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Synthesis, Crystal Structure and Characterization of Polynuclear Potassium(I), Copper(II) and Cobalt(II) Complex with Acetylacetonethylenediamine

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SYNTHESIS, CRYSTAL STRUCTURE AND CHARACTERIZATION OF POLYNUCLEAR POTASSIUM(I), COPPER(II) AND COBALT(II) COMPLEX WITH ACETYLACETONETHYLENEDIAMINE

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The title complex [K{Cu(acen)}_3]_2[Co(NCS)_4] · 1/4CH_3OH (acen = acetylacetonethylenediamine anion) has been prepared and characterized. Single-crystal x-ray analysis reveals that the complex crystallizes in space group *P*1 with *a*=11.442(2), *b*=15.098(3), *c*=28.500(4) Å, α =82.77(1), β =83.58(1), γ =85.07(1)°. The crystal consists of the complex [K{Cu(acen)}_3]⁺ cations, [Co(NCS)_4]²⁻ anions and methanol molecules. Three [Cu(acen)] molecules function as bridging ligands through phenolic O atoms to one K⁺ to give the tetranuclear [K{Cu(acen)}_3]⁺ cation. Each copper(II) atom in the cation is in a square-planar geometry, being coordinated by two oxygen atoms and two nitrogen atoms from a quadridentate acen ligand. The cobalt(II) atom is coordinated by four nitrogen atoms of thiocyanate ligands, forming a deformed tetrahedral environment. The IR and UV–Vis spectra have also been investigated.

Keywords: Copper(II); Cobalt(II); Acen; Polynuclear complex; Crystal structure

INTRODUCTION

Multinuclear metal complexes are of great interest not only in elucidating the magnetic coupling between metal ions [1,2], but also in model compounds of the active sites of multi-metalloenzymes [3,4]. For the synthesis of hetero-metal polynuclear complexes, two synthetic methods have been employed. One is the method that uses a polynucleating ligand exhibiting multi-inequivalent coordination sites. The other is the method that uses a "ligand complex" which involves coordination ability to other metal ions. The latter method has advantages for syntheses of hetero-metal complexes with the systematic combination of metal ions and homo-metal complexes with inequivalent coordination geometries. A few "ligand complexes" are known. N,N'-ethylenebis (salicylideneaminato)copper(II) or zinc(II) (hereafter abbreviated as [Cu(salen)] or [Zn(salen)]) and derivatives can act as electrically neutral bidentate "ligand complexes" through the μ -phenoxo bridge [5,6]. Because of similar structures, divalent transition

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metal complexes with acetylacetonethylenediamine (abbreviated as [M(acen)] (M=Cu, Ni, Co) can be "ligand complexes". In this article, we report the synthesis, crystal structure and characterization of a potassium(I), copper(II) and cobalt(II) polynuclear complex by use the neutral ligand complex [Cu(acen)].

EXPERIMENTAL

Preparation

[Cu(acen)] and K₂[Co(NCS)₄] were prepared by literature procedure [7,8]. To a methanol solution (15 mL) of [Cu(acen)] (2 mmol, 560 mg) was added a methanol solution of K₂Co(NCS)₄ (1 mmol, 440 mg) with stirring. The resulting solution was allowed to stand at room temperature; three days later dark blue prism crystals suitable for single-crystal X-ray determination were formed. C, H and N analysis with an Erba 1160 instrument supported the composition [K{Cu(acen)}₃]₂[Co(NCS)₄] · 1/4CH₃OH. Anal. Calcd. for C_{76.25}H₁₀₉N₁₆O_{12.25}S₄CoCu₆K₂(%): C, 43.74; H, 5.21; N, 10.71. Found: C, 43.68; H, 5.43; N, 10.98. Infrared spectra were recorded using a Nicolet 205 Spectrophotometer (4000–400 cm⁻¹) with a crystalline sample spread on KBr pellets. Electronic spectra were measured in methanol by using a Shimadzu UV-260 spectrophotometer.

Crystal Structure Determination

A single crystal with dimensions $0.48 \times 0.46 \times 0.28$ mm was mounted on a glass fiber and used for the structure determination. Diffraction intensity data were collected on a Siemens P4 diffractometer up to $(2\theta)_{max}$ of 50.0 with graphite-monochromatized Mo-K α radiation ($\lambda = 0.71073$ Å) using the ω scan technique. A total of 16986 independent reflections were collected, among which 9068 reflections were considered as observed [$I > 2\sigma(I)$] and used for the structure refinement. Usual Lp and empirical absorption corrections were applied.

The structure was solved by direct methods followed by Fourier synthesis. The structure was refined on F^2 by full-matrix least-squares methods. Hydrogen atoms were generated geometrically and allowed to ride on their parent carbon and nitrogen atoms. The carbon atoms of C(6) and C(7), C(30) and C(31), C(66) and C(67) were disordered over two orientations. Anisotropic refinement including all non-H atoms, using the SHELXTL software package [9], converged to agreement factors R = 0.0417 and $R_w = 0.0990$, where $w = 1/[\sigma^2(F_o^2) + (0.0568P)^2]$. The highest peak in the final difference Fourier map was $0.658 \text{ e } \text{Å}^{-3}$. Atomic scattering factors used were taken from International Tables for X-ray crystallography [10].

RESULTS AND DISCUSSION

Crystal Structure

Crystal data: C_{76.25}H₁₀₉N₁₆O_{12.25}S₄CoCu₆K₂, M = 2092.40, triclinic, space group $P\overline{1}$, *a*=11.442(2), *b*=15.098(3), *c*=28.500(4) Å, *α*=82.77(1), *β*=83.58(1), *γ*=85.07(1)°, *V*=4840.7(2) Å³, *Z*=2, *D_c*=1.436 g cm⁻³, *F*(000)=2159, μ (Mo-K α)=1.693 mm⁻¹.

