The Crystal and Molecular Structure of π-Cyclooctenyl-π-cycloocta-1,5-dienecobalt, $Co(C_8H_{13})(C_8H_{12})$

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The crystal structure of π-cyclooctenyl-π-cycloocta-1,5-dienecobalt, $Co(C_8H_{13})(C_8H_{12})$, has been established by successive Fourier analyses. The atomic parameters were refined by least-squares techniques using three-dimensional X-ray data to an R factor of 0.125. The complex molecule crystallizes in the space group $P2_1/c$ with four molecules in the unit cell of dimensions: $a=10.78$, $b=7.30$, $c=17.81$ Å, $\beta=104.2°$. The four cobalt atoms lie nearly on the face-centered positions in the unit cell and are sandwiched between the two ligands, cyclooctenyl C_8H_{13} and cyclooctadiene C_8H_{12}. The seven nearest Co···C distances range from 2.02 Å to 2.09 Å. Atoms Co, C(1), C(3) and the respective centers of the two double bonds, C(9)–C(16) and C(12)–C(13), in C_8H_{12} ring are coplanar to within 0.08 Å. The conformation of C_8H_{13} is of the tub form and C_8H_{12} of the boat form. The two lengths of the double bonds in C_8H_{12} are 1.41 Å and 1.39 Å, while those in the allyl part in C_8H_{13} are 1.35 Å and 1.46 Å, respectively. The average distance of the remaining twelve C–C bonds is 1.54 Å.

π-Cyclooctenyl-π-cycloocta-1,5-dienecobalt was prepared by Otsuka and Rossi.[1] They reported the formation of $CoH(dp)_2$ [dp=1,2-bis(diphenylphosphino)-ethane] when this complex was treated with an excess of dp and the release of cyclooctene upon thermal decomposition. The latter is in contrast to the thermal decomposition of bis(cycloocta-1,5-diene)nickel, $Ni(C_8H_{12})_2$ which yields only cyclooctadiene and metallic nickel. On the basis of a NMR and IR study, they proposed two possible molecular structures in each of which two hydrogen atoms on the octenyl ligand are found at exceptionally short distances from the cobalt atom. Thus the reactivity of this complex was attributed to the proximity of the two hydrogen atoms to the cobalt atom. In order to clarify the postulated structures, particular emphasis being laid on the role of the hydrogen atoms, we have undertaken a three-dimensional X-ray crystal analysis of $Co(C_8H_{13})(C_8H_{12})$. A preliminary account of this work has already been reported.[2]

Experimental

Crystals of π-cyclooctenyl-π-cycloocta-1,5-dienecobalt were kindly provided by Professor S. Otsuka. They were recrystallized as brilliant black plates from *n*-hexane solutions. Specimens used in this investigation were sealed in thin-walled glass capillaries and were held below 0°C during experiments to prevent oxidative and thermal decompositions. Oscillation and Weissenberg photographs taken with Fe$K\alpha$ radiation exhibited a monoclinic symmetry with space group $P2_1/c$. The lattice parameters were obtained from (0kl) and (h0l) Weissenberg photographs superimposed by silicon powder patterns and were refined by a least-squares method. In order to collect the three-dimensional intensity data, equi-inclination integrating Weissenberg photographs were taken with Mn-filtered Fe$K\alpha$ radiation from 0kl to 6kl and from h0l to h4l, using a multiple-film technique. The intensities were visually estimated using a calibrated scale. Thus, 1043 independent non-zero reflections were observed. These relative intensities were corrected for Lorentz and polarization factors and were placed on an absolute scale by Wilson's methods. No absorption correction was applied since $\mu R \simeq 1$. The crystal data are summarized in Table 1.

Table 1. Crystal data of π-cyclooctenyl-π-cycloocta-1,5-dienecobalt, $Co(C_8H_{13})(C_8H_{12})$

Monoclinic	$a=10.78\pm0.03$ Å
	$b=7.30\pm0.02$
	$c=17.81\pm0.04$
	$\beta=104.2\pm0.1°$
U	1361.6 Å^3
Dc	1.35 g/cm^3
Z	4
Space group	$P2_1/c$
μ	30.5 cm^{-1} (for Fe$K\alpha$)

Structure Determination

A three-dimensional sharpened Patterson function showed three large peaks at (1/2, 0, 1/2), (1/2, 1/2, 0), and (0, 1/2, 1/2). This vector set implies that the arrangement of the cobalt atoms is of the face-centered type so that these atoms lie either on the two sets of special positions (centers of symmetry) or on the general positions with $x \fallingdotseq 1/4$, $y \fallingdotseq 0$, $z \fallingdotseq 1/4$. The latter case was chosen because the complex molecule was expected to be noncentro-symmetric. The symbolic addition procedure was applied, but this attempt was not successful owing to a pseudo-symmetry arising from the arrangement of the cobalt atoms.

The positions of the cobalt atom were refined by a diagonal-matrix least-squares method, and a Fourier synthesis phased on the metal atom alone was carried out. All of the sixteen carbon atoms were satisfactorily located by successive Fourier analyses. After several cycles of refinement with isotropic temperature factors for all the atoms, the discrepancy factor R, $R=\sum||F_o|-|F_c||/\sum|F_o|$, dropped to 0.16. The positional and anisotropic thermal parameters were further refined by a block-diagonal-matrix least-squares method to the R value of 0.125. The final atomic coordinates and

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1) S. Otsuka and M. Rossi, *J. Chem. Soc., A*, **1968**, 2630.

2) S. Koda, A. Takenaka, and T. Watanabé, *Chem. Commun.*, **1969**, 1293.

TABLE 2 (a). THE FINAL ATOMIC COORDINATES WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Co	0.2460(3)	−0.0066(4)	0.2565(2)	C-9	0.2032(22)	−0.0258(34)	0.3606(11)
C-1	0.0896(19)	−0.1571(29)	0.1954(11)	C-10	0.2584(24)	0.1469(33)	0.4125(13)
C-2	0.0944(19)	0.0260(30)	0.1640(10)	C-11	0.3096(29)	0.2925(32)	0.3715(16)
C-3	0.2003(20)	0.0858(30)	0.1435(12)	C-12	0.3491(23)	0.2301(30)	0.2990(14)
C-4	0.2932(24)	−0.0230(38)	0.1031(13)	C-13	0.4320(21)	0.0831(31)	0.2942(12)
C-5	0.2201(25)	−0.1117(34)	0.0247(13)	C-14	0.4996(20)	−0.0285(40)	0.3696(13)
C-6	0.1024(22)	−0.2263(30)	0.0283(11)	C-15	0.4257(20)	−0.1932(34)	0.3855(13)
C-7	0.1186(21)	−0.3753(31)	0.0874(12)	C-16	0.2800(22)	−0.1728(30)	0.3516(11)
C-8	0.1565(22)	−0.3253(27)	0.1745(12)				

