AD-A050 502 CALIFORNIA UNIV LOS ANGELES DEPT OF CHEMISTRY F/G 7/2
STRUCTURES OF METALLOCARBORANES. IX. CRYSTAL AND MOLECULAR STRU--ETC(U)
JAN 78 G E HARDY, K P CALLAHAN, M F HAWTHORNE N00014-76-C-0390
UNCLASSIFIED TR-100 NL

1 OF 2
AD A050502

END
DATE FILMED
4 -78
DDC

CONT.

OFFICE OF NAVAL RESEARCH

Contract No. N00014-76-C-0390

Task No. NR 053-608

TECHNICAL REPORT NO. 100

TR-100, CONTRIB-3915

Structures of Metallocarboranes. IX. Crystal and Molecular Structure of the Ten-Vertex Heterobimetallocarborane 2,3-Di-η-cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8), 2,3-$(\eta$-$C_5H_5)_2$-(2,3)-NiCo-10-CB_7H_8.

By

G. E. Hardy, K. P. Callahan, M. F. Hawthorne*

Prepared for Publication
in
Inorganic Chemistry

18 Jan 78

29 P.

N00014-76-C-0390

Department of Chemistry
University of California
Los Angeles, California 90024

January 18, 1978

†Present address: Brown University, Chemistry Department, Providence, R.I. 02912

[Contribution No. 3915 from the Department of Chemistry,
University of California, Los Angeles, California 90024]

Structures of Metallocarboranes. IX.

Crystal and Molecular Structure of the Ten-Vertex Heterobimetallocarborane 2,3-Di-η-cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8), $2,3\text{-}(\eta\text{-}C_5H_5)_2\text{-}(2,3)\text{-}NiCo\text{-}10\text{-}CB_7H_8$[1]

By

G. E. Hardy, K. P. Callahan[†], and M. F. Hawthorne*

Department of Chemistry
University of California
Los Angeles, California 90024

[†]Present address: Brown University, Chemistry Department, Providence, R.I. 02912

ABSTRACT

A complete three dimensional crystal structure determination of the title compound was carried out. Crystal data: Space group C2/c, $\underline{a}$ = 15.794(4), $\underline{b}$ = 7.955(2), $\underline{c}$ = 24.273(7) Å, $\underline{\beta}$ = 104.12(2)°, $\underline{z}$ = 8, d_o = 1.55(2), d_c = 1.54. Diffraction data to $2\theta_{max} = 50^{o}$ were obtained with a Syntex $P\bar{1}$ automated diffractometer (MoK_{α} radiation) and the structure was solved by conventional Patterson, Fourier and full matrix least-squares techniques to a conventional R = 0.047 for 2048 independent non-zero reflections. The molecule has the bicapped square antiprismal geometry expected for a closo ten-vertex polyhedron. The two metal atoms are indistinguishable and occupy adjacent sites in the same equatorial belt. The carbon atom resides in the four-coordinate site non-adjacent to the two metal atoms.

INTRODUCTION

Polyhedral expansion of the monocarbacobaltacarborane anion[2,3] $[C_5H_5Co-CB_7H_8]^-$ with $NiBr_2$·2 glyme in the presence of $C_5H_5^-$ affords several neutral isomeric complexes of the formula $(C_5H_5)_2NiCoCB_7H_8$ which contain formal Ni(IV) and Co(III) vertices,[4,5] and which are isoelectronic with $(C_5H_5)_2Co_2C_2B_6H_8$. The structure of one isomer of the latter has previously been reported;[6a] the mixed cobalt-nickel compounds exist in more numerous isomeric forms. An x-ray structural investigation of one isomer of this complex is reported herein.

UNIT CELL AND SPACE GROUP

A sample of the compound was furnished by Dr. C. G. Salentine. It was found to be stable to both air and x-rays. Preliminary x-ray diffraction photographs of the black crystals indicated monoclinic symmetry with systematic absences indicative of space groups C2/c or Cc. The density, measured by flotation, was 1.55(2) g cm^{-3}, in good agreement with the calculated density of 1.54(z = 8).