TABLE I Atomic coordinates $(\times 10^4)$ and equivalent isotropic displacement parameters (Å² × 10³). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

Atom	X	Y	Ζ	$U_{ m eq}$
Cu(1)	448(1)	1256(1)	4908(1)	53(1)
Cu(2)	5193(1)	2080(1)	1913(1)	60(1)
Cu(3)	5256(1)	2632(1)	3232(1)	58(1)
Cu(4)	7136(1)	1246(1)	-108(1)	60(1)
Cu(5)	1314(1)	3682(1)	5066(1)	58(1)
Cu(6)	9619(1)	3555(1)	101(1)	70(1)
Co	2054(1)	7371(1)	2592(1)	92(1)
K(1)	2591(1)	2414(1)	4115(1)	61(1)
K(2)	7432(1)	2292(1)	901(1)	69(1)
S(1)	4389(2)	7700(1)	3785(1)	108(1)
S(2)	-403(1)	5010(1)	2730(1)	104(1)
S(3)	686(2)	10306(1)	2072(1)	114(1)
S(4)	5288(2)	6853(1)	1477(1)	143(1)
O(1)	881(2)	1223(2)	4235(1)	61(1)
O(2)	2093(2)	1348(2)	4956(1)	65(1)
O(3)	6531(2)	1330(2)	1701(1)	64(1)
O(4)	5997(3)	3043(2)	1558(1)	86(1)
O(5)	4534(2)	1686(2)	3635(1)	65(1)
O(6)	3849(3)	3346(2)	3385(1)	68(1)
O(7)	8395(3)	1140(2)	296(1)	67(1)
O(8)	6046(3)	1410(2)	443(1)	63(1)
O(9)	2857(2)	3594(2)	4723(1)	62(1)
O(10)	724(3)	3451(2)	4491(1)	68(1)
O(11)	9348(3)	3240(2)	774(1)	78(1)
O(12)	7956(3)	3492(2)	81(1)	76(1)
O(13)	7142(16)	-2114(14)	2895(9)	237(18)
N(1)	-1197(3)	1143(2)	4859(1)	54(1)
N(2)	-15(3)	1333(2)	5574(1)	62(1)
N(3)	4346(3)	1110(3)	2249(1)	66(1)
N(4)	3834(3)	2845(3)	2109(1)	69(1)
N(5)	6590(3)	1878(3)	3010(1)	68(1)
N(6)	6076(4)	3614(3)	2900(2)	73(1)
N(7)	8178(4)	1347(3)	-682(1)	69(1)
N(8)	5890(4)	1138(3)	-503(1)	65(1)
N(9)	1900(4)	3926(2)	5639(1)	64(1)
N(10)	-235(3)	3827(2)	5401(2)	63(1)
N(11)	11270(4)	3699(3)	121(2)	77(1)
N(12)	9938(5)	3861(3)	-570(2)	85(1)
N(13)	2795(5)	7446(4)	3169(2)	106(2)
N(14)	935(5)	6432(4)	2680(2)	103(2)
N(15)	1284(5)	8539(4)	2398(2)	96(2)
N(16)	3347(5)	7077(4)	2109(2)	106(2)
C(1)	743(5)	1089(4)	3436(2)	100(2)
C(2)	152(4)	1105(3)	3933(2)	61(1)
C(3)	-1007(4)	1012(3)	4033(2)	66(1)
C(4)	-1679(4)	1066(3)	4478(2)	62(1)
C(5)	-2999(4)	1047(4)	4491(2)	100(2)
C(6)	-1910(19)	1045(9)	5331(5)	62(5)
C(7)	-1300(5)	1446(13)	5688(9)	76(7)
C(8)	220(5)	1409(4)	6413(2)	106(2)
C(9)	701(6)	1394(3)	5894(2)	74(2)
C(10)	1925(5)	1429(3)	5782(2)	77(2)
C(11)	2546(4)	1407(3)	5340(2)	68(1)
C(12)	3865(4)	1436(4)	5281(2)	91(2)
C(13)	7675(4)	34(4)	1510(2)	88(2)
C(14)	6576(4)	462(4)	1746(2)	66(1)
C(15)	5724(5)	-44(3)	2000(2)	76(2)
C(16)	4668(5)	274(4)	2258(2)	75(2)
C(17)	3955(5)	-453(4)	2549(2)	114(2)

(Continued)