TABLE 2 (b). THE ANISOTROPIC TEMPERATURE FACTORS IN THE FORM OF
$\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{23}kl+B_{31}lh)\}$
(Standard deviations in parentheses)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{31}
Co	0.0067(3)	0.0078(5)	0.0016(1)	−0.0006(9)	0.0001(6)	0.0005(3)
C-1	0.0040(23)	0.0078(47)	0.0017(8)	−0.0033(52)	0.0013(31)	−0.0017(21)
C-2	0.0061(23)	0.0088(49)	0.0008(7)	0.0036(59)	−0.0035(32)	−0.0041(19)
C-3	0.0080(27)	0.0054(43)	0.0018(8)	0.0017(57)	−0.0018(32)	−0.0001(24)
C-4	0.0118(31)	0.0169(63)	0.0025(9)	−0.0167(79)	−0.0032(43)	0.0034(27)
C-5	0.0120(33)	0.0137(58)	0.0020(9)	−0.0086(73)	−0.0029(39)	0.0047(27)
C-6	0.0091(28)	0.0075(48)	0.0010(7)	0.0012(60)	0.0018(32)	−0.0023(23)
C-7	0.0050(24)	0.0097(51)	0.0023(8)	−0.0016(56)	−0.0018(34)	−0.0008(23)
C-8	0.0094(28)	0.0002(41)	0.0021(9)	−0.0036(53)	−0.0032(30)	0.0005(25)
C-9	0.0100(27)	0.0132(58)	0.0011(7)	−0.0017(70)	0.0002(36)	0.0008(22)
C-10	0.0095(30)	0.0126(56)	0.0027(9)	−0.0010(66)	−0.0087(38)	0.0037(27)
C-11	0.0178(42)	0.0040(49)	0.0042(12)	−0.0068(75)	−0.0025(41)	0.0060(36)
C-12	0.0100(30)	0.0048(48)	0.0033(10)	−0.0136(63)	−0.0021(37)	−0.0001(27)
C-13	0.0068(27)	0.0088(46)	0.0023(9)	−0.0156(58)	−0.0049(35)	0.0007(24)
C-14	0.0035(22)	0.0270(77)	0.0027(9)	0.0014(71)	0.0079(47)	−0.0030(22)
C-15	0.0032(23)	0.0161(58)	0.0029(10)	0.0049(60)	0.0054(39)	−0.0006(24)
C-16	0.0098(28)	0.0090(48)	0.0009(7)	0.0002(61)	−0.0001(30)	0.0033(23)

anisotropic temperature factors of the form: $\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{23}kl+B_{31}lh)\}$ together with their estimated standard deviations are given in Table 2(a) and (b). The observed and calculated structure factors are listed in Table 3. The scattering factors of Co^{+1} and C were taken from International Tables for X-ray Crystallography (1962). The oxidation state of the cobalt atom will be discussed later. All the numerical calculations were carried out on a FACOM 270-20 computer of this University using the programs written in our laboratory.

Results and Discussion

Figure 1 shows the view of the molecule along the *b*-axis, where the hydrogen atoms are given in positions postulated on the assumption of the conventional bond distances and angles. The numbering scheme for the carbon and hydrogen atoms are also shown. Interatomic bond distances and angles and their estimated standard deviations are summarized in Table 4 (a) and (b).

As is shown in Fig. 1, the cobalt atom is sandwiched between the two ligands, cyclooctenyl C_8H_{13}, and cyclooctadiene C_8H_{12}. Interatomic distances from the metal atom to the seven nearest carbon atoms, C(1), C(2), C(3), C(9), C(12), C(13), and C(16), fall in the range from 2.02 Å to 2.09 Å. Atoms Co, C(1), C(3), and the respective centers of the two double bonds, C(9)–C(16) and C(12)–C(13), in C_8H_{12} ring are coplanar to within 0.08 Å. We shall designate the plane thus described as the Co-plane. The equation of the plane and the deviations of the respective atoms from the plane are listed in Table 5. Figures 2 and 3 represent the geometry around the cobalt atom which are the projections along the directions parallel and normal

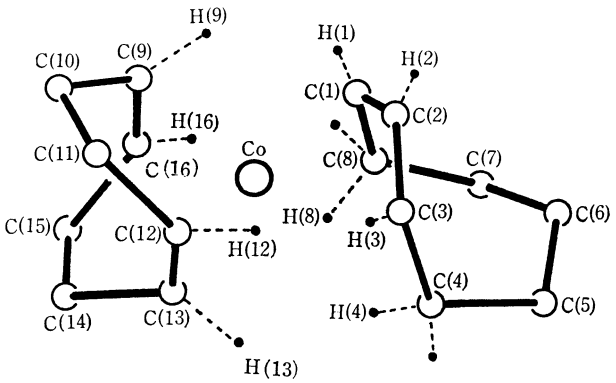

Fig. 1. The molecular structure viewed along the *b* axis.