COLLECTION AND REFINEMENT OF X-RAY DATA

Intensity data were collected on a Syntex $P\bar{1}$ automated diffractometer equipped with scintillation counter and pulse height analyzer. A graphite crystal was used to produce monochromatic MoK_α radiation (λ = 0.71069 Å). Fifteen automatically centered reflections were used in the determination of the lattice parameters; a = 15.794(4)Å, b = 7.955(2)Å, c = 24.273(7)Å, β = 104.12(2)°. Intensity data were collected on a small crystal of irregular shape (average diameter about 0.1 mm) with a θ-2θ scan technique to a limit of 2θ = 50°. Reflections were scanned at a constant rate of 2.0°/min from 1° below the

$K_{\alpha 1}$ reflection to 1.0^{o} above the $K_{\alpha 2}$ reflection. Background was measured at each end of the scan. The total time counting background was equal to the scan time for each reflection. The intensities of three standard reflections were measured after every 97 reflections. No significant change in the intensities of these reflections was observed in the course of the data collection.

The reflections were corrected for Lorentz and polarization effects. The intensity of a reflection, $\underline{I}(\underline{hkl})$, and $\sigma[\underline{I}(\underline{hkl})]$, its estimated standard deviation, were calculated according to the equations $\underline{I} = CT - (t_c/t_b)(B1+B2)/2$ and $\sigma = \{\sigma_s^2 + [(0.041)^2]\}^{1/2}$, where $\underline{I}$ is the net integrated intensity, CT is the total integrated count, t_c and t_b are the times employed for counting the scan and background, respectively, B1 and B2 are the background counts on the low and high sides of the reflection, and σ_s is the standard deviation in the intensity due to counting statistics. Reflections having intensities less than three times their standard deviations were defined as unobserved and not included in subsequent calculations. Because of the small and irregular shape of the crystal, no absorption correction was applied.

SOLUTION AND REFINEMENT OF THE STRUCTURE

The coordinates of the two metal atoms were determined by the solution of a three-dimensional Patterson map, and a Fourier map based on these positions revealed the positions of all the non-hydrogen cage atoms. Successive Fourier maps were used to identify the positions of the cyclopentadienyl carbon atoms. Full matrix least-squares refinement of these parameters was followed by a Fourier difference map in which all the cage hydrogen atoms except H9 were located. Idealized positions for the cyclopentadienyl hydrogen atoms and for H9 were calculated, and the position of all hydrogen atoms were refined in subsequent least-squares cycles. The position of the carbon atom was identified by short bond distances to its neighbors and its small temperature factor when

refined as a boron atom. No distinction could be made between the two metal sites and therefore they were both assigned scattering factors which corresponded to the average of the nickel and cobalt scattering factors. In the final refinement, the positions of all atoms and anisotropic thermal parameters for all non-hydrogen atoms were refined. The temperature factors for the hydrogen atoms were set at 2.0. This refinement converged to R = 4.7%.

The programs used in this structure determination, the scattering factors and the refinement techniques, were the same as those used in the preceding paper.[1]

The final observed atomic fractional coordinates are collected in Table I. Anisotropic thermal parameters are presented in Table II. The final observed calculated structure factors are available.[7]

THE MOLECULAR STRUCTURE AND DISCUSSION

Intramolecular distances and their estimated standard deviations (esd's) are listed in Table IIIa. Average bond distances, with their root-mean-square deviations, are collected in Table IIIb. The individual bond angles and their associated esd's are presented in Table IV. The structure of $(C_5H_5)_2NiCoCB_7H_8$ is shown in Figure 1, which also illustrates the numbering system employed.[8]

The structure of the complex may be described as a distorted bicapped square antiprism, a 10-vertex closed polyhedron comprised of seven boron, one carbon, one cobalt, and one nickel atom vertices. The carbon and boron atoms are further bonded to terminal hydrogen atoms, while the metal vertices are attached to η-cyclopentadienyl ligands. The metals occupy adjacent equatorial positions on the polyhedral framework, 2.4492(11)Å apart, while the apical positions are occupied by one boron atom and the carbon atom. The metals reside in the same equatorial belt, the belt closest to the apical boron atom and furthest removed from the apical carbon atom. The positions occupied by the metals are totally equivalent in the polyhedron, and there is consequent

random orientation of the two metals such that specification of the unique positions of the cobalt or nickel vertices is impossible. Instead, an averaged "half-nickel, half-cobalt" atom is seen at those two sites. The polyhedron exhibits mirror symmetry; the mirror plane, which includes atoms B1, B6, B8 and C10, is not crystallographically required but related bond distances are equal within three standard deviations.

