 0.1204 (5) & 0.8231 (3) & 0.07\\ C(11) & 0.0745 (4) & -0.0424 (5) & 0.7848 (4) & 0.08\\ C(12) & 0.0318 (4) & 0.2971 (5) & 0.8673 (4) & 0.05\\ C(13) & 0.2366 (3) & -0.2126 (4) & 0.8231 (3) & 0.05\\ C(14) & 0.1824 (3) & -0.2647 (4) & 0.7831 (3) & 0.05\\ C(15) & 0.1987 (3) & -0.3147 (4) & 0.7288 (3) & 0.06\\ C(16) & 0.2668 (3) & -0.3135 (4) & 0.7135 (3) & 0.06\\ C(16) & 0.2668 (3) & -0.3135 (4) & 0.7135 (3) & 0.06\\ C(17) & 0.3199 (3) & -0.2608 (5) & 0.7550 (4) & 0.07\\ C(18) & 0.3057 (3) & -0.2108 (4) & 0.8100 (3) & 0.06\\ C(19) & 0.2830 (4) & -0.3656 (5) & 0.6525 (4) & 0.09\\ C(20) & 0.2791 (3) & 0.5284 (4) & 0.9511 (3) & 0.05\\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06\\ C(22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.08\\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09\\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & 0.5465 (5) & 0.9249 (4) & 0.88\\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16\\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04\\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06\\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08\\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08\\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08\\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04\\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.2828 (4) & 0.8237 (3) & 0.04\\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06\\ C(34) & 0.4586 (3) & 0.3707 (4) & 0.8405 (2) & 0.04\\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.05\\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.06\\ C(33) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06\\ C(43) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.06\\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.06\\ C(43) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.06\\ C(44) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.06\\ C(48) $	38 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5 (2)
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(2)
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2 (2)
$\begin{array}{cccccc} C(20) & 0.2791 (3) & 0.2284 (4) & 0.9911 (3) & 0.05 \\ C(21) & 0.3087 (4) & 0.5538 (4) & 1.0151 (3) & 0.06 \\ C(22) & 0.2653 (5) & 0.5975 (5) & 1.0548 (4) & 0.08 \\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09 \\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(25) & 0.2078 (4) & 0.5465 (5) & 0.9249 (4) & 0.08 \\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0440 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.06 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.083 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(47) & 0.1326 (3) & -0.0005 (6) & 1.0491 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & $	0(2)
$\begin{array}{ccccccc} C(21) & 0.3087(4) & 0.3338(4) & 1.0151(3) & 0.06\\ C(22) & 0.2653(5) & 0.5975(5) & 1.0548(4) & 0.08\\ C(23) & 0.1932(5) & 0.6133(5) & 1.0303(5) & 0.09\\ C(24) & 0.1649(5) & 0.5887(6) & 0.9652(5) & 0.10\\ C(25) & 0.2078(4) & 0.5465(5) & 0.9249(4) & 0.08\\ C(26) & 0.1439(6) & 0.6554(6) & 1.0748(6) & 0.16\\ C(27) & 0.3285(3) & -0.0854(4) & 0.9670(3) & 0.04\\ C(28) & 0.3455(4) & -0.1792(4) & 0.9904(3) & 0.06\\ C(29) & 0.4075(4) & -0.1951(5) & 1.0400(4) & 0.08\\ C(30) & 0.4508(4) & -0.1209(7) & 1.0666(4) & 0.08\\ C(31) & 0.4345(4) & -0.0292(6) & 1.0445(4) & 0.08\\ C(32) & 0.3739(3) & -0.0111(5) & 0.9947(3) & 0.06\\ C(33) & 0.3914(3) & 0.3350(4) & 0.9793(3) & 0.04\\ C(34) & 0.4586(3) & 0.3813(5) & 0.9961(3) & 0.06\\ C(35) & 0.5068(3) & 0.3585(5) & 1.0544(3) & 0.07\\ C(36) & 0.4890(4) & 0.2900(6) & 1.0971(3) & 0.08\\ C(37) & 0.4232(4) & 0.2420(6) & 1.0807(3) & 0.08\\ C(38) & 0.3758(3) & 0.2641(4) & 1.0213(3) & 0.06\\ C(39) & 0.3859(3) & 0.3707(4) & 0.8405(2) & 0.044\\ C(40) & 0.4139(3) & 0.2828(4) & 0.8237(3) & 0.055\\ C(41) & 0.4623(3) & 0.2792(5) & 0.7798(3) & 0.056\\ C(42) & 0.4817(4) & 0.3639(6) & 0.7520(3) & 0.077\\ C(43) & 0.4531(4) & 0.4502(5) & 0.7673(4) & 0.08\\ C(44) & 0.4055(4) & 0.4555(4) & 0.8117(3) & 0.06\\ C(45) & 0.1804(3) & -0.0385(4) & 0.9690(3) & 0.044\\ C(46) & 0.1787(3) & 0.052(4) & 0.9690(3) & 0.06\\ C(47) & 0.1326(3) & 0.0710(5) & 1.0341(3) & 0.06\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(49) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(41) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(42) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(43) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.066\\ C(47) & 0.1326(3) & 0.0710(5) & 1.0341(3) & 0.066\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(48) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(49) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.077\\ C(49) & 0.0882(3) & -0.0005(6) & 1.0491(3) & 0.07$	2(2)
$\begin{array}{ccccccc} C(22) & 0.2053 (5) & 0.5975 (5) & 1.0548 (4) & 0.08 \\ C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09 \\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10 \\ C(25) & 0.2078 (4) & 0.5465 (5) & 0.9249 (4) & 0.08 \\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(33) & 0.3719 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.05 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.06 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.07 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.86 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.06 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9900 (3) & 0.06 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.06 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(49) & 0.081 (2) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(41) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(42) & 0.081 (2) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(43) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(44) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07 \\ C(48) & 0.0882 (3)$	6(2)