TABLE 3. OBSERVED AND CALCULATED STRUCTURE FACTORS

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	0	2	92.05	-125.87	6	0	12	16.84	-22.48	-6	0	10	36.15	38.25	1	1	15	28.23	22.32	5	1	12	13.67	-21.38	-3	1	5	97.49	-103.16
0	0	4	38.55	-18.32	8	0	0	38.94	35.16	-6	0	12	49.68	-44.82	2	1	0	91.98	73.67	5	1	13	21.58	-26.71	-3	1	7	76.43	87.91
0	0	6	33.26	-35.88	8	0	2	20.51	-13.36	-6	0	14	30.12	26.76	2	1	1	36.77	-26.01	6	1	0	26.09	-18.86	-3	1	8	12.83	-10.97
0	0	8	90.36	83.90	8	0	4	34.01	36.91	-7	0	4	22.02	-22.72	2	1	2	41.69	-28.14	6	1	1	13.28	-12.49	-3	1	9	52.36	-57.89
0	0	10	57.23	-46.35	8	0	6	32.03	-34.93	-7	0	6	11.16	-9.97	2	1	4	6.53	2.29	6	1	2	11.77	7.82	-3	1	11	51.42	53.18
0	0	12	38.15	32.79	8	0	8	27.54	34.07	-7	0	8	33.95	-27.49	2	1	5	49.90	40.07	6	1	6	16.05	-16.52	-3	1	13	40.39	-47.67
0	0	14	37.83	-31.70	9	0	0	17.47	18.44	-7	0	10	29.66	25.73	2	1	6	14.62	19.62	6	1	7	15.21	-17.57	-3	1	15	20.79	20.50
0	0	16	18.17	12.53	10	0	0	7.63	-7.57	-7	0	12	16.56	-17.26	2	1	7	44.69	-39.88	6	1	9	7.12	7.39	-3	1	17	19.47	-22.36
1	0	2	37.91	31.87	10	0	2	21.79	30.82	-7	0	14	19.77	17.96	2	1	8	19.48	-13.65	6	1	11	5.47	-4.69	-4	1	1	20.80	-20.91
1	0	4	6.15	-6.42	-1	0	4	63.98	61.12	-8	0	2	46.50	-42.21	2	1	9	29.11	-24.03	7	1	0	19.26	-17.18	-4	1	2	37.19	-21.77
1	0	6	20.22	13.79	-1	0	6	49.54	39.05	-8	0	4	47.20	40.23	2	1	10	19.15	16.43	7	1	1	48.97	43.35	-4	1	3	47.04	35.96
1	0	8	67.63	-65.52	-1	0	8	11.42	19.78	-8	0	6	55.66	-46.67	2	1	12	19.35	-17.58	7	1	3	40.14	-43.50	-4	1	4	18.22	11.20
1	0	10	21.21	18.85	-1	0	10	50.55	-48.50	-8	0	8	19.15	13.69	2	1	13	31.06	33.64	7	1	5	21.07	23.43	-4	1	5	17.77	-18.16
1	0	12	23.04	-21.74	-1	0	12	75.77	75.31	-8	0	10	33.12	-32.31	2	1	15	21.51	-22.15	7	1	7	18.96	-18.17	-4	1	6	23.45	-18.90
1	0	16	20.47	-19.37	-1	0	14	16.59	-15.84	-8	0	12	33.47	33.98	3	1	0	52.59	36.12	7	1	9	24.99	24.57	-4	1	7	17.83	14.11
2	0	0	112.95	-161.42	-2	0	2	146.84	186.38	-8	0	14	26.00	-27.26	3	1	1	110.01	99.13	9	1	1	13.01	-11.76	-4	1	9	34.37	-37.57
2	0	2	54.87	-35.65	-2	0	4	83.58	-94.38	-9	0	2	10.45	-9.81	3	1	2	39.77	27.99	9	1	3	20.72	27.40	-4	1	11	23.08	27.63
2	0	4	6.99	-10.17	-2	0	6	93.26	104.11	-9	0	4	25.81	25.36	3	1	3	63.85	-62.42	9	1	5	20.75	-32.64	-4	1	13	12.85	-13.78
2	0	6	27.76	39.76	-2	0	8	78.77	-75.63	-9	0	6	17.94	-22.93	3	1	4	30.01	-26.00	-1	1	1	137.15	191.53	-4	1	15	12.18	8.76
2	0	8	80.99	-84.60	-2	0	10	67.28	70.01	-9	0	8	13.96	11.30	3	1	5	52.24	54.09	-1	1	2	15.43	11.53	-4	1	17	24.90	-29.92
2	0	10	72.68	66.01	-2	0	12	39.73	-38.42	-10	0	2	22.00	22.97	3	1	6	29.34	-24.27	-1	1	3	84.29	-97.09	-5	1	1	102.34	91.96
2	0	12	71.09	-68.48	-2	0	14	31.54	30.42	-10	0	4	26.99	-25.56	3	1	7	85.67	-79.85	-1	1	5	75.33	84.07	-5	1	2	28.60	-16.89
2	0	14	30.17	20.69	-2	0	16	9.28	-6.53	-10	0	6	30.06	29.94	3	1	8	10.19	-11.62	-1	1	6	25.82	-19.75	-5	1	3	41.06	-35.39
2	0	16	20.42	-22.33	-2	0	18	19.93	28.15	0	1	1	17.44	-11.75	3	1	9	71.49	73.59	-1	1	7	52.76	-61.80	-5	1	4	17.49	-13.35
3	0	0	53.70	-51.18	-3	0	2	38.80	43.31	0	1	2	54.18	47.44	3	1	10	25.18	24.62	-1	1	8	12.99	7.29	-5	1	5	55.55	49.01
3	0	2	50.35	-40.16	-3	0	4	16.08	-13.47	0	1	3	42.90	40.62	3	1	11	47.05	-46.82	-1	1	9	76.58	81.78	-5	1	7	44.18	-44.20
3	0	4	37.75	26.12	-3	0	6	10.88	-4.36	0	1	5	14.41	5.00	3	1	12	9.84	-8.38	-1	1	10	13.89	11.76	-5	1	9	36.87	37.49
3	0	6	33.43	-33.82	-3	0	10	20.01	18.64	0	1	6	74.55	64.79	3	1	13	35.10	30.39	-1	1	11	50.73	-52.82	-5	1	11	38.42	-41.01
3	0	8	10.52	-9.47	-3	0	12	42.51	-40.07	0	1	7	41.68	33.74	3	1	14	14.38	-19.78	-1	1	13	28.53	31.95	-5	1	13	41.38	43.00
3	0	10	18.97	15.95	-3	0	14	41.26	37.54	0	1	8	24.62	-17.31	3	1	15	14.28	-13.99	-1	1	14	17.91	16.62	-5	1	15	19.79	-15.85
3	0	12	21.67	20.21	-3	0	16	15.49	-13.93	0	1	9	32.04	-32.92	4	1	0	14.19	-9.52	-1	1	15	18.31	-12.41	-5	1	16	5.94	-5.23
3	0	14	35.21	-32.49	-4	0	2	43.46	-44.50	0	1	11	29.02	29.91	4	1	1	6.93	6.86	-1	1	17	21.83	22.14	-5	1	17	12.21	14.16