TABLE I Continued

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Atom	X	Y	Ζ	Uea
$\begin{array}{c} C(18) & 323(10) & 1230(1) & 233(2) & 97(2) \\ C(20) & 2550(5) & 4220(4) & 2153(2) & 109(2) \\ C(21) & 3693(4) & 3705(4) & 2000(2) & 73(2) \\ C(22) & 4581(5) & 4205(4) & 1728(2) & 80(2) \\ C(23) & 5610(5) & 3876(4) & 1524(2) & 86(2) \\ C(24) & 6405(6) & 4508(4) & 1209(2) & 146(3) \\ C(25) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ C(26) & 4848(4) & 836(4) & 3638(2) & 63(1) \\ C(27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ C(28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ C(29) & 7708(4) & 4488(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 73(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -3224(2) & 78(2) \\ C(44) & 3932(5) & 1637(4) & -1205(2) & 108(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -5372(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 403(3) & 455(2) & 00(2) \\ C(45) & 313(4) & 3791(3) & 4878(2) & 67(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 405(3) & 5521(2) & 74(2) \\ C(55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ C(44) & 3932(5) & 925(5) & 1451(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 2265(4) & 6162(2) & 102(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(70) & 7967(6) & 3883(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 5257(16) & 2269(2) & 80(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C($	C(18)	2201(5)	1420(5)	2530(2)	07(2)
$\begin{array}{c ccccc} C(20) & 2550(5) & 4220(4) & 2153(2) & 190(2) \\ C(21) & 3693(4) & 3705(4) & 2000(2) & 73(2) \\ C(23) & 5610(5) & 3876(4) & 1728(2) & 86(2) \\ C(24) & 6405(6) & 4508(4) & 1209(2) & 146(3) \\ C(25) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ C(26) & 4484(4) & 836(4) & 3638(2) & 63(1) \\ C(27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ C(28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ C(29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 834(4) \\ C(31) & 7313(5) & 3512(8) & 2769(4) & 92(4) \\ C(32) & 6569(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75C(\\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 66(1) \\ C(39) & 9948(4) & 1135(3) & -1324(2) & 66(1) \\ C(39) & 9948(4) & 1351(3) & -722(2) & 70(1) \\ C(39) & 9948(4) & 1351(3) & -722(2) & 70(1) \\ C(39) & 9948(4) & 1351(3) & -7324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1105(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 108(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & 4572(2) & 78(2) \\ C(44) & 43932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4730(4) & 4041(4) & 5512(2) & 70(2) \\ C(50) & 3813(4) & 379(1) & 4878(2) & 67(1) \\ C(51) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 78(2) \\ C(54) & 4737(4) & 1207(3) & 4578(2) & 67(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 78(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(56) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(70) & 767(6) & 3868(4) & -749(2) & 97($	C(10)	2886(5)	1430(3)	2339(2) 2343(2)	97(2)
$\begin{array}{c} C(2) & 2.53(4) & 3705(4) & 2000(2) & 73(2) \\ C(2) & 4581(5) & 4205(4) & 1728(2) & 80(2) \\ C(2) & 6405(6) & 4508(4) & 129(2) & 146(3) \\ C(25) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ C(26) & 4848(4) & 836(4) & 3638(2) & 63(1) \\ C(27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ C(28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ C(29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7433(8) & 2350(7) & 2670(3) & 83(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 1-324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1657(4) & -1205(2) & 108(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 86(2) \\ C(44) & 4393(5) & 951(4) & -716(2) & 86(2) \\ C(45) & 4772(5) & 1130(3) & -332(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 932(2) & 78(2) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4084(4) & 5877(2) & 87(2) \\ C(53) & -1297(4) & 3676(3) & 3744(2) & 74(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & 11207(8) & 3827(13) & -7309) & 118(6) \\ C(66) & 1180(0) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11207(8) & 3827(13) & -7309) & 118(6) \\ C(66) & 11207(8) & 3827(13) & -7309) & 118(6) \\ C(66) & 11207(8) & 3827(13) & -7309) & 118(6) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1249(2) & 250(3) \\ C(76) & 4167(6)$	C(20)	2550(5)	4220(4)	2153(2)	109(2)
$\begin{array}{ccccc} (22) & 35610(5) & 3126(4) & 1728(2) & 80(2) \\ (23) & 5610(5) & 3876(4) & 1524(2) & 86(2) \\ (24) & 6405(6) & 4508(4) & 1209(2) & 146(3) \\ (25) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ (26) & 4848(4) & 836(4) & 3638(2) & 73(1) \\ (27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ (28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ (29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ (20) & 7433(8) & 2350(7) & 2670(3) & 83(4) \\ (31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ (32) & 5639(5) & 5184(4) & 2559(2) & 129(3) \\ (33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ (23) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ (23) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ (23) & 3699(4) & 1182(3) & 142(2) & 66(1) \\ (239) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ (240) & 9295(5) & 1451(3) & -722(2) & 708(1) \\ (241) & 9967(5) & 1637(4) & -1105(2) & 108(2) \\ (242) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ (243) & 6401(5) & 967(4) & -797(2) & 85(2) \\ (244) & 4392(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4392(5) & 951(4) & -716(2) & 88(2) \\ (245) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ (246) & 4307(4) & 1279(3) & 932(2) & 69(1) \\ (248) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ (244) & 3932(5) & 951(4) & -716(2) & 88(2) \\ (245) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ (246) & 4307(4) & 1279(3) & 932(2) & 69(1) \\ (248) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ (249) & 735(5) & 3881(4) & 6045(2) & 80(2) \\ (249) & 735(5) & 3881(4) & 6045(2) & 80(2) \\ (250) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ (55) & -197(5) & 4008(4) & 5877(2) & 87(2) \\ (56) & -2403(4) & 40041(4) & 5512(2) & 1002(2) \\ (57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ (56) & 1209(4) & 3751(5) & 3481(4) & 608(2) & 87(2) \\ (76) & -187(2) & 366(4) & -872(2) & 96(2) \\ (76) & 7182(5) & 35515(3) & 4719(2) & 70(2) \\ (56) & 1309(4) & 3827(13) & -7309(9) & 118(6) \\ (56) & 9198(7) & 3956(4) & -730(9) & 118(6) \\ (56) & 1180(0) & 4071(11) & -336(4) & 108(2) \\ (77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1024(5) & 9268(5) $	C(21)	3693(4)	3705(4)	2000(2)	73(2)