$\begin{array}{cccccc} C(23) & 0.1932 (5) & 0.6133 (5) & 1.0303 (5) & 0.09\\ C(24) & 0.1649 (5) & 0.5887 (6) & 0.9652 (5) & 0.10\\ C(25) & 0.2078 (4) & 0.5465 (5) & 0.9249 (4) & 0.08\\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16\\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04\\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06\\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08\\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08\\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08\\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04\\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06\\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07\\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08\\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08\\ C(38) & 0.3788 (3) & 0.2641 (4) & 1.0213 (3) & 0.06\\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04\\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.054\\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.065\\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079\\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.088\\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066\\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044\\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066\\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) &$	6(2)
$\begin{array}{ccccc} C(24) & 0.1649 (s) & 0.3887 (6) & 0.9652 (s) & 0.10 \\ C(25) & 0.2078 (4) & 0.5465 (s) & 0.9249 (4) & 0.08 \\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.04400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.33813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.06 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.077 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.082 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & $	0(3)
$\begin{array}{ccccccc} C(25) & 0.2078 (4) & 0.3465 (5) & 0.9249 (4) & 0.08 \\ C(26) & 0.1439 (6) & 0.6554 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.055 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.055 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.077 \\ C(43) & 0.4531 (4) & 0.4552 (4) & 0.8117 (3) & 0.066 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0522 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & $	8 (3)
$\begin{array}{cccccc} C(20) & 0.1439 (6) & 0.0534 (6) & 1.0748 (6) & 0.16 \\ C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04 \\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.044 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.054 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.064 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.072 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.082 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(40) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) $	8 (2)
$\begin{array}{ccccccc} C(27) & 0.3285 (3) & -0.0854 (4) & 0.9670 (3) & 0.04\\ C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.06\\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08\\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08\\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08\\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06\\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04\\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06\\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07\\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08\\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08\\ C(38) & 0.3758 (3) & 0.26241 (4) & 1.0213 (3) & 0.06\\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.047\\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.055\\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7673 (4) & 0.083\\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079\\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.083\\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066\\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -$	2 (4)
$\begin{array}{ccccc} C(28) & 0.3455 (4) & -0.1792 (4) & 0.9904 (3) & 0.066 \\ C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.054 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.066 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.088 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.064 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) $	9(1)
$\begin{array}{ccccccc} C(29) & 0.4075 (4) & -0.1951 (5) & 1.0400 (4) & 0.08 \\ C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.044 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0971 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.044 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.056 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.066 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.083 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0811 (2) & 0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0881 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0882 (3) & -0.0005 (6) & 1.0491$	5 (2)
$\begin{array}{cccccc} C(30) & 0.4508 (4) & -0.1209 (7) & 1.0666 (4) & 0.08 \\ C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3583 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.044 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.056 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.066 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.077 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.082 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.070 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.070 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.070 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.0005 (6) & 1.0491 (3) & 0.071 \\ C(49) & 0.0891 (2) & -0.071 \\ C(49) & 0.0891 (2) & -0.071 \\ C(49) & 0.0891 (2) & -0.071 \\ C(49) & 0$	3 (2)