4	0	0	75.73	70.70	-4	0	4	54.21	47.21	0	1	12	36.83	33.40	4	1	2	27.57	-26.06	-2	1	1	27.67	-13.09	-6	1	1	6.27	6.93
4	0	2	77.78	-70.83	-4	0	6	69.43	-69.00	0	1	13	26.90	-27.61	4	1	3	22.70	23.82	-2	1	2	13.65	-7.00	-6	1	2	11.54	3.14
4	0	4	46.13	45.37	-4	0	8	63.68	66.02	0	1	16	8.56	7.24	4	1	4	38.56	33.83	-2	1	3	33.17	-24.79	-6	1	4	24.83	-19.64
4	0	6	75.34	-73.42	-4	0	10	66.92	-62.36	0	1	17	12.81	-15.58	4	1	7	11.20	-7.57	-2	1	4	57.84	-50.07	-6	1	5	7.91	5.67
4	0	8	92.33	96.71	-4	0	12	49.14	49.36	1	1	0	43.49	28.71	4	1	8	10.68	-12.34	-2	1	6	9.10	-6.77	-6	1	6	12.74	-12.50
4	0	10	64.05	-60.79	-4	0	14	30.89	-24.92	1	1	1	117.00	-138.62	4	1	11	24.27	29.26	-2	1	7	8.89	-8.43	-6	1	7	28.92	-30.78
4	0	12	23.54	17.21	-4	0	16	20.84	16.43	1	1	2	60.95	45.56	4	1	13	27.04	-31.32	-2	1	8	41.00	39.81	-6	1	9	41.19	44.81
4	0	14	12.18	-12.08	-5	0	2	49.99	-42.16	1	1	3	12.12	17.57	4	1	14	5.07	7.03	-2	1	9	31.82	30.44	-6	1	11	21.25	-24.34
5	0	0	32.28	-27.26	-5	0	4	36.90	33.83	1	1	4	40.22	29.47	5	1	0	17.21	8.37	-2	1	10	23.00	-19.89	-6	1	13	16.52	21.49
5	0	2	25.13	18.18	-5	0	8	34.44	39.59	1	1	5	26.65	-33.61	5	1	1	94.90	-88.25	-2	1	11	29.34	-29.82	-6	1	15	11.41	-13.01
5	0	4	10.27	15.20	-5	0	10	21.56	-22.41	1	1	6	34.63	19.29	5	1	2	28.04	-28.59	-2	1	12	9.65	-9.96	-6	1	16	11.41	-13.73
5	0	12	19.29	-19.21	-5	0	12	17.65	21.01	1	1	7	77.67	77.05	5	1	3	67.09	66.37	-2	1	13	32.13	33.80	-7	1	1	58.55	-55.74
6	0	0	78.18	-80.15	-5	0	14	23.76	-24.03	1	1	8	12.09	9.63	5	1	5	58.71	-64.15	-2	1	15	20.62	-20.17	-7	1	3	56.66	53.35
6	0	2	55.70	53.34	-5	0	16	24.83	26.27	1	1	9	86.26	-76.74	5	1	7	53.14	52.35	-2	1	17	20.09	23.51	-7	1	5	64.34	-59.49
6	0	4	47.74	-52.47	-6	0	2	52.31	46.01	1	1	11	41.46	37.01	5	1	8	11.11	15.15	-3	1	1	64.24	-61.54	-7	1	7	40.28	35.96
6	0	6	51.38	52.86	-6	0	4	58.79	-67.18	1	1	12	19.87	19.65	5	1	9	34.89	-31.32	-3	1	2	20.20	-12.31	-7	1	9	21.72	-25.06
6	0	8	43.26	-36.93	-6	0	6	47.77	51.01	1	1	13	44.15	-40.68	5	1	10	9.70	-7.52	-3	1	3	10.13	9.89	-7	1	11	20.84	24.75
6	0	10	19.79	15.78	-6	0	8	20.60	-21.53	1	1	14	11.30	-7.59	5	1	11	21.85	23.51	-3	1	4	19.64	16.78	-7	1	12	14.03	-13.50
-7	1	13	30.85	-31.37	2	2	4	76.63	-78.28	7	2	0	23.71	-21.63	-4	2	1	8.51	13.11	-8	2	6	43.66	-41.19	2	3	9	15.54	16.96
-7	1	15	21.70	22.70	2	2	6	71.63	76.94	7	2	4	14.53	14.06	-4	2	2	36.64	-39.34	-8	2	7	10.14	11.09	2	3	10	12.55	13.68
-8	1	2	25.67	17.61	2	2	7	12.89	4.16	7	2	5	15.68	-16.80	-4	2	3	16.27	14.88	-8	2	8	32.93	32.72	2	3	11	10.93	-9.85
-8	1	3	18.17	20.33	2	2	8	64.39	-65.93	7	2	6	18.77	-17.90	-4	2	4	37.20	42.35	-8	2	10	18.32	-17.09	2	3	13	10.03	9.84
-8	1	4	16.82	22.88	2	2	9	10.60	-11.60	7	2	7	8.65	-9.92	-4	2	5	10.14	5.31	-8	2	12	20.60	19.47	2	3	14	8.24	-4.02
-8	1	9	19.52	-26.91	2	2	10	61.34	61.16	7	2	9	10.04	11.48	-4	2	6	65.58	-65.56	-8	2	13	11.70	-12.54	3	3	0	33.98	-30.32
-8	1	11	29.12	16.06	2	2	12	28.88	-26.47	8	2	0	32.34	33.92	-4	2	8	56.47	55.92	-8	2	14	15.68	-19.85	3	3	1	88.69	79.86
-8	1	13	18.47	-21.12	2	2	13	11.73	-13.27	8	2	2	36.62	-37.04	-4	2	9	11.04	15.15	-9	2	2	18.27	-20.00	3	3	3	75.90	-72.29
-9	1	1	17.45	20.30	2	2	14	26.22	26.15	8	2	4	15.40	14.91	-4	2	10	36.37	-39.41	-9	2	5	15.88	15.85	3	3	4	17.93	-16.73
-9	1	3	35.69	-36.74	3	2	0	55.67	-42.60	8	2	5	8.21	-10.84	-4	2	11	8.42	-13.18	-9	2	8	11.96	7.84	3	3	5	54.46	54.73
-9	1	5	42.13	42.40	3	2	1	15.27	6.08	8	2	6	20.74	-27.20	-4	2	12	20.07	16.69	-9	2	10	18.14	-21.01	3	3	6	21.18	-22.78
-9	1	7	22.73	-18.13	3	2	2	27.05	22.64	10	2	0	11.66	-12.81	-4	2	13	11.45	10.54	-9	2	11	9.34	10.27	3	3	7	49.79	-51.07
-9	1	9	15.93	14.75	3	2	3	31.72	-21.04	-1	2	2	78.61	18.80	-4	2	14	32.19	-32.49	-9	2	12	15.40	21.09	3	3	9	49.59	51.71
10	1	1	6.67	9.21	3	2	4	34.49	35.64	-1	2	3	101.35	-88.82	-4	2	16	26.80	28.40	-10	2	2	14.93	19.97	3	3	10	10.76	6.76
10	1	2	9.78	-12.41	3	2	5	19.73	16.43	-1	2	5	6.41	2.23	-4	2	17	4.46	-4.73	-10	2	4	27.73	-32.35	3	3	11	26.32	-25.46
10	1	3	14.13	-17.11	3	2	6	9.27	-8.68	-1	2	6	39.32	-41.08	-5	2	1	41.68	-32.36	-10	2	5	10.88	-11.07	3	3	13	19.35	16.61