This compound is a close analog of the bimetallocarborane $(C_5H_5)_2Co_2C_2B_6H_8$, whose structure has been previously reported.[6] This latter species has the same overall geometry, with the two cobalt atoms occupying different equatorial belts, (still in adjacent polyhedral positions at a distance of 2.489(1)Å) and the two carbon atoms at the two low-coordinate apical positions. Rationalizations of the energetic relationship between these two geometries are complicated by the observation that while $(C_5H_5)Co_2C_2B_6H_8$ thermally rearranges to give an isomer with non-adjacent metal vertices, the isomer of $(C_5H_5)CoNiCB_7H_8$ studied here is stable to thermal rearrangement at 450°C. Both $(C_5H_5)_2Co_2C_2B_6H_8$ and $(C_5H_5)_2NiCoCB_7H_8$ fit the theoretical models of closo-metallocarboranes[9] in that they are constituted of n = 10 polyhedral atoms and 2n + 2 electron pairs or 22 framework electrons. Another 10-vertex complex $(C_5H_5)_2Fe_2C_2B_6H_8$, whose structure was recently reported,[10] is two electrons short of the 2n + 2 rule and exhibits major distortion from the idealized closo structure of a bicapped square antiprism. The symmetrical structure and lack of distortion (other than that produced by the presence of heteroatoms) found for $(C_5H_5)_2NiCoCB_7H_8$ is good evidence for the validity of the electron-counting scheme and lends further justification to the idea previously put forth[9,11] that $\{C_5H_5Co\}$ is electronically equivalent to {BH} and that $\{C_5H_5Ni\}$ is equivalent to a polyhedral {CH} group, for similar geometries are observed in the electronically similar complexes $(C_5H_5)_2NiCoCB_7H_8$, $(C_5H_5)_2Co_2C_2B_6H_8$,[6] $(CoC_2B_7H_9)_2^-$,[12] $C_2B_8H_{10}$,[13]

and $B_{10}H_{10}^{2-}$.[14] Within experimental errors, all equivalent bond distances are the same in this series of compounds.[15]

Although it is impossible to discern between the cobalt and nickel atoms, it is interesting that the metal-metal distance is significantly shorter than is the Co-Co distance in $(C_5H_5)_2Co_2C_2B_6H_8$. It should be noted that "tropical"[12] bond distances in bicapped square antiprisms are generally found to be longer than "equatorial" bond distances, thus diminishing the significance of this observation.

The cyclopentadienyl rings, while exhibiting the large librational motion typical in compounds of this type studied at room temperature, exhibit D_{5h} symmetry, as expected. The metal-carbon distances to the cyclopentadienyl rings are again equal within experimental error, further establishing the positional disorder of the metals.

Acknowledgments

We thank Dr. C. Salentine for providing the sample. We also thank the Office of Naval Research for partial support of this work and the UCLA Campus Computing Network for computer time.

Supplementary Material available.[7]