$\begin{array}{ccccc} 1 & 150(10) & 125(1) & 1124(2) & 60(2) \\ (224) & 6405(6) & 4508(4) & 1294(2) & 146(3) \\ (225) & 4459(5) & 224(3) & 3955(2) & 92(2) \\ (226) & 4848(4) & 836(4) & 3638(2) & 63(1) \\ (277) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ (28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ (29) & 7708(4) & 488(4) & 2543(2) & 106(2) \\ (30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ (231) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ (232) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ (233) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (234) & 4521(5) & 4772(4) & 3020(2) & 83(2) \\ (235) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ (236) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ (237) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ (238) & 9499(4) & 1182(3) & -1242(2) & 66(1) \\ (240) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ (241) & 9967(5) & 1637(4) & -1105(2) & 108(2) \\ (243) & 6401(5) & 967(4) & -979(2) & 85(2) \\ (243) & 6401(5) & 967(4) & -979(2) & 85(2) \\ (243) & 6401(5) & 967(4) & -979(2) & 85(2) \\ (243) & 6401(5) & 967(4) & -979(2) & 85(2) \\ (244) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ (244) & 4303(3) & 455(2) & 60(1) \\ (244) & 4303(3) & 455(2) & 60(1) \\ (245) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ (246) & 4307(4) & 1279(3) & 93(2) & 78(2) \\ (249) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (249) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (250) & 3813(4) & 7791(3) & 4878(2) & 67(1) \\ (241) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ (252) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ (251) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ (252) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ (253) & 3333(5) & 4225(4) & 6162(2) & 102(2) \\ (254) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ (255) & -197(5) & 4084(4) & 8577(2) & 87(2) \\ (256) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ (256) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ (256) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ (256) & -2403(4) & 406(4) & 187(2) & 87(2) \\ (256) & -2403(4) & 406(4) & 187(2) & 87(2) \\ (256) & -2403(4) & 406(4) & 187(2) & 87(2) \\ (256) & -2403(4) & 406(4) & 149(6) & 186(2) \\ (266) & -1860(20) & 4071(11) & -335(4) & 108$	C(21)	4581(5)	4205(4)	1728(2)	80(2)
$\begin{array}{cccc} (22) & 5016(5) & 5016(7) & 1241(2) & 501(2) \\ (225) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ (226) & 448(4) & 836(4) & 538(2) & 63(1) \\ (27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ (28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ (29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ (230) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ (231) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ (232) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ (233) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (24) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ (233) & 5644(6) & 4442(3) & 1242(2) & 89(2) \\ (234) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ (235) & 3699(5) & 4209(4) & 3442(2) & 112(2) \\ (236) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ (237) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ (248) & 9499(4) & 1182(3) & 1442(2) & 66(1) \\ (239) & 9938(4) & 1351(3) & -3242(2) & 78(2) \\ (240) & 2925(5) & 1451(3) & -722(2) & 70(1) \\ (241) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ (242) & 7505(5) & 1441(4) & -1105(2) & 86(2) \\ (243) & 4601(5) & 967(4) & -979(2) & 85(2) \\ (244) & 9332(5) & 951(4) & -716(2) & 88(2) \\ (244) & 9332(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 455(2) & 60(1) \\ (244) & 4933(3) & 515(3) & 4414(4) & 5812(2) & 102(2) \\ (55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (25) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (55) & -197(4) & 367(3) & -730(9) & 118(6) \\ (56) & -1806(2) & 477(1) & -336(4) & 108(7) \\ (56) & -1309(4) & 3827(13) & -730(9) & 118(6) \\ (56) & 1309(4) & 3827(13) & -730(9) & 118(6) \\ (56) & 13809(4) & 3827(13) & -730(9) & 118(6)$	C(22)	5610(5)	3876(4)	1524(2)	86(2)
$\begin{array}{ccccc} C(25) & 4059(5) & 224(3) & 3955(2) & 92(2) \\ C(26) & 44848(4) & 836(4) & 3638(2) & 63(1) \\ C(27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ C(28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ C(29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & -1324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(11) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(11) \\ C(47) & 4914(4) & 1279(3) & 393(2) & 69(1) \\ C(47) & 4914(4) & 1279(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(11) \\ C(51) & 3838(4) & 4025(3) & 5521(2) & 71(2) \\ C(55) & -197(5) & 4088(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3081(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3081(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3081(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 30881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3088(4) & -749(2) & 97(2) \\ C(55) & -197(5) & 3088(4) & -749(2) & 97(2) \\ C(55) & -197(5) & 3088(4) & -749(2) & 97(2) \\ C(55) & -1399(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(57) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 2749(2) & 97(2) \\$	C(24)	6405(6)	4508(4)	1209(2)	146(3)
$\begin{array}{ccccc} (26) & 4848(4) & 836(4) & 3638(2) & 63(1) \\ (27) & 8812(4) & 503(4) & 3381(2) & 73(1) \\ (28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ (29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ (30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ (23) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ (23) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ (23) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (23) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (23) & 35644(6) & 4442(5) & 2841(2) & 82(2) \\ (23) & 35699(5) & 4206(4) & 3275(2) & 75(2) \\ (236) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ (237) & 10314(4) & 1041(4) & 5242(2) & 89(2) \\ (238) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ (239) & 9938(4) & 1351(3) & -722(2) & 70(1) \\ (241) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ (242) & 7505(5) & 1461(4) & -716(2) & 88(2) \\ (243) & 4601(5) & 967(4) & -979(2) & 88(2) \\ (244) & 3932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 3932(5) & 951(4) & -716(2) & 88(2) \\ (244) & 4303(3) & 455(2) & 60(1) \\ (247) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ (247) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ (247) & 4914(4) & 1403(3) & 5697(2) & 71(1) \\ (248) & 4262(4) & 1539(4) & 933(2) & 78(2) \\ (249) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (249) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (250) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ (249) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (250) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ (251) & 3988(4) & 4025(3) & 5297(2) & 71(1) \\ (253) & 3339(5) & 4265(4) & 6162(2) & 1002(2) \\ (253) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ (254) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ (255) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ (265) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ (265) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ (265) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ (266) & 11860(2) & 4071(11) & -336(4) & 108(7) \\ (267) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ (268) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ (266) & 11860(2) & 4071(11) & -336(4) & 108(7) \\ (267) & 1202(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 7740(19) $	C(25)	4059(5)	224(3)	3955(2)	92(2)