10	1	6	12.02	11.59	3	2	11	25.64	-24.50	-1	2	7	54.60	52.95	-5	2	3	16.46	13.77	-10	2	6	22.23	22.45	3	3	14	10.26	13.47
10	1	7	12.53	-14.56	3	2	12	34.56	37.56	-1	2	9	21.04	-22.45	-5	2	4	47.82	37.42	-10	2	8	14.44	-17.21	4	3	0	26.21	21.30
10	1	9	10.12	15.89	3	2	14	26.74	-30.08	-1	2	10	28.03	-27.53	-5	2	5	21.04	13.35	0	3	1	9.26	15.23	4	3	1	6.47	5.04
0	2	0	72.32	81.30	3	2	15	14.22	16.25	-1	2	12	31.07	32.52	-5	2	6	21.44	-22.24	0	3	2	11.79	-16.72	4	3	2	24.65	-22.14
0	2	1	9.04	-2.90	4	2	0	97.29	102.45	-1	2	13	13.47	9.42	-5	2	8	34.84	31.64	0	3	3	13.32	-15.48	4	3	4	14.35	-12.69
0	2	2	83.83	-92.55	4	2	1	24.65	24.62	-1	2	14	15.95	-15.72	-5	2	10	33.09	-36.96	0	3	4	30.56	24.16	4	3	5	14.86	-11.74
0	2	4	45.52	55.77	4	2	2	84.47	-91.85	-1	2	16	24.92	16.71	-5	2	11	16.21	-15.96	0	3	5	35.63	-34.15	4	3	6	17.31	12.58
0	2	6	72.48	-74.04	4	2	3	14.15	-14.30	-1	2	17	6.95	7.89	-5	2	12	12.88	15.01	0	3	6	17.83	13.69	4	3	7	16.59	17.99
0	2	8	71.25	75.04	4	2	4	78.16	79.69	-2	2	1	14.75	5.67	-5	2	13	14.41	17.27	0	3	8	28.77	-28.55	4	3	8	8.23	9.49
0	2	9	50.03	40.06	4	2	5	9.64	-10.07	-2	2	2	15.96	24.75	-5	2	16	10.38	10.84	0	3	9	24.64	-27.92	4	3	9	9.50	-9.62
0	2	10	60.48	-63.79	4	2	6	47.65	-45.94	-2	2	3	13.66	-6.97	-6	2	1	21.10	-17.54	0	3	10	12.11	-11.18	4	3	11	11.58	9.48
0	2	11	17.26	15.17	4	2	8	53.69	52.79	-2	2	4	89.17	-83.74	-6	2	2	60.42	53.18	0	3	11	46.43	46.90	4	3	13	12.70	-19.32
0	2	12	52.96	49.26	4	2	9	11.26	8.68	-2	2	5	11.66	-14.66	-6	2	4	57.37	-61.18	0	3	12	13.44	16.01	5	3	0	14.30	-11.84
0	2	14	23.25	-23.34	4	2	10	29.26	-26.63	-2	2	6	77.13	80.49	-6	2	6	65.09	63.14	0	3	13	7.22	-3.42	5	3	1	52.45	-42.91
0	2	15	10.66	-9.32	4	2	12	22.16	22.29	-2	2	7	15.30	-16.10	-6	2	7	14.15	-12.10	1	3	0	15.16	17.49	5	3	2	7.44	3.80
0	2	16	23.00	24.61	4	2	14	25.66	-29.24	-2	2	8	60.11	-64.29	-6	2	8	26.89	-24.94	1	3	1	87.85	-84.13	5	3	3	64.53	62.56
1	2	1	16.07	-11.14	5	2	0	18.54	14.64	-2	2	9	29.82	-28.69	-6	2	10	28.01	31.07	1	3	2	12.61	-12.45	5	3	4	11.09	8.78
1	2	2	57.17	-45.51	5	2	1	9.32	-5.51	-2	2	10	29.85	31.54	-6	2	12	27.67	-29.58	1	3	3	70.89	59.13	5	3	5	36.75	-40.51
1	2	3	19.79	11.57	5	2	2	6.31	-5.01	-2	2	12	47.78	-52.67	-6	2	13	8.26	-7.28	1	3	4	20.17	16.60	5	3	6	9.55	10.88
1	2	4	34.02	-25.98	5	2	3	10.19	10.15	-2	2	13	14.84	10.54	-6	2	14	21.67	21.41	1	3	5	55.03	-53.57	5	3	7	32.73	33.06
1	2	5	51.18	39.95	5	2	4	7.08	2.68	-2	2	14	44.15	44.00	-6	2	15	13.71	14.03	1	3	6	24.33	-20.04	5	3	8	14.93	18.54
1	2	6	44.30	38.87	5	2	5	23.47	20.32	-2	2	16	25.66	-27.10	-6	2	16	12.48	-15.81	1	3	7	76.49	72.61	5	3	9	26.64	-27.30
1	2	7	11.84	-11.82	5	2	6	25.23	26.84	-3	2	1	54.18	37.45	-7	2	4	18.29	12.52	1	3	9	60.65	-61.33	5	3	11	22.76	25.32
1	2	8	9.20	-4.36	5	2	7	21.67	-20.78	-3	2	2	36.23	22.53	-7	2	6	16.77	11.49	1	3	11	56.10	51.80	5	3	12	10.74	14.65
1	2	10	14.22	13.43	5	2	8	14.97	-15.84	-3	2	3	54.98	41.54	-7	2	7	16.77	-8.73	1	3	13	26.92	-25.42	6	3	0	7.72	5.62
1	2	11	30.13	27.09	5	2	10	9.55	7.77	-3	2	4	9.83	-4.68	-7	2	8	35.03	-35.00	1	3	14	8.47	-10.79	6	3	1	12.76	-12.10
1	2	12	13.56	-14.24	5	2	11	7.18	5.99	-3	2	5	62.91	-57.37	-7	2	10	39.42	44.88	1	3	15	26.26	27.52	6	3	2	12.92	-15.27
1	2	13	23.94	-22.47	5	2	12	16.08	-19.35	-3	2	6	9.64	-5.70	-7	2	12	15.87	-15.88	2	3	0	8.25	-12.34	6	3	3	12.41	10.52
1	2	14	22.06	20.63	6	2	0	52.98	-46.17	-3	2	7	17.14	-8.22	-7	2	13	11.82	-10.76	2	3	1	46.29	-33.59	6	3	4	24.68	22.92
1	2	16	14.27	-15.91	6	2	2	69.61	73.79	-3	2	8	34.64	-36.27	-7	2	14	10.30	9.24	2	3	2	16.91	12.76	6	3	5	26.00	28.76
2	2	0	77.23	-75.49	6	2	4	48.51	-50.26	-3	2	10	26.12	26.85	-8	2	2	29.41	-30.00	2	3	4	24.49	-20.55	6	3	6	7.34	8.91
2	2	1	15.63	-11.85	6	2	6	18.26	15.41	-3	2	12	18.70	-19.44	-8	2	3	20.85	-18.53	2	3	5	41.54	33.36	6	3	7	14.66	-14.62
2	2	2	100.99	99.81	6	2	8	22.82	-20.85	-3	2	15	14.45	-14.29	-8	2	4	37.55	37.53	2	3	6	23.71	-20.54	6	3	9	7.76	-9.65
2	2	3	46.22	34.97	6	2	10	25.35	29.94	-3	2	16	29.70	-32.13	-8	2	5	14.66	11.09	2	3	8	7.59	-10.72	7	3	1	46.56	47.97