References

1. Part VIII. Preceding paper.
2. D. F. Dustin and M. F. Hawthorne, Inorg. Chem., 12, 1380 (1973).
3. K. P. Callahan, C. E. Strouse, A. L. Sims and M. F. Hawthorne, Inorg. Chem., 13, 1393 (1974).
4. C. G. Salentine and M. F. Hawthorne, J. Chem. Soc., Chem. Commun., 560 (1973).
5. C. G. Salentine and M. F. Hawthorne, J. Amer. Chem. Soc., 97, 6382 (1975).
6. E. L. Hoel, C. E. Strouse and M. F. Hawthorne, Inorg. Chem., 13, 1388 (1974).
7. See paragraph at end of paper regarding supplementary information.
8. R. M. Adams, Pure Appl. Chem., 30, 683 (1972).
9. C. J. Jones, W. J. Evans and M. F. Hawthorne, J. Chem. Soc., Chem. Commun., 543 (1973); K. Wade, ibid., 792 (1971).
10. K. P. Callahan, W. J. Evans, F. Y. Lo, C. E. Strouse and M. F. Hawthorne, J. Amer. Chem. Soc., 97, 296 (1975).
11. C. J. Jones, J. N. Francis and M. F. Hawthorne, J. Amer. Chem. Soc., 95, 7633 (1973).
12. D. St. Clair, A. Zalkin and D. H. Templeton, Inorg. Chem., 11, 377 (1972).
13. T. F. Koetzle and W. N. Lipscomb, Inorg. Chem., 9, 2279 (1970).
14. R. D. Dobrott and W. N. Lipscomb, J. Chem. Phys., 37, 1779 (1962).
15. See Reference 6 for a compilation.

TABLE I

Final Atomic Parameters[a]

Atom	x	y	z
M2	0.21175(4)	0.61403(10)	0.36659(3)
M3	0.36816(4)	0.61233(10)	0.37044(3)
B1	0.2730(5)	0.4860(9)	0.3172(3)
B4	0.3455(6)	0.3492(9)	0.3619(3)
B5	0.2289(5)	0.3506(9)	0.3579(4)
B6	0.3133(4)	0.5962(0)	0.4404(3)
B7	0.3931(5)	0.4177(9)	0.4308(3)
B8	0.3051(6)	0.2697(10)	0.4187(4)
B9	0.2243(5)	0.4215(9)	0.4277(3)
C10	0.3208(4)	0.4129(8)	0.4664(3)
Cp1	0.1722(6)	0.8495(11)	0.3364(8)
Cp2	0.1257(9)	0.7368(22)	0.3024(4)
Cp3	0.0813(7)	0.6434(13)	0.3329(9)
Cp4	0.1046(7)	0.7121(22)	0.3873(8)
Cp5	0.1588(10)	0.8352(19)	0.3871(5)
Cp6	0.4948(7)	0.6750(23)	0.3805(11)
Cp7	0.4573(15)	0.7959(29)	0.4011(6)
Cp8	0.3984(9)	0.8544(12)	0.3577(13)
Cp9	0.3995(11)	0.7682(31)	0.3113(6)
Cp10	0.4608(14)	0.6562(18)	0.3272(11)
CpH1	0.211(4)	0.921(7)	0.334(3)
CpH2	0.129(4)	0.735(8)	0.271(3)
CpH3	0.049(4)	0.561(7)	0.328(3)
CpH4	0.085(4)	0.679(8)	0.412(3)
CpH5	0.174(4)	0.880(9)	0.413(3)
CpH6	0.523(4)	0.618(8)	0.399(3)
CpH7	0.473(4)	0.820(8)	0.429(3)
CpH8	0.365(4)	0.917(7)	0.352(3)
CpH9	0.368(4)	0.771(7)	0.277(3)

Table I. Final Atomic Parameters (cont'd)

Atom	x	y	z
CpH10	0.473(4)	0.594(7)	0.309(3)
B1H	0.259(3)	0.494(7)	0.272(2)
B4H	0.375(4)	0.293(7)	0.335(2)
B5H	0.181(3)	0.275(7)	0.337(2)
B6H	0.320(3)	0.690(7)	0.468(2)
B7H	0.454(4)	0.412(7)	0.449(2)
B8H	0.306(3)	0.137(6)	0.432(2)
B9H	0.164(4)	0.390(7)	0.444(2)
C10H	0.334(4)	0.387(7)	0.506(2)

[a]Values in parentheses are estimated standard deviations and refer to the last digit of the preceding number.