$\begin{array}{ccccc} (27) & 5812(4) & 503(4) & 3381(2) & 73(1) \\ (28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ (29) & 7708(4) & 458(4) & 2543(2) & 106(2) \\ (30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ (31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ (32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ (33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ (34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ (25) & 3599(5) & 4206(4) & 3275(2) & 75(2) \\ (23) & 53699(5) & 4206(4) & 3275(2) & 75(2) \\ (23) & 53699(5) & 4209(4) & 3442(2) & 112(2) \\ (37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ (38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ (23) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ (2(4) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ (41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ (2(4) & 3032(5) & 951(4) & -716(2) & 88(2) \\ (2(4) & 4307(4) & 1279(3) & -333(2) & 68(1) \\ (2(4) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ (2(4) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ (2(4) & 4307(4) & 1279(3) & 93(2) & 78(2) \\ (2(4) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ (2(5) & -197(5) & 4059(3) & 5697(2) & 71(1) \\ (2(5) & 3838(4) & 4025(3) & 5321(2) & 74(2) \\ (2(5) & -2403(4) & 4041(4) & 5817(2) & 87(2) \\ (2(5) & -197(5) & 4088(4) & 5877(2) & 87(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ (2(5) & -197(5) & 3433(3) & 5217(2) & 71(2) \\ (2(5) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ (5(5) & -197(5) & 3405(4) & 954(2) & 93(2) \\ (5(6) & 11860(2) & 4071(11) & -336(4) & 108(7) \\ (2(7) & 1207(8) & 3827(13) & -730(9) & 118(6) \\ (16(6) & 11860(2) & 4071(11) & -336(4) & 108(7) \\ (2(6) & 1180(2) & 4071(11) & -336(4) & 108(7) \\ (2(7) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ (77) & 1740(19) & -2357(16) & 24339(12) & 250(30) \\ \end{array}$	C(26)	4848(4)	836(4)	3638(2)	63(1)
$\begin{array}{cccccc} C(28) & 6672(4) & 1006(5) & 3079(2) & 74(2) \\ C(29) & 7708(4) & 438(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 88(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 55321(2) & 74(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 78(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -1207(5) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5521(2) & 74(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -120(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -120(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -120(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -120(5) & 3813(3) & 5217(2) & 71(2) \\ C(56) & -120(5) & 3827(13) & -730(9) & 118(6) \\ C(60) & -617(5) & 3414(4) & 494(2) & 81(2) \\ C(61) & 1187(4) & 3661(4) & -479(2) & 97(2) \\ C(71) & 1727(8) & 3827(13) & -730(9) & 118(6) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(76) & 11027(8) & 3827(13) & -730(9) & 118(6) \\ C(76) & 11027(8) & 3827(13) & -730(9) & 118(6) \\ C(76) & 11027(5) & 75$	C(27)	5812(4)	503(4)	3381(2)	73(1)
$\begin{array}{cccccc} C(29) & 7708(4) & 1458(4) & 2543(2) & 106(2) \\ C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1105(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 108(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 55321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(51) & 3898(4) & 4025(3) & 55321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(51) & 3898(4) & 4025(3) & 55321(2) & 74(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -12403(4) & 4041(4) & 5112(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(1) \\ C(56) & -1207(4) & 3676(3) & 4744(2) & 74(2) \\ C(56) & -1207(4) & 3676(3) & 4744(2) & 74(2) \\ C(56) & -1207(4) & 3676(3) & 4744(2) & 74(2) \\ C(56) & 11207(8) & 3228(4) & 1068(2) & 842(2) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 1024$	C(28)	6672(4)	1006(5)	3079(2)	74(2)
$\begin{array}{cccccc} C(30) & 7453(8) & 2350(7) & 2670(3) & 83(4) \\ C(31) & 7313(5) & 3312(8) & 2769(4) & 92(4) \\ C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4777(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1105(2) & 108(2) \\ C(42) & 7505(5) & 14461(4) & -1105(2) & 88(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(47) & 4914(4) & 13716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 3881(4) & 6045(2) & 89(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 103(3) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(56) & -120(5) & 3823(3) & 5217(2) & 71(1) \\ C(56) & -120(5) & 3827(1) & -730(9) & 118(6) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 70$	C(29)	7708(4)	458(4)	2543(2)	106(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(30)	7453(8)	2350(7)	2670(3)	83(4)
$\begin{array}{cccccc} C(32) & 6369(5) & 5184(4) & 2559(2) & 129(3) \\ C(33) & 5644(6) & 4442(5) & 2841(2) & 82(2) \\ C(34) & 4521(5) & 4727(4) & 3020(2) & 83(2) \\ C(35) & 3699(5) & 4206(4) & 3275(2) & 75(2) \\ C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 88(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(44) & 43932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4084(4) & 5877(2) & 87(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 102(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(1) \\ C(53) & 3139(5) & 4265(4) & 6162(2) & 102(2) \\ C(57) & -1227(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1227(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 118207(6) & 3688(4) & -749(2) & 97(2) \\ C(70) & 7967(6) & 388(4) & -749(2) & 97(2) \\ C(71) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(72) & 6116(5) & 6600(4) & -213(2) & 108(3) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 1369(5) & 5843(4) & 700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 698(4) & 1849(2) & 93(2) $	C(31)	7313(5)	3312(8)	2769(4)	92(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(32)	6369(5)	5184(4)	2559(2)	129(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(33)	5644(6)	4442(5)	2841(2)	82(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(34)	4521(5)	4727(4)	3020(2)	83(2)
$\begin{array}{ccccc} C(36) & 2507(5) & 4209(4) & 3442(2) & 112(2) \\ C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 14461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -1403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(56) & -1403(4) & 4041(4) & 5512(2) & 103(3) \\ C(60) & -617(5) & 3405(4) & 954(2) & 93(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(66) & 9185(7) & 3955(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & $	C(35)	3699(5)	4206(4)	3275(2)	75(2)
$\begin{array}{cccccc} C(37) & 10314(4) & 1041(4) & 524(2) & 89(2) \\ C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9238(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5597(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 81(2) \\ C(77) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(36)	2507(5)	4209(4)	3442(2)	112(2)
$\begin{array}{ccccc} C(38) & 9499(4) & 1182(3) & 142(2) & 66(1) \\ C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 8877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -1207(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11260(2) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(37)	10314(4)	1041(4)	524(2)	89(2)