TABLE 3. Continued

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	3	2	18.63	25.46	-3	3	13	23.98	-21.71	-7	3	13	20.93	-22.95	3	4	8	20.64	-21.35	-2	4	9	20.65	18.71	-7	4	1	14.60	-15.81
7	3	3	47.96	-51.14	-3	3	14	10.14	-7.86	-7	3	14	5.77	-4.74	3	4	10	10.20	-13.83	-2	4	10	29.67	34.64	-7	4	6	12.11	12.85
7	3	4	10.09	-12.13	-3	3	15	40.96	44.27	-8	3	1	10.20	-7.16	3	4	12	14.69	16.70	-2	4	11	17.65	-18.05	-7	4	8	20.36	-17.56
7	3	5	23.36	24.99	-4	3	1	30.53	-21.14	-8	3	4	7.31	8.37	4	4	0	50.05	46.39	-2	4	12	25.48	-24.40	-7	4	10	15.48	15.15
7	3	7	23.34	-28.31	-4	3	2	29.59	18.01	-8	3	7	13.97	15.78	4	4	1	8.24	7.37	-2	4	13	15.50	-20.11	-7	4	11	8.90	-11.38
7	3	8	4.53	-5.23	-4	3	3	44.38	39.83	-8	3	9	22.27	-25.25	4	4	2	64.14	-66.73	-2	4	14	22.12	23.97	-7	4	12	12.23	-14.46
8	3	0	7.08	-6.52	-4	3	4	25.43	17.10	-8	3	11	26.57	29.70	4	4	4	29.29	29.87	-2	4	15	10.70	12.79	-8	4	1	20.95	5.43
8	3	1	6.88	6.18	-4	3	5	15.69	-16.90	-8	3	12	7.35	-7.51	4	4	6	41.09	-41.75	-3	4	1	8.88	-2.93	-8	4	2	12.63	-23.77
8	3	2	6.61	3.77	-4	3	6	15.54	21.14	-9	3	1	19.30	25.26	4	4	8	21.99	20.77	-3	4	3	6.48	-1.32	-8	4	3	26.36	13.87
8	3	5	8.05	-4.02	-4	3	7	13.76	-6.75	-9	3	3	20.99	-27.89	4	4	10	25.60	-26.31	-3	4	4	21.48	-19.22	-8	4	6	18.46	-14.89
8	3	6	4.14	-3.36	-4	3	8	10.10	10.82	-9	3	5	20.81	18.96	4	4	11	8.50	-10.75	-3	4	5	26.10	23.13	-8	4	7	10.85	-14.00
9	3	0	5.56	11.60	-4	3	9	14.13	-16.46	-9	3	7	21.14	-20.68	4	4	12	5.20	26.76	-3	4	6	17.38	19.38	-8	4	8	18.65	15.92
9	3	1	25.51	-29.41	-4	3	10	12.36	-11.02	-9	3	9	15.45	19.74	5	4	0	8.24	-8.23	-3	4	9	21.18	-22.77	-8	4	10	21.13	-17.89
9	3	2	4.71	-4.96	-4	3	11	30.22	31.98	0	4	0	63.60	65.74	5	4	1	8.31	7.13	-3	4	10	45.58	47.09	-9	4	2	7.22	-10.70
9	3	3	23.17	28.94	-4	3	12	18.78	21.21	0	4	1	11.06	-7.67	5	4	2	21.53	-19.24	-3	4	11	13.85	8.43	-9	4	4	8.88	12.95
-1	3	1	82.00	83.74	-4	3	13	13.64	-13.20	0	4	2	59.87	-68.21	5	4	7	11.73	13.95	-3	4	12	19.09	-21.23	-9	4	6	6.87	-10.05
-1	3	3	77.82	-75.87	-4	3	15	13.11	14.31	0	4	3	15.82	-13.21	5	4	9	9.50	8.21	-3	4	14	12.88	17.36	-9	4	7	5.37	-7.27
-1	3	5	34.57	41.55	-4	3	16	6.70	-2.74	0	4	4	48.66	49.22	5	4	10	12.33	17.40	-4	4	1	10.16	10.28	0	5	2	18.01	-17.17
-1	3	6	14.16	9.35	-5	3	1	40.39	33.01	0	4	5	13.14	20.73	6	4	0	31.11	-25.39	-4	4	2	49.14	-45.45	0	5	3	20.22	16.34
-1	3	7	58.64	-57.84	-5	3	2	8.47	-2.87	0	4	6	41.42	-43.01	6	4	2	43.84	42.73	-4	4	4	48.50	45.77	0	5	5	12.80	-11.68
-1	3	8	23.86	-19.41	-5	3	3	61.00	-66.12	0	4	7	12.23	-12.06	6	4	3	21.10	25.67	-4	4	5	35.38	33.46	0	5	10	10.59	11.59
-1	3	9	39.37	39.60	-5	3	4	12.38	-12.10	0	4	8	56.93	61.67	6	4	4	38.08	-40.11	-4	4	6	65.09	-66.74	0	5	11	23.14	23.65
-1	3	10	10.87	-13.10	-5	3	5	62.17	66.10	0	4	10	44.82	-46.87	6	4	5	7.41	-12.64	-4	4	7	30.96	-30.60	1	5	1	51.90	-44.91
-1	3	11	47.74	-46.30	-5	3	6	16.71	12.40	0	4	11	11.49	-9.64	6	4	6	22.55	24.97	-4	4	8	58.52	59.32	1	5	2	13.57	-12.45
-1	3	13	45.22	45.97	-5	3	7	49.11	-51.14	0	4	12	23.67	21.90	6	4	7	8.79	9.54	-4	4	9	8.22	8.60	1	5	3	51.31	46.07
-1	3	15	35.00	-38.31	-5	3	9	44.24	49.34	0	4	13	15.63	16.08	6	4	8	17.38	-20.59	-4	4	10	23.74	-23.63	1	5	4	30.47	27.27
-1	3	16	4.37	-5.33	-5	3	10	24.46	27.19	0	4	14	29.14	-32.68	7	4	0	15.41	-14.70	-4	4	11	17.24	17.84	1	5	5	52.89	-51.30
-2	3	1	19.26	17.89	-5	3	11	28.83	-32.27	1	4	0	9.58	-10.32	7	4	2	14.59	16.13	-4	4	12	20.78	24.73	1	5	6	29.94	-30.34
-2	3	2	12.93	11.38	-5	3	14	8.80	8.41	1	4	1	7.13	6.62	7	4	5	8.32	8.41	-4	4	14	9.03	-11.28	1	5	7	45.24	47.16
-2	3	3	17.69	10.61	-5	3	15	13.70	-15.73	1	4	2	20.36	17.68	8	4	0	22.22	26.18	-4	4	15	6.78	-9.19	1	5	8	21.67	25.41
-2	3	4	28.42	-27.79	-6	3	1	7.69	-4.97	1	4	3	7.80	-4.30	8	4	1	17.26	28.00	-5	4	1	7.98	6.15	1	5	9	28.74	-27.67
-2	3	5	9.50	2.35	-6	3	2	17.75	-14.82	1	4	4	13.85	-8.67	8	4	2	30.70	-40.86	-5	4	4	9.90	8.08	1	5	11	28.00	32.07
-2	3	6	17.58	10.69	-6	3	3	10.18	-6.43	1	4	6	25.95	21.64	8	4	3	15.98	-20.28	-5	4	6	30.70	-25.08	2	5	3	12.46	-10.00
-2	3	8	12.06	-5.28	-6	3	4	9.13	-7.20	1	4	10	17.17	13.03	8	4	4	27.23	32.67	-5	4	7	20.51	15.00	2	5	4	12.41	15.42
-2	3	9	17.02	19.38	-6	3	5	35.05	35.07	1	4	12	15.55	-12.28	-1	4	2	11.95	-13.09	-5	4	10	22.39	-24.85	2	5	5	21.24	17.81
-2	3	10	7.69	-4.43	-6	3	6	11.57	-8.68	2	4	0	63.42	-50.91	-1	4	3	11.07	5.74	-5	4	12	22.53	24.02	2	5	11	14.62	-16.96
-2	3	11	46.35	-49.94	-6	3	7	24.11	-25.18	2	4	1	44.56	-35.82	-1	4	4	36.08	34.46	-5	4	13	7.27	5.09	3	5	0	24.21	-26.93
-2	3	12	12.98	-12.67	-6	3	8	15.20	11.53	2	4	2	87.59	81.65	-1	4	6	10.94	-8.29	-5	4	14	4.80	-6.53	3	5	1	50.88	50.72
-2	3	13	22.03	24.94	-6	3	9	22.08	22.48	2	4	3	30.50	27.18	-1	4	7	17.69	-15.30	-6	4	1	21.35	22.86	3	5	2	48.56	42.28
-2	3	14	13.84	-12.45	-6	3	11	18.16	-20.26	2	4	4	52.15	-51.80	-1	4	8	11.14	10.95	-6	4	2	25.95	22.99	3	5	3	68.86	-65.38
-2	3	15	14.71	-14.00	-6	3	14	12.03	11.31	2	4	5	15.90	-13.69	-1	4	10	36.16	-38.57	-6	4	3	15.50	-15.91	3	5	5	34.69	31.93
-3	3	1	69.16	-62.72	-6	3	15	8.94	-12.14	2	4	6	51.19	51.92	-1	4	12	23.25	23.10	-6	4	4	39.95	-36.36	3	5	7	27.92	-26.19
-3	3	3	68.47	70.50	-7	3	1	13.53	-7.68	2	4	8	55.16	-53.55	-2	4	1	7.19	4.48	-6	4	5	20.27	-18.55	3	5	9	26.06	26.70
-3	3	4	28.48	19.70	-7	3	3	25.95	24.33	2	4	10	24.97	23.37	-2	4	2	71.72	63.64	-6	4	6	34.30	29.23	3	5	11	24.94	-35.32
-3	3	5	71.21	-66.08	-7	3	5	47.74	-46.71	2	4	12	25.48	-26.95	-2	4	3	9.72	-4.04	-6	4	7	23.49	23.68	4	5	1	18.46	-18.47
-3	3	6	12.90	-11.06	-7	3	6	10.98	-11.35	2	4	13	11.05	-12.20	-2	4	4	68.95	-60.19	-6	4	8	47.09	-44.67	4	5	6	7.95	-5.75
-3	3	7	64.03	68.62	-7	3	7	43.07	42.95	3	4	1	11.42	-7.22	-2	4	5	33.82	-30.07	-6	4	9	10.84	-5.72	4	5	7	16.42	-15.92
-3	3	8	28.88	29.07	-7	3	8	7.55	-3.60	3	4	3	10.24	-6.47	-2	4	6	61.03	63.09	-6	4	10	27.96	27.74	5	5	0	11.71	13.16
-3	3	9	38.01	-37.32	-7	3	9	24.33	-24.06	3	4	4	12.98	12.95	-2	4	7	13.60	16.52	-6	4	11	6.75	1.36	5	5	1	57.38	-58.90
-3	3	12	16.46	-17.84	-7	3	11	31.53	31.76	3	4	6	16.07	-17.68	-2	4	8	35.69	-31.56	-6	4	12	28.67	-29.47	5	5	2	8.01	-9.09