TABLE II

Anisotropic Thermal Parameters x 10^4[a]

Atom	B11	B22	B33	B12	B13	B23
M2	27.2(4)	117.2(15)	12.8(2)	-4.3(6)	5.6(2)	5.1(4)
M3	27.5(4)	113.7(15)	14.9(2)	3.0(6)	5.9(2)	5.4(5)
B1	46(4)	149(13)	12.1(13)	-20(6)	3.6(17)	-11(4)
B4	69(5)	101(14)	21(2)	16(6)	15(2)	-11(4)
B5	57(4)	114(15)	21(2)	-31(6)	6(2)	-8(4)
B6	50(4)	155(14)	9.6(12)	4(6)	3.7(16)	-6(4)
B7	45(4)	131(15)	17.2(16)	13(6)	4.7(19)	6(4)
B8	66(5)	125(14)	23(2)	-5(6)	12(2)	12(4)
B9	58(4)	127(15)	19(2)	-13(6)	8(2)	16(4)
C10	64(4)	171(14)	15.1(13)	9(5)	7.7(17)	12(4)
Cp1	37(4)	169(17)	64(5)	31(6)	20(4)	53(7)
Cp2	84(7)	485(36)	17(2)	118(13)	5(3)	45(8)
Cp3	42(5)	215(23)	65(5)	-25(8)	-23(5)	9(9)
Cp4	48(6)	459(38)	57(6)	92(12)	42(5)	102(13)
Cp5	92(10)	301(37)	33(3)	107(16)	7(4)	-25(7)
Cp6	32(4)	493(45)	78(7)	1(11)	-4(5)	129(14)
Cp7	125(11)	540(42)	38(3)	-207(18)	35(5)	-62(11)
Cp8	51(6)	112(18)	115(9)	11(7)	43(6)	55(10)
Cp9	82(9)	588(51)	30(3)	130(18)	-8(4)	89(10)
Cp10	116(11)	333(36)	74(6)	-52(16)	79(7)	-44(12)

[a]See footnote a of Table I. The anisotropic temperature factor T is defined as $T = \exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}\ell^2 + 2B_{12}hk + 2B_{13}h\ell + 2B_{23}k\ell)]$. Thermal ellipsoids are depicted in the figure.

TABLE IIIa

Interatomic Distances[a]

Atoms	Distance, Å	Atoms	Distance, Å
I. Distances around Metal Atoms			
M2-M3	2.4492(11)	M3-Cp6	2.018(10)
M2-Cp1	2.052(8)	M3-Cp7	2.040(9)
M2-Cp2	2.049(7)	M3-Cp8	2.027(8)
M2-Cp3	2.037(9)	M3-Cp9	2.048(10)
M2-Cp4	2.034(10)	M3-Cp10	2.028(10)
M2-Cp5	2.060(9)	M3-B1	1.998(6)
M2-B1	1.993(8)	M3-B4	2.126(7)
M2-B5	2.129(7)	M3-B6	2.090(8)
M2-B6	2.097(6)	M3-B7	2.102(7)
M2-B9	2.109(7)		
II. Distances in Cyclopentadienyl Rings			
Cp1-Cp2	1.315(15)	Cp6-Cp7	1.293(19)
Cp1-Cp5	1.304(15)	Cp6-Cp10	1.281(19)
Cp2-Cp3	1.360(17)	Cp7-Cp8	1.310(18)
Cp3-Cp4	1.393(18)	Cp8-Cp9	1.322(20)
Cp4-Cp5	1.302(17)	Cp9-Cp10	1.303(18)
III. Boron-Boron Distances			
B1-B4	1.750(10)	B5-B9	1.803(13)
B1-B5	1.720(11)	B6-B7	1.949(10)
B4-B5	1.820(12)	B6-B9	1.947(10)
B4-B7	1.745(11)	B7-B8	1.790(11)
B4-B8	1.771(13)	B8-B9	1.808(12)
B5-B8	1.781(11)		

Table IIIa. Interatomic Distances (cont'd)

IV. Boron-Carbon Distances

B6-C10	1.582(9)	B8-C10	1.600(11)
B7-C10	1.591(11)	B9-C10	1.584(9)