$\begin{array}{ccccc} C(31) & 0.4345 (4) & -0.0292 (6) & 1.0445 (4) & 0.08 \\ C(32) & 0.3739 (3) & -0.0111 (5) & 0.9947 (3) & 0.06 \\ C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04 \\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.05 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.069 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.07 \\ C(43) & 0.4531 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0811 (2) & 0.0905 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 0.0912 (3) & 0.074 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 0.0912 (3)$	8 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3 (2)
$\begin{array}{cccccc} C(33) & 0.3914 (3) & 0.3350 (4) & 0.9793 (3) & 0.04\\ C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06\\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07\\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08\\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08\\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08\\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06\\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04\\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.056\\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.06\\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.07\\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.08\\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066\\ C(42) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044\\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066\\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07\\ C(49) & 0.0891 (2) & 0.0805 (6) & 0.2916 (6) & 0.0716 (6) \\ 0.0781 (2) & 0.0805 (6) & 0.0411 (2) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.076\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6) & 0.0491 (3) & 0.071\\ C(48) & 0.0882 (3) & -0.0005 (6$	5 (2)
$\begin{array}{ccccc} C(34) & 0.4586 (3) & 0.3813 (5) & 0.9961 (3) & 0.06 \\ C(35) & 0.5068 (3) & 0.3585 (5) & 1.0544 (3) & 0.07 \\ C(36) & 0.4890 (4) & 0.2900 (6) & 1.0971 (3) & 0.08 \\ C(37) & 0.4232 (4) & 0.2420 (6) & 1.0807 (3) & 0.08 \\ C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06 \\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.044 \\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.056 \\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.066 \\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.079 \\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.082 \\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066 \\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044 \\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066 \\ C(47) & 0.1326 (3) & -0.0005 (6) & 1.0341 (3) & 0.066 \\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0821 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0821 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 1.0491 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 0.0912 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.0005 (6) & 0.0912 (3) & 0.077 \\ C(49) & 0.0812 (3) & -0.072 (3) & 0.071 \\ C(49) & 0.0812 (3) & -0.072 (3) & 0.071 \\ C(49) & $	7 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 (2)
$\begin{array}{ccccccc} C(38) & 0.3758 (3) & 0.2641 (4) & 1.0213 (3) & 0.06\\ C(39) & 0.3859 (3) & 0.3707 (4) & 0.8405 (2) & 0.04'\\ C(40) & 0.4139 (3) & 0.2828 (4) & 0.8237 (3) & 0.056\\ C(41) & 0.4623 (3) & 0.2792 (5) & 0.7798 (3) & 0.066\\ C(42) & 0.4817 (4) & 0.3639 (6) & 0.7520 (3) & 0.07'\\ C(43) & 0.4531 (4) & 0.4502 (5) & 0.7673 (4) & 0.082\\ C(44) & 0.4055 (4) & 0.4555 (4) & 0.8117 (3) & 0.066\\ C(45) & 0.1804 (3) & -0.0385 (4) & 0.9609 (3) & 0.044\\ C(46) & 0.1787 (3) & 0.0525 (4) & 0.9900 (3) & 0.066\\ C(47) & 0.1326 (3) & 0.0710 (5) & 1.0341 (3) & 0.066\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07'\\ C(48) & 0.0882 (3) & -0.0005 (6) & 1.0491 (3) & 0.07'\\ C(49) & 0.0801 (2) & 0.0900 (6) & 1.0210 (4) & 0.07'\\ \end{array}$	5 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	7 (1)
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ə (2)
C(44)         0.4055 (4)         0.4555 (4)         0.8117 (3)         0.066           C(45)         0.1804 (3)         -0.0385 (4)         0.9609 (3)         0.044           C(46)         0.1787 (3)         0.0525 (4)         0.9900 (3)         0.066           C(47)         0.1326 (3)         0.0710 (5)         1.0341 (3)         0.066           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.070           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.070	3 (2)
C(45)         0.1804 (3)         -0.0385 (4)         0.9609 (3)         0.044           C(46)         0.1787 (3)         0.0525 (4)         0.9900 (3)         0.066           C(47)         0.1326 (3)         0.0710 (5)         1.0341 (3)         0.066           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.076           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.077	ຈັດວິ
C(46)         0.1787 (3)         0.0525 (4)         0.9900 (3)         0.066           C(47)         0.1326 (3)         0.0710 (5)         1.0341 (3)         0.066           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.070           C(48)         0.0882 (3)         -0.0005 (6)         1.0491 (3)         0.070	ŧŵ
C(47) 0.1326 (3) 0.0710 (5) 1.0341 (3) 0.066 C(48) 0.0882 (3) -0.0005 (6) 1.0491 (3) 0.070 C(49) 0.0891 (3) 0.07005 (6) 1.0491 (3) 0.070	າຂັ້
C(48) 0.0882 (3) -0.0005 (6) 1.0491 (3) 0.07( C(49) 0.0891 (3) 0.0805 (6) 1.0491 (3) 0.07(	5 (2)
C(49) 0.0901 (2) 0.0900 (5) 1.0210 (4) 0.077	$\dot{(2)}$
C(43) $0.0031(3)$ $-0.0090(3)$ $1.0210(4)$ $0.012$	\$ (2)
C(50) 0.1348 (3) -0.1096 (4) 0.9770 (3) 0.061	(2)