5	5	3	39.04	36.91	-5	5	12	6.17	-7.96	-2	6	9	8.95	-11.02
5	5	5	19.76	-18.11	-6	5	2	12.18	12.24	-2	6	10	14.89	11.61
5	5	7	18.69	24.23	-6	5	3	7.71	-12.09	-3	6	1	11.91	-10.08
5	5	8	4.28	-5.19	-6	5	7	9.98	-7.07	-3	6	2	26.58	29.86
6	5	0	10.67	7.12	-6	5	8	10.54	-10.79	-3	6	4	25.86	-26.66
6	5	1	7.36	-6.61	-6	5	9	13.88	14.53	-4	6	1	12.21	11.20
6	5	3	16.89	20.42	-6	5	11	17.05	-18.87	-4	6	2	22.87	-21.79
6	5	4	6.22	-7.89	0	6	0	56.45	51.97	-4	6	3	14.85	-16.99
6	5	6	7.06	8.36	0	6	1	13.39	18.38	-4	6	4	30.35	28.84
-1	5	1	65.25	59.99	0	6	2	44.04	-44.98	-4	6	6	38.21	-42.35
-1	5	2	23.46	-23.72	0	6	3	13.08	15.01	-4	6	8	28.39	33.02
-1	5	3	47.06	-44.28	0	6	4	22.16	18.12	-4	6	10	10.89	-17.78
-1	5	5	41.09	40.76	0	6	6	33.25	-33.15	-5	6	3	10.08	-12.19
-1	5	6	19.15	20.20	0	6	7	27.15	-30.36	-5	6	4	17.54	18.25
-1	5	7	51.16	-46.98	0	6	8	28.62	27.39	-5	6	5	9.53	-5.90
-1	5	9	27.70	29.40	0	6	9	15.34	15.45	-5	6	6	11.04	-12.88
-1	5	10	16.33	15.12	0	6	10	23.22	-26.71	-5	6	8	7.10	8.83
-1	5	11	23.34	-25.68	2	6	0	44.02	-44.23	-6	6	2	19.77	23.04
-1	5	12	8.97	-10.46	2	6	1	12.60	-12.14	-6	6	3	9.82	12.89
-1	5	13	20.39	24.43	2	6	2	39.26	36.40	-6	6	4	15.51	-14.90
-2	5	1	12.42	11.10	2	6	3	20.99	15.59	-6	6	5	12.28	-14.66
-2	5	5	37.35	35.91	2	6	4	30.96	-25.67	-6	6	6	23.99	25.19
-2	5	11	19.27	-19.29	2	6	5	15.73	-14.05	0	7	1	10.03	-11.77
-2	5	13	17.18	20.92	2	6	6	35.97	37.50	0	7	2	9.80	-7.98
-3	5	1	34.87	-29.02	2	6	7	16.30	11.22	0	7	5	10.94	10.11
-3	5	3	49.45	46.11	2	6	8	31.26	-30.58	1	7	0	21.07	22.76
-3	5	5	49.88	-47.59	3	6	1	11.69	9.74	1	7	1	39.80	-37.25
-3	5	6	26.63	-22.93	3	6	4	18.25	20.32	1	7	2	17.37	-18.72
-3	5	7	59.65	59.11	4	6	0	38.49	38.12	1	7	3	25.05	23.29
-3	5	9	26.54	-25.35	4	6	1	18.70	20.95	1	7	4	8.61	-9.75
-3	5	10	10.12	7.80	4	6	2	35.07	-33.76	1	7	5	21.74	-28.78
-3	5	11	18.35	24.78	4	6	3	7.69	-7.69	2	7	2	8.33	-9.35
-3	5	12	7.92	8.95	4	6	4	29.36	27.61	3	7	0	14.98	-11.96
-3	5	13	13.53	-17.23	4	6	6	23.00	-30.47	3	7	1	37.44	38.50
-4	5	4	9.24	-11.20	5	6	0	9.87	-10.05	-1	7	1	30.85	26.23
-4	5	5	12.96	-10.92	5	6	1	6.72	-8.39	-1	7	2	23.09	26.37
-4	5	7	21.62	22.50	5	6	2	8.98	12.83	-1	7	3	28.14	-24.63
-4	5	9	16.17	-18.29	5	6	3	9.17	-9.00	-1	7	5	23.79	23.12
-4	5	10	13.00	-17.10	6	6	0	27.87	-32.92	-2	7	1	12.82	14.54
-4	5	11	20.33	20.53	6	6	1	7.87	-11.69	-2	7	3	25.90	-30.58
-4	5	13	8.17	-10.73	6	6	2	25.87	33.85	-3	7	1	26.52	-32.03
-5	5	1	20.92	18.45	-1	6	2	24.39	-25.62	-3	7	3	12.62	16.42
-5	5	3	23.59	-23.94	-1	6	8	15.62	-15.52	-3	7	5	23.33	-28.94
-5	5	5	30.18	27.99	-1	6	10	16.20	-17.19					
-5	5	6	17.21	16.02	-2	6	1	22.05	-22.60					
-5	5	7	41.36	-45.39	-2	6	2	42.05	41.55					
-5	5	8	11.79	-11.57	-2	6	4	40.85	-38.85					
-5	5	9	29.90	31.61	-2	6	6	34.51	33.41					
-5	5	10	9.07	-8.63	-2	6	7	15.37	14.64					
-5	5	11	23.41	-27.30	-2	6	8	26.57	-26.13					

Table 4 (a). Interatomic distances (Å)
(Standard deviations in parentheses)

Co-C(1)=2.08(2)	C(3)-C(4)=1.58(4)
Co-C(2)=2.03(2)	C(4)-C(5)=1.57(3)
Co-C(3)=2.06(2)	C(5)-C(6)=1.54(4)
Co-C(9)=2.02(2)	C(6)-C(7)=1.49(3)
Co-C(12)=2.09(2)	C(7)-C(8)=1.55(3)
Co-C(13)=2.06(2)	C(8)-C(1)=1.52(3)
Co-C(16)=2.04(2)	C(9)-C(10)=1.59(3)
	C(10)-C(11)=1.47(4)
Co-C(4)=2.90(3)	C(11)-C(12)=1.53(4)
Co-C(8)=2.79(2)	C(13)-C(14)=1.59(3)
	C(14)-C(15)=1.51(4)
C(1)-C(2)=1.46(3)	C(15)-C(16)=1.55(3)
C(2)-C(3)=1.35(3)	
C(9)-C(16)=1.39(3)	
C(12)-C(13)=1.41(3)	
C(4)···C(8)=3.09(4)	
C(9)···C(12)=3.89(4)	
C(13)··C(16)=2.84(3)	
C(2)···C(6)=3.06(3)	
C(10)··C(15)=3.17(4)	
C(11)··C(14)=3.12(4)	

Table 4 (b). Bond angles (°).
(Standard deviations in parentheses)

C(1)-Co-C(2)=41.4 (0.8)
C(2)-Co-C(3)=38.6 (0.9)
C(1)-Co-C(3)=72.2 (0.8)
C(9)-Co-C(12)=86.9 (1.0)
C(16)-Co-C(13)=87.5 (0.9)
C(1)-C(2)-C(3)=120.8 (1.9)
C(2)-C(3)-C(4)=129.1 (2.0)
C(8)-C(1)-C(2)=125.8 (1.9)
C(10)-C(9)-C(16)=122.1 (1.9)
C(9)-C(16)-C(15)=127.4 (1.9)
C(11)-C(12)-C(13)=126.2 (2.1)
C(12)-C(13)-C(14)=120.3 (2.1)
C(3)-C(4)-C(5)=112.2 (1.9)
C(4)-C(5)-C(6)=115.4 (2.0)
C(5)-C(6)-C(7)=118.1 (1.7)
C(6)-C(7)-C(8)=119.4 (1.8)
C(7)-C(8)-C(1)=114.4 (1.6)
C(9)-C(10)-C(11)=114.7 (2.0)
C(10)-C(11)-C(12)=114.8 (1.6)
C(13)-C(14)-C(15)=114.5 (1.7)
C(14)-C(15)-C(16)=112.5 (1.8)

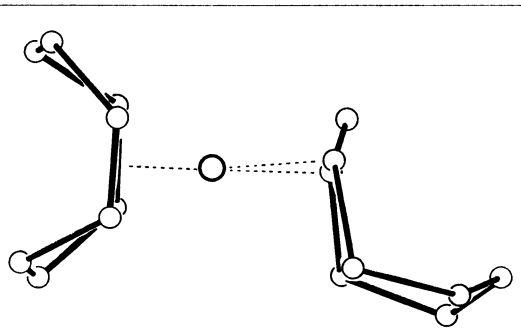

Fig. 2. The molecule viewed along a direction parallel to the Co-plane.