$\begin{array}{ccccc} C(39) & 9938(4) & 1351(3) & -324(2) & 78(2) \\ C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5521(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 8877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(64) & 11817(4) & 3641(4) & 4944(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(66) & 11800(20) & 4071(11) & -336(4) & 108(7) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 832(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 832(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(73) & 3475(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(38)	9499(4)	1182(3)	142(2)	66(1)
$\begin{array}{cccc} C(40) & 9295(5) & 1451(3) & -722(2) & 70(1) \\ C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(66) & 9185(7) & 3956(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(77) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(77) & 736(5) & 5843(4) & 2700(2) & 81(2) \\ C(77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(39)	9938(4)	1351(3)	-324(2)	78(2)
$\begin{array}{ccccc} C(41) & 9967(5) & 1637(4) & -1205(2) & 108(2) \\ C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5817(2) & 71(2) \\ C(56) & -2403(4) & 4041(4) & 5912(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5812(2) & 102(2) \\ C(56) & -2403(4) & 4041(4) & 5817(2) & 87(2) \\ C(56) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 1180(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3883(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 5843(4) & 2700(2) & 81(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) &$	C(40)	9295(5)	1451(3)	-722(2)	70(1)
$\begin{array}{ccccc} C(42) & 7505(5) & 1461(4) & -1105(2) & 86(2) \\ C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 40025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3888(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 5843(4) & 2700(2) & 81(3) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(41)	9967(5)	1637(4)	-1205(2)	108(2)
$\begin{array}{ccccc} C(43) & 6401(5) & 967(4) & -979(2) & 85(2) \\ C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(1) & -730(9) & 118(6) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & -700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(42)	7505(5)	1461(4)	-1105(2)	86(2)
$\begin{array}{ccccc} C(44) & 3932(5) & 951(4) & -716(2) & 88(2) \\ C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ C(77) & 7740(19) & -2357(16)$	C(43)	6401(5)	967(4)	-979(2)	85(2)
$\begin{array}{ccccc} C(45) & 4772(5) & 1130(3) & -373(2) & 68(1) \\ C(46) & 4307(4) & 1279(3) & 93(2) & 69(1) \\ C(47) & 4914(4) & 1403(3) & 455(2) & 60(1) \\ C(48) & 4262(4) & 1539(4) & 932(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3827(13) & -730(9) & 118(6) \\ C(66) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(44)	3932(5)	951(4)	-716(2)	88(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(45)	4772(5)	1130(3)	-373(2)	68(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(46)	4307(4)	12/9(3)	93(2)	69(1)
$\begin{array}{ccccc} C(48) & 4202(4) & 1539(4) & 952(2) & 78(2) \\ C(49) & 4897(4) & 3716(4) & 4520(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(47)	4914(4)	1403(3)	455(2)	60(1)
$\begin{array}{cccc} C(47) & 487/(4) & 57/16(4) & 4220(2) & 91(2) \\ C(50) & 3813(4) & 3791(3) & 4878(2) & 67(1) \\ C(51) & 3898(4) & 4025(3) & 5321(2) & 74(2) \\ C(52) & 2971(5) & 4059(3) & 5697(2) & 71(1) \\ C(53) & 3339(5) & 4265(4) & 6162(2) & 102(2) \\ C(54) & 975(5) & 3881(4) & 6045(2) & 89(2) \\ C(55) & -197(5) & 4084(4) & 5877(2) & 87(2) \\ C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 24391(2) & 250(30) \\ \end{array}$	C(48)	4202(4)	1339(4)	932(2) 4520(2)	78(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(49) C(50)	4697(4) 2812(4)	3710(4)	4320(2)	91(2) 67(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(50)	3898(4)	4025(3)	5321(2)	74(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(51)	2971(5)	4059(3)	5697(2)	71(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(53)	3339(5)	4265(4)	6162(2)	102(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(54)	975(5)	3881(4)	6045(2)	89(2)
$\begin{array}{cccccc} C(56) & -2403(4) & 4041(4) & 5512(2) & 102(2) \\ C(57) & -1226(5) & 3833(3) & 5217(2) & 71(2) \\ C(58) & -1297(4) & 3676(3) & 4744(2) & 74(2) \\ C(59) & -381(5) & 3515(3) & 4419(2) & 67(1) \\ C(60) & -617(5) & 3414(4) & 3916(2) & 87(2) \\ C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(55)	-197(5)	4084(4)	5877(2)	87(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(56)	-2403(4)	4041(4)	5512(2)	102(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(57)	-1226(5)	3833(3)	5217(2)	71(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(58)	-1297(4)	3676(3)	4744(2)	74(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(59)	-381(5)	3515(3)	4419(2)	67(1)
$\begin{array}{ccccccc} C(61) & 9674(5) & 2913(5) & 1587(2) & 133(3) \\ C(62) & 1013(5) & 3208(4) & 1068(2) & 84(2) \\ C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(60)	-617(5)	3414(4)	3916(2)	87(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(61)	9674(5)	2913(5)	1587(2)	133(3)
$\begin{array}{cccccc} C(63) & 1127(5) & 3405(4) & 954(2) & 93(2) \\ C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(62)	1013(5)	3208(4)	1068(2)	84(2)
$\begin{array}{cccccc} C(64) & 11817(4) & 3641(4) & 494(2) & 81(2) \\ C(65) & 13099(4) & 3821(4) & 466(3) & 118(2) \\ C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(63)	1127(5)	3405(4)	954(2)	93(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(64)	11817(4)	3641(4)	494(2)	81(2)
$\begin{array}{ccccc} C(66) & 11860(20) & 4071(11) & -336(4) & 108(7) \\ C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(65)	13099(4)	3821(4)	466(3)	118(2)
$\begin{array}{cccccc} C(67) & 11207(8) & 3827(13) & -730(9) & 118(6) \\ C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(66)	11860(20)	4071(11)	-336(4)	108(7)
$\begin{array}{ccccc} C(68) & 9519(6) & 4196(5) & -1409(2) & 148(3) \\ C(69) & 9185(7) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(67)	11207(8)	3827(13)	-730(9)	118(6)
$\begin{array}{cccc} C(59) & 9185(1) & 3956(4) & -872(2) & 96(2) \\ C(70) & 7967(6) & 3868(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(68)	9519(6)	4196(5)	-1409(2)	148(3)
$\begin{array}{cccccccc} C(70) & 7907(6) & 3808(4) & -749(2) & 97(2) \\ C(71) & 7424(5) & 3657(3) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(69)	9185(7)	3956(4)	-8/2(2)	96(2)
$\begin{array}{ccccccc} C(71) & 7424(5) & 5657(5) & -298(3) & 83(2) \\ C(72) & 6116(5) & 3600(4) & -213(2) & 108(2) \\ C(73) & 3475(5) & 7554(4) & 3419(2) & 76(2) \\ C(74) & 369(5) & 5843(4) & 2700(2) & 81(2) \\ C(75) & 1024(5) & 9268(5) & 2269(2) & 80(2) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(70)	/96/(6)	3868(4)	-/49(2)	97(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(71)	/424(5)	3057(3)	-298(3)	83(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(72)	0110(5)	3000(4) 7554(4)	-213(2) 2410(2)	108(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(74)	34/3(3)	7334(4) 5842(4)	3+19(2) 2700(2)	70(2) 81(2)
$\begin{array}{ccccc} C(76) & 1027(5) & 1200(5) & 1200(5) & 1200(5) & 002(5) \\ C(76) & 4167(6) & 6984(4) & 1849(2) & 93(2) \\ C(77) & 7740(19) & -2357(16) & 2439(12) & 250(30) \\ \end{array}$	C(75)	1024(5)	9268(5)	2769(2)	80(2)
C(77) $7740(19)$ $-2357(16)$ $2439(12)$ $250(30)$	C(76)	4167(6)	6984(4)	1849(2)	93(2)
	C(77)	7740(19)	-2357(16)	2439(12)	250(30)