Cl(1)	0.0210 (2)	0.2650	(2)	0.6341 (2)	0.167 (1)
Cl(2)	0.0491 (2)	0.0716	(3)	0.6059 (2)	0.226 (2)
CGI	0.0790 (5)	0.1722	(7)	0.6512 (5)	0.132 (4)
0(01)	0.011 0 (0)		<b>、</b>		
	Table 2. Ge	eometric	: param	eters (Å, °)	
Ir(1)Ir(	) <u> </u>	307 (1)	N(3)—N	J(4)	1.376 (6)
$I_{r}(1) = I(2)$	1) 21	075 (4)	N(3)-C	2(8)	1.337 (7)
Ir(1) = N(1)	$\frac{1}{3}$ 2.0	091 (4)	N(4)C	(9)	1.332 (7)
$I_{r}(2) = N(2)$	2) 2(	068 (4)	0(1)-0	C(1)	1.174 (7)
Ir(2) = N(4)	4) 2.0	073 (4)	0(2)0	C(2)	1.165 (7)
Ir(1) - C(1)	1) 1.	797 (6)	C(3)-C	2(5)	1.371 (8)
Ir(2) - C(2)	2) 1.	810 (6)	C(3)-C	2(6)	1.493 (9)
Ir(1) - P(1)	Ú 2.	224 (1)	C(4)—C	2(5)	1.377 (8)
Ir(2) - P(2)	2) 2.	224 (1)	C(4)C	C(7)	1.494 (8)
P(1)-O(	3) 1.	629 (4)	C(8)-C	C(10)	1.365 (9)
P(2)-O(4	4) 1.	633 (4)	C(8)C	C(11)	1.488 (9)
N(1) - N(	ź) 1.	370 (6)	C(9)-C	C(10)	1.377 (9)
N(1) - C(1)	3) 1.	349 (7)	C(9)-C	C(12)	1.493 (9)
N(2)-C	4) 1.	334 (7)			
P(1)Ir(1	1)—N(3) 9	2.3 (1)	lr(2)—P	P(2)—C(39)	117.8 (2)
P(1) - Ir(1)	í)—C(1) 9	91.0 (2)	lr(1)—N	N(1) - N(2)	117.9 (3)
N(1) lr(	1)—N(3) 8	35.1 (2)	Ir(1)—N	N(1)—C(3)	135.1 (3)
N(1)lr(	1)—C(1) 9	91.6 (2)	C(3)—N	N(1)—N(2)	106.8 (4)
P(1)Ir(	1)—N(1) 17	17.4 (1)	lr(2)N	N(2)—N(1)	117.1 (3)
N(3)-lr(	1)—C(1) 17	76.3 (2)	lr(2)—N	√(2)—C(4)	133.0 (3)
P(2)-Ir(2	2)—N(2) 9	92.5 (1)	C(4)—N	N(2)—N(1)	109.3 (4)
P(2)—Ir(2	2)—C(2) 9	91.8 (2)	Ir(1)—N	N(3)—N(4)	117.2 (3)
N(2)Ir(	2)—N(4) 8	33.1 (2)	Ir(1)—N	N(3)—C(8)	134.3 (4)
P(2) - Ir(2)	2)—N(4) 17	74.2(1)	C(8)—N	N(3)—N(4)	108.4 (4)
N(2)Ir(	2)-C(2) 17	74.1 (2)	C(9)—N	N(4)—N(3)	107.4 (4)
N(4)—lr(	2)—C(2) 9	92.9 (2)	Ir(2)—N	N(4)—N(3)	118.0 (3)
Ir(1)—C(	1)O(1) 17	79.3 (5)	Ir(2)—N	N(4)—C(9)	134.5 (4)
Ir(2)—C(	2)—O(2) 17	78.0(5)	C(5)—C	C(3) - N(1)	109.2 (5)
Lr(1)P(	1)—0(3) 11	19.3 (1)	C(5)—C	C(4)—N(2)	108.2 (5)
lr(1)P(	1)—C(27) 11	6.5 (2)	C(4)C	C(5) - C(3)	106.5 (5)
Lr(1)—P(	1)—C(45) 1	6.4 (2)	C(10)-	C(8) - N(3)	108.6 (5)
Ir(2)—P(3	2)0(4) 1	19.7 (1)	C(10)-	-C(9)—N(4)	109.1 (5)
lr(2) - P(2)	2)—C(33) 11	16.2 (2)	C(9)—C	J(10)C(8)	106.5 (5)