Table 5. Some least-squares planes within the molecule, with deviations (Å) of the atoms from the plane

a) Co-plane
$0.6827X-0.7107Y-0.3320Z=0.2488$
distance from this plane

center of C(9)-C(16)	−0.06 Å
center of C(12)-C(13)	0.06
C(1)	0.07
C(3)	−0.07
Co	0.08

b) Plane C(1)-C(3)-C(4)-C(8)
$0.5097X+0.0510Y+0.7078Z=2.9196$
distance from this plane

C(1)	−0.02 Å
C(3)	0.02
C(4)	−0.02
C(8)	0.02

c) Plane C(9)-C(12)-C(13)-C(16)
$0.3342X+0.1751Y+0.8159Z=5.9179$
distance from this plane

C(9)	0.02 Å
C(12)	−0.02
C(13)	0.02
C(16)	−0.02

In the above equations, X, Y, and Z are the rectangular coordinates in Å unit, where $X=x+z\cos\beta$, $Y=y$, $Z=z\sin\beta$.

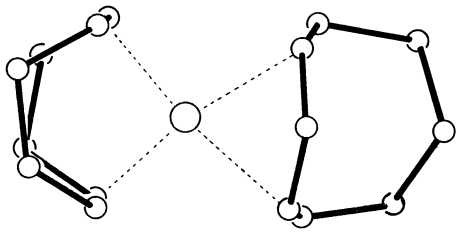

Fig. 3. The molecule viewed along the direction normal to the Co-plane.

to the Co-plane respectively. The planar configuration of the cobalt atom with the allyl part of the cyclooctenyl ligand (C(1)-C(2)-C(3)) and the two double bond centers of the cycloocta-1,5-diene ligand is clearly shown in Figs. 2 and 3. The formal oxidation state of the cobalt atom is suggested to be +1 by the reaction absorbing carbon monoxide to give a carbonyl complex, $Co(CO)(C_8H_{13})(C_8H_{12})$, from which hydridocarbonylphosphine complexes, $CoH(CO)L_3$ ($L=PPh_3$ or $PMePh_2$), are derived.[3] Thus the cobalt atom attains an outer configuration of sixteen electrons by forming the complex with the two ligands. In this case, the allyl part in the octenyl ligand acts as a four-electron bidentate donor.

The two carbon-carbon bond lengths in the allyl part differ somewhat; C(1)-C(2)=1.46 Å and C(2)-C(3)=1.35 Å. On the other hand, the three interatomic distances between the cobalt and the three carbon atoms, C(1), C(2), and C(3), are 2.08 Å, 2.03 Å, and 2.06 Å, respectively. Taking the standard deviations into con-

3) S. Otsuka and M. Rossi, *J. Chem. Soc., A*, **1969**, 497.

sideration, the bonding of the allyl group to the cobalt atom is probably symmetrical. In the NMR spectrum of this complex too, signals of the symmetrical π-allyl group have been found.[1]

The average bond length of the two double bonds, C(9)–C(16) and C(12)–C(13), is 1.40 Å, giving the bond order of 1.5.[4] The remaining twelve C–C interatomic distances in the two ligands are found to be in the range 1.47 Å to 1.59 Å. These are comparable to the reported values of the single bond length in several complexes of this type.[5,6] Some of the bond angles are found definitely larger either than 109.5° for sp^3 or than 120° for sp^2 (Table 4 (a) and (b)).

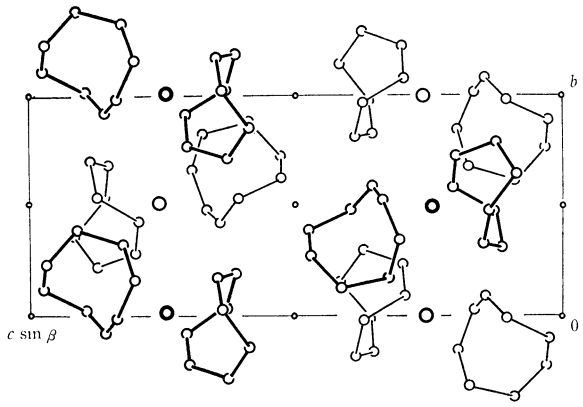

Fig. 4. The crystal structure viewed along the *a* axis.

Atoms C(9), C(12), C(13), and C(16) deviate by only 0.02 Å from a least-squares plane, and atoms C(1), C(3), C(4), and C(8) also approach planarity. The dihedral angles between the Co-plane and plane C(9)–C(12)–C(13)–C(16), plane C(1)–C(3)–C(4)–C(8) and plane C(1)–C(2)–C(3) are 93°, 100°, and 108°, respectively. The equations of these planes and deviations of the respective carbon atoms from the planes are summarized in Table 5.

The cyclooctenyl ring is of the tub form. The two parts of the ligand, C(8)–C(1)–C(2)–C(3) and C(1)–C(2)–C(3)–C(4), deviate from the planar *cis*-conformation. The angles of twist around the two bonds, C(1)–C(2) and C(2)–C(3), are 32° and 38°, respectively. The cycloocta-1,5-diene ring is of the boat form. The conformation of C(9)–C(10)–C(11)–C(12) is incompletely eclipsed; the C(11)–C(12) and C(9)–C(10) groups are skewed around the C(11)–C(12) bond, the dihedral angle between the C(9)–C(10)–C(11) and C(10)–C(11)–C(12) planes being 22°. This twisting probably arises from the repulsion between hydrogen atoms attached to the carbon atoms concerned. The conformation of C(13)–C(14)–C(15)–C(16) is similar to that of C(9)–C(10)–C(11)–C(12). Here, the dihedral angle is 27°.

Positions of the hydrogen atoms attached to all the sixteen carbon atoms were calculated based upon a C–H distance of 1.08 Å and H–C–H bond angles of 120° for sp^2 and 109.5° for sp^3. No abnormally short interatomic distances between Co and H have been found. However, there are two short interatomic distances between hydrogen atoms: H(3)···H(12) and H(4)···H(8) are 1.73 Å and 1.87 Å, respectively, which are comparable to those reported for $Ni(C_8H_{12})_2$.[5]

The arrangement of molecules in the crystal viewed along the *a* and *b* axes is shown in Figs. 4 and 5. The crystal contains discrete molecular units of π-cyclooctenyl-π-cycloocta-1,5-dienecobalt, separated by normal van der Waals distances. The shortest C···C intermolecular distances are 3.84 Å for sp^3–sp^3 and 3.66 Å for sp^2–sp^3.

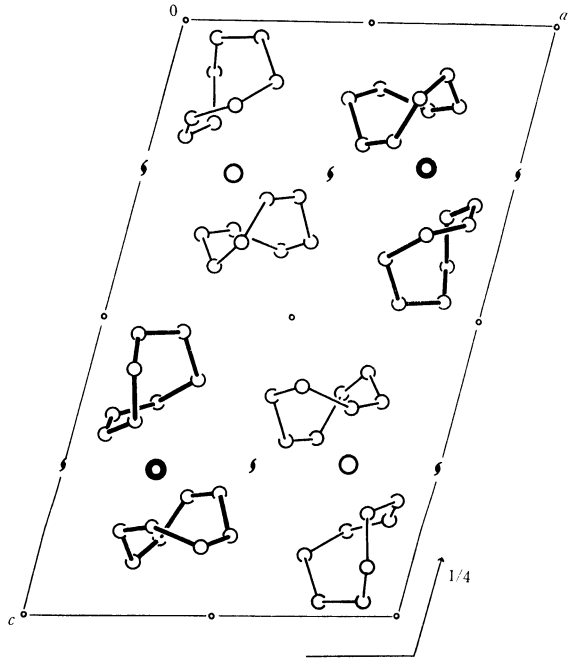

Fig. 5. The crystal structure viewed along the *b* axis.

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4) L. Pauling, "The Nature of the Chemical Bond" 3rd Edition, Cornell University Press, New York (1960), p. 236.

5) H. Dierks and H. Dietrich, *Z. Krist.*, **122**, 1 (1965).

6) J. Coetzer and G. Gafner, *Acta Crystallogr.*, **B26**, 985 (1970).