V. Carbon-Hydrogen Distances

C10-CH10	0.95(5)	Cp6-CpH6	0.71(6)
Cp1-CpH1	0.85(6)	Cp7-CpH7	0.70(6)
Cp2-CpH2	0.79(6)	Cp8-CpH8	0.72(6)
Cp3-CpH3	0.82(6)	Cp9-CpH9	0.86(5)
Cp4-CpH4	0.78(7)	Cp10-CpH10	0.73(6)
Cp5-CpH5	0.71(6)		

VI. Boron-Hydrogen Distances

B1-BH1	1.06(5)	B7-BH7	0.96(5)
B4-BH4	0.99(6)	B8-BH8	1.10(5)
B5-BH5	1.00(5)	B9-BH9	1.15(6)
B6-BH6	1.00(5)		

[a]See footnote a of Table I.

TABLE IIIb

Average Bond Lengths

Atoms	No.	Range[a], Å	Average[b], Å
M-C	10	2.018(10)-2.060(9)	2.039(13)
M-B	8	1.993(8)-2.129(7)	2.08(5)
C-C	10	1.281(19)-1.393(18)	1.32(3)
B-B	11	1.720(11)-1.949(10)	1.81(8)
B-C	4	1.582(9)-1.600(11)	1.589(8)
C-H	11	0.70(6)-0.95(5)	0.78(8)
B-H	7	0.96(5)-1.15(6)	1.04(7)

[a]See footnote a of Table I. [b]ESD's for average bond lengths were calculated using the internal routine of an HP-45 calculator.

TABLE IV

Interatomic Angles[a]

Atoms 1,2,3	Angle, Deg	Atoms 1,2,3	Angle, Deg
	I. Angles around Metals		
	A. C_5H_5-M-C_5H_5		
Cp1-M2-Cp2	37.4(4)	Cp6-M3-Cp7	37.2(5)
Cp2-M2-Cp3	38.9(5)	Cp7-M3-Cp8	37.6(5)
Cp3-M2-Cp4	40.0(5)	Cp8-M3-Cp9	37.9(6)
Cp4-M2-Cp5	37.1(5)	Cp9-M3-Cp10	37.3(5)
Cp5-M2-Cp1	37.0(4)	Cp10-M3-Cp6	36.9(6)
Cp1-M2-Cp3	64.0(4)	Cp6-M3-Cp8	61.3(5)
Cp3-M2-Cp5	64.5(5)	Cp8-M3-Cp10	62.0(5)
Cp2-M2-Cp4	64.4(5)	Cp7-M3-Cp9	63.8(5)
Cp2-M2-Cp5	62.9(4)	Cp6-M3-Cp9	62.1(5)
Cp4-M2-Cp1	62.6(4)	Cp7-M3-Cp10	62.9(5)
	B. C_5H_5-M-CB_7H_8		
Cp1-M2-B1	113.7(5)	Cp6-M3-B1	140.3(9)
Cp1-M2-B5	153.9(6)	Cp6-M3-B4	113.2(6)
Cp1-M2-B6	118.0(5)	Cp6-M3-B6	120.8(8)
Cp1-M2-B9	152.0(6)	Cp6-M3-B7	95.0(4)
Cp2-M2-B1	96.6(4)	Cp7-M3-B1	160.1(7)
Cp2-M2-B5	118.1(5)	Cp7-M3-B4	145.7(9)
Cp2-M2-B6	155.4(6)	Cp7-M3-B6	97.7(4)
Cp2-M2-B9	144.4(6)	Cp7-M3-B7	106.2(7)
Cp3-M2-B1	114.1(6)	Cp8-M3-B1	123.2(8)
Cp3-M2-B5	102.3(3)	Cp8-M3-B4	164.1(8)
Cp3-M2-B6	147.0(7)	Cp8-M3-B6	110.1(8)

Table IV. Interatomic Angles (cont'd)