Weights were taken as  $1/\sigma^2(F_o^2)$ ; variances  $[\sigma^2(F_o^2)]$  derived from counting statistics plus an additional term,  $(0.014I)^2$ ; variances of the merged data by propagation of error plus another additional term,  $(0.014\langle I \rangle)^2$ . Goodness of fit for merging data was 1.02;  $R_{merge}$  for duplicates, 0.020. Dispersion corrections were taken from Cromer & Waber (1974). The final *R* for  $F_o^2$ >  $3\sigma$  was 0.0235; the final wR, 0.0022. Since the calculated absorption correction increased the goodness of fit for merging, an absorption coefficient corresponding to 30% of the calculated value was used.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55976 (41 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST1021]

#### References

- Beveridge, K. A, Bushnell, G. W., Dixon, K. R., Eadie, D. T., Stobart, S. R., Atwood, J. L. & Zaworotko, M. J. (1982). J. Am. Chem. Soc. 104, 920-921.
- Beveridge, K. A., Bushnell, G. W. & Stobart, S. R. (1983). Organometallics, 2, 1447-1451.
- Coleman, A. W., Eadie, D. T., Stobart, S. R., Zaworotko, M. J. & Atwood, J. L. (1982). J. Am. Chem. Soc. 104, 922–923.
- Cromer, D. T. & Waber, J. T. (1974). International Tables for X-ray Crystallography, Vol. IV, pp. 99-101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

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- Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana. Abstract B14, pp. 29-30.
- Farid, R. S., Chang, I.-J., Winkler, J. R. & Gray, H. B. (1993). In preparation.
- Fox, L. S. (1989). PhD dissertation, California Institute of Technology, USA.
- Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Louie, B. M., Rettig, S. J., Storr, A. & Trotter, J. (1984). Can. J. Chem. 62, 1057–1067.
- Nussbaum, S., Rettig, S. J., Storr, A. & Trotter, J. (1985). Can. J. Chem. 63, 692-702.
- Schagen, J. D., Straver, L., van Meurs, F. & Williams, G. (1989). CAD-4 manual. Version 5.0. Enraf-Nonius, Delft, The Netherlands.
- Uson, R., Oro, L. A., Ciriano, M. A., Pinillos, M. T., Tiripicchio, A. & Carmellini, M. (1981). J. Organomet. Chem. 205, 247-257.

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# Structure of [N, N'-o-Phenylenebis-(salicylideneaminato)]iron(III) Chloride as a Five-Coordinate Monomer

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## Abstract

The crystal contains three independent five-coordinate monomers of chloro{2,2'-[o-phenylenebis(nitrilomethylidyne)]diphenolato-N, N', O, O'}iron(III). The distances Fe(1)—Fe(1A), Fe(1)—Fe(1B) and Fe(1A)—Fe(1B) are 7.175 (1), 7.683 (1) and 7.207 (1) Å, respectively. The planes of the ligand groups of the two neighbouring molecules bend away from each other.

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