IADLEI	I Dolla dista	thees (A) and angles ()	
Cu(1)–O(1)	1.931(3)	Cu(1)–O(2)	1.921(3)
Cu(1) - N(1)	1.926(3)	Cu(1) - N(2)	1.928(4)
Cu(2)–O(4)	1.906(3)	Cu(2) - O(3)	1.912(3)
Cu(2) - N(4)	1.930(4)	Cu(2) - N(3)	1.920(4)
Cu(3)-O(5)	1.904(3)	Cu(3)–O(6)	1.899(3)
Cu(3) - N(5)	1.921(4)	Cu(3) - N(6)	1.913(4)
Cu(4) - O(8)	1.920(3)	Cu(4) - O(7)	1.926(3)
Cu(4) - N(8)	1.944(4)	Cu(4) - N(7)	1.913(4)
Cu(5) - O(9)	1.922(3)	Cu(5) - O(10)	1.922(4)
Cu(5) - N(9)	1.922(4)	Cu(5) - N(10)	1.925(4)
Cu(6)–O(12)	1.921(3)	Cu(6)–O(11)	1.915(3)
Cu(6) - N(12)	1.911(5)	Cu(6) - N(11)	1.928(4)
Co-N(13)	1.953(5)	Co-N(4)	1.964(5)
Co-N(15)	1.946(6)	Co-N(6)	1.966(6)
K(1) - O(1)	2.735(3)	K(1) - O(2)	2.748(3)
K(1) - O(5)	2.702(3)	K(1)–O(6)	2.704(3)
K(1)–O(9)	2.695(3)	K(1) - O(10)	2.737(3)
K(2) - O(3)	2.698(3)	K(2) - O(4)	2.651(3)
K(2) - O(7)	2.684(3)	K(2) - O(8)	2.696(3)
K(2) - O(11)	2.684(3)	K(2) - O(12)	2.812(4)
C(6)-C(7)	1.509(5)	C(18) - C(19)	1.453(7)
C(30) - C(31)	1.506(5)	C(42) - C(43)	1.508(7)
C(54)-C(55)	1.468(7)	C(66)–C(67)	1.510(5)
S(1) - C(73)	1.604(6)	S(2)-C(74)	1.587(6)
S(3) - C(75)	1.626(7)	S(4)–C(76)	1.586(7)
N(13)-C(73)	1.145(6)	N(14)-C(74)	1.137(6)
N(15)-C(75)	1.141(7)	N(16)-C(76)	1.138(7)
N(1)-Cu(1)-N(2)	85.80(16)	N(1)-Cu(1)-O(1)	93.39(14)
N(1)-Cu(1)-O(2)	179.08(14)	N(2)-Cu(1)-O(1)	177.79(15)
N(2)-Cu(1)-O(2)	94.35(15)	O(1)-Cu(1)-O(2)	86.49(13)
N(3)-Cu(2)-N(4)	85.95(19)	N(3)-Cu(2)-O(3)	94.66(17)
N(3)-Cu(2)-O(4)	177.68(17)	N(4)-Cu(2)-O(3)	178.55(15)
N(4)-Cu(2)-O(4)	93.59(17)	O(3)–Cu(2)–O(4)	85.74(14)
N(5)-Cu(3)-N(6)	86.35(19)	N(5)–Cu(3)–O(5)	94.09(16)
N(5)–Cu(3)–O(6)	172.99(15)	N(6)-Cu(3)-O(5)	172.23(16)
N(6)–Cu(5)–O(6)	94.37(18)	O(5)–Cu(3)–O(6)	86.13(13)
N(7)-Cu(4)-N(8)	86.78(18)	N(7)-Cu(4)-O(7)	93.79(16)
N(7)-Cu(4)-O(8)	168.07(15)	N(8)-Cu(4)-O(7)	170.55(15)
N(8)-Cu(4)-O(8)	93.13(15)	O(7)-Cu(4)-O(8)	88.26(13)
N(9)-Cu(5)-N(10)	86.19(12)	N(9)-Cu(5)-O(9)	93.60(15)
N(9)-Cu(5)-O(10)	179.39(15)	N(10)-Cu(5)-O(9)	177.40(14)
N(10)-Cu(5)-O(10)	93.74(16)	O(9)-Cu(5)-O(10)	86.45(13)
N(11)-Cu(6)-N(12)	85.2(2)	N(11)-Cu(6)-O(11)	93.19(17)
N(11)-Cu(6)-O(12)	176.43(17)	N(12)-Cu(6)-O(11)	178.32(19)
N(12)-Cu(6)-O(12)	94.44(19)	O(11)-Cu(6)-O(12)	87.17(15)
N(13)-Co-N(14)	112.2(2)	N(13)-Co-N(15)	108.3(2)
N(13)-Co-N(16)	105.8(2)	N(14)–Co–N(15)	111.3(2)
N(14)–Co–N(16)	109.3(2)	N(15)-Co-N(16)	109.9(2)
C(73)–N(13)–Co	161.6(5)	C(74)–N(14)–Co	172.9(6)
C(75) - N(15) - Co	168.3(6)	C(76)–N(16)–Co	171.6(6)
N(13)-C(73)-S(1)	177.9(6)	N(14)-C(74)-S(2)	179.1(7)
N(15) = C(75) = S(3)	178.3(6)	N(16)-C(76)-S(4)	178.5(7)