Cp3-M2-B9	106.1(6)	Cp8-M3-B7	142.7(9)
Cp4-M2-B1	154.0(7)	Cp9-M3-B1	97.1(4)
Cp4-M2-B6	108.9(6)	Cp9-M3-B6	145.7(9)
Cp4-M2-B9	92.6(4)	Cp9-M3-B7	154.0(7)
Cp5-M2-B1	150.0(6)	Cp10-M3-B1	106.1(7)
Cp5-M2-B5	158.9(7)	Cp10-M3-B4	104.2(4)
Cp5-M2-B6	97.0(3)	Cp10-M3-B6	157.7(8)
Cp5-M2-B9	115.1(6)	Cp10-M3-B7	116.9(8)

C. Boron-Metal-Boron

B1-M2-B5	49.2(3)	B1-M3-B4	50.1(3)
B1-M2-B6	95.5(3)	B1-M3-B6	95.6(3)
B1-M2-B9	94.4(3)	B1-M3-B7	93.6(3)
B5-M2-B6	85.9(3)	B4-M3-B6	85.7(3)
B5-M2-B9	50.4(3)	B4-M3-B7	48.7(3)
B6-M2-B9	55.1(3)	B6-M3-B7	55.4(3)

D. Boron-Metal-Metal

B1-M2-M3	52.2(2)	B6-M2-M3	54.1(2)
B5-M2-M3	81.2(2)	B9-M2-M3	92.8(2)

E. Carbon-Metal-Metal

Cp1-M2-M3	103.5(3)	Cp4-M2-M3	152.2(6)
Cp2-M2-M3	120.5(4)	Cp5-M2-M3	117.4(5)
Cp3-M2-M3	158.2(7)		

Table IV. Interatomic Angles (cont'd)

II. B-B-B Angles

B4-B1-B5	63.3(8)	B7-B6-B9	85.6(5)
B1-B4-B5	57.6(4)	B4-B7-B6	101.6(5)
B1-B4-B7	117.6(5)	B4-B7-B8	60.1(5)
B1-B4-B8	113.5(6)	B6-B7-B8	90.0(5)
B5-B4-B7	104.1(6)	B4-B8-B5	61.7(4)
B5-B4-B8	59.5(8)	B4-B8-B7	58.7(5)
B7-B4-B8	61.2(5)	B4-B8-B9	104.7(5)
B1-B5-B4	59.2(4)	B5-B8-B7	103.8(5)
B1-B5-B8	114.5(6)	B5-B8-B9	60.3(5)
B1-B5-B9	117.3(5)	B7-B8-B9	94.8(5)
B4-B5-B8	58.9(5)	B5-B9-B8	59.1(5)
B8-B5-B9	60.6(5)	B6-B9-B8	89.6(5)

III. C-B-B Angles

C10-B6-B7	52.3(4)	C10-B8-B5	107.2(6)
C10-B6-B9	52.1(4)	C10-B8-B7	55.6(4)
C10-B7-B4	108.3(6)	C10-B8-B9	55.0(4)
C10-B7-B6	51.9(4)	C10-B9-B5	106.9(7)
C10-B7-B8	56.1(5)	C10-B9-B6	52.0(4)
C10-B8-B4	106.7(6)	C10-B9-B8	55.8(4)

IV. B-C-B Angles

B6-C10-B7	75.8(5)	B7-C10-B8	68.3(5)
B6-C10-B8	112.6(5)	B7-C10-B9	113.0(6)
B6-C10-B9	75.9(4)	B8-C10-B9	69.2(5)

V. Cyclopentadienyl Ring Angles

Cp2-Cp1-Cp5	109.8(12)	Cp7-Cp6-Cp10	111.0(13)
Cp1-Cp2-Cp3	108.3(10)	Cp6-Cp7-Cp8	104.8(13)
Cp2-Cp3-Cp4	104.4(9)	Cp7-Cp8-Cp9	110.3(13)
Cp3-Cp4-Cp5	108.3(12)	Cp8-Cp9-Cp10	105.3(12)
Cp4-Cp5-Cp1	109.1(12)	Cp9-Cp10-Cp6	108.6(14)

[a]See footnote a of Table I.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: Technical Report 100