TABLE II Bond distances (Å) and angles (°)

Fractional atomic coordinates and equivalent isotropic thermal parameters for all non-H atoms are listed in Table I. Selected bond distances and angles are listed in Table II.

The polynuclear complex consists of two $[K{Cu(acen)}_3]^+$ cations and one $[Co(NCS)_4]^{2-}$ anion. As shown in Fig. 1, each copper(II) atom in the cation assumes a square-planar coordination geometry, with two amido nitrogen atoms and two



FIGURE 1 An ORTEP view of the $[K{Cu(acen)}_3]^+$ cations with atom labels, showing 35% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

oxygen atoms of quadridentate acen ligand. The average bond distances of Cu–O and Cu–N are 1.917(3) and 1.923(4)Å, respectively, which are both shorter than the corresponding distances of [Cu(acen)] [11]. Each potassium ion in the cation is surrounded octahedrally by the six phenolic oxygen atoms from three quadridentate acen ligands. These K–O distances are in the range of 2.651(3)–2.812(4)Å and the values are close to those of 2.672(7)–2.866(9)Å found for K₂[NiL]·2DMF·2H₂O (H₄L = 1,2-bis(2-hydroxybenzamido)ethane) [12], 2.682(5)–2.873(5)Å found for K₂[Cu(hbab)]·5DMF (hbab = 1,2-bis(2-hydrobenzamido)benzene) [13] and consistent with the average distance of 2.8 ± 0.1 Å of potassium crown ether complexes [14]. The most striking feature of the crystal structure is that six phenolic oxygen atoms from three [Cu(acen)] molecules function as μ_2 -O bridging ligands to one K⁺ to give a tetranuclear [K{Cu(acen)}₃]⁺ cation. This structure feature is different from those observed in other phenolic oxygen bridging complexes [12,13], in which the phenolic oxygen atoms act as μ_3 -O bridging ligands to K⁺ to give a one-dimensional chain structure.

The cobalt(II) atom in the anion possesses four thiocyanate ligands, each attached to the metal by the nitrogen atom, giving rise to a deformed tetrahedral environment around the cobalt(II) center. The Co–N distances are in the range of 1.946(6)–1.966(6)Å. Co–N–C linkages are bent with angles varying from 161.6(5) to 172.9(6) and N–Co–N angle in the range of 105.8(2)–112.2(2), which are in agreement with the corresponding distances and angles found in $[Cu(cyclam)][Co(NCS)_4]$ (cyclam = 1,4,8,11-tetraazacyclotetradecane) [15]. The thiocyanate groups are almost linear with a mean value of the N–C–S angles of 178.5(6)°. The C–N average distance of 1.140(6) Å and C–S average distance of 1.601(7) Å in the SCN[–] moiety show the normal structure of the thiocyanate in the complex.

The C–C distance from 1.468(7) to 1.510(5) Å in the Cu–N–C–C–N ring of the complex is below that expected for a sp³ hybrid C–C single bond (1.54 Å) [16]. The corresponding C–C bond distance in Cu(acen) [11], Cu(acen) $\cdot 1/2H_2O$ [17], and Cu(acen) $\cdot H_2O$ [18] are 1.55, 1.43, and 1.55 Å, respectively.

Packing diagram of the polynuclear complex as shown in Fig. 2.

Spectroscopic Properties

The infrared spectrum of the complex exhibits a sharp and strong band at 2072 cm^{-1} , which correspond to the $\nu(\text{CN})$ stretching mode of SCN⁻, indicating the presence of



FIGURE 2 Packing diagram of the polynuclear complex.

nitrogen-bonded thiocyanates (Co–NCS) [15]. The weak band corresponding to ν (CS) vibration appears at 870 cm⁻¹, and the δ (NCS) bending mode is observed at 465 cm⁻¹ as a shoulder. The peak at 1605 cm⁻¹ was assigned to the C=N stretching vibration in the complex. Compared with 1640 cm⁻¹ for the C=N stretching vibration of free acen, the 35 cm⁻¹ shift to low wavelength strongly suggests coordination of the Schiff base nitrogen atoms of acen in the complex. The peak at 1530 cm⁻¹ was attributed to a C–O stretching mode in the spectrum of the complex. The shift of the ν (C–O) band to higher frequency compared with that of the "ligand complex" [Cu(acen)] (1510 cm⁻¹) is the result of an increased constraint of the oxygen atoms due to polynucleation [19].

The reflectance electronic spectrum on the crystalline sample in methanol solvent exhibits a broad absorption at 312 nm and shoulders at 329 and 339 nm. It is reasonable to assign these bands to charge-transfer bands. It is possible that the charge transfer in this case is due to MLCT. At high wavelength the complex shows a broad band centred at 545 nm, which can be assigned to the copper d-d transitions.

Supplementary Material

Full lists of crystallographic data are available from the author upon request.

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