2. GOVT ACCESSION NO.

3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle): Structures of Metallocarboranes. IX. Crystal and Molecular Structure of the Ten-Vertex Heterobimetallocarborane 2,3-Di-η-cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8), 2,3-$(\eta\text{-}C_5H_5)_2$-(2,3)-NiCo-10-CB_7H_8

5. TYPE OF REPORT & PERIOD COVERED: Interim

6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s): G. E. Hardy, K. P. Callahan, and M. F. Hawthorne

8. CONTRACT OR GRANT NUMBER(s): N00014-76-C-0390

9. PERFORMING ORGANIZATION NAME AND ADDRESS: The University of California, Department of Chemistry, Los Angeles, California 90024

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: NR 053-608

11. CONTROLLING OFFICE NAME AND ADDRESS: Chemistry Branch, Office of Naval Research, Washington, D.C. 20360

12. REPORT DATE: January 16, 1978

13. NUMBER OF PAGES: 16 (Suppl. mat'l separate)

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)

15. SECURITY CLASS. (of this report): Unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Metallocarborane.
Crystal structure.
Bimetallic compound.
Nickelacarborane.
Cobaltacarborane.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A complete three dimensional crystal structure determination of the title compound was carried out. Crystal data: Space group C2/c, a = 15.794(4), b = 7.955(2), c = 24.273(7) Å, β = 104.12(2)°, z = 8, d_o = 1.55(2), d_c = 1.54. Diffraction data to $2\theta_{max}$ = 50° were obtained with a Syntex PT automated diffractometer (MoK_α radiation) and the structure was solved by conventional Patterson, Fourier and full matrix least-squares techniques to a conventional R = 0.047 for 2048 independent non-zero reflections. The molecule has the bicapped square antiprismal geometry expected for a closo ten-vertex polyhedron. The two metal

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-014-6601

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

20. (Abstract, cont'd)

atoms are indistinguishable and occupy adjacent sites in the same equatorial belt. The carbon atom resides in the four-coordinate site non-adjacent to the two metal atoms.

APPENDIX

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Office of Naval Research Arlington, Virginia 22217 Attn: Code 472	2
Office of Naval Research Arlington, Virginia 22217 Attn: Code 102IP 1	6
ONR Branch Office 536 S. Clark Street Chicago, Illinois 60605 Attn: Dr. Jerry Smith	1
ONR Branch Office 715 Broadway New York, New York 10003 Attn: Scientific Dept.	1
ONR Branch Office 1030 East Green Street Pasadena, California 91106 Attn: Dr. R. J. Marcus	1
ONR Branch Office 760 Market St., Rm. 447 San Francisco, Calif. 94102 Attn: Dr. P. A. Miller	1
ONR Branch Office 495 Summer Street Boston, Massachusetts 02210 Attn: Dr. L. H. Peebles	1
Director Naval Research Laboratory Washington, D.C. 20390 Attn: Code 6100	1
The Asst. Secretary of the Navy (R&D) Department of the Navy Room 4E736, Pentagon Washington, D.C. 20350	1
Commander Naval Air Systems Command Department of the Navy Washington, D.C. 20360 Attn: Code 310C (H. Rosenwasser)	1
Defense Documentation Center Building 5, Cameron Station Alexandria, Virginia 22314	12
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, N.C. 27709 Attn: CRD-AA-IP	1
Naval Ocean Systems Center San Diego, California 92152 Attn: Mr. Joe McCartney	1
Naval Weapons Center China Lake, California 93555 Attn: Head, Chemistry Division	1
Naval Civil Engineering Laboratory Port Hueneme, California 93041 Attn: Mr. W. S. Haynes	1
Professor O. Heinz Department of Physics & Chemistry Naval Postgraduate School Monterey, California 93940	1
Dr. A. L. Slafkosky Scientific Advisor Commandant of the Marine Corps (Code RD-1) Washington, D.C. 20380	1
Office of Naval Research Arlington, Virginia 22217 Attn: Dr. Richard S. Miller	1
Dr. R. M. Grimes University of Virginia Department of Chemistry Charlottesville, Virginia 22901	1
Dr. M. Tsutsui Texas A&M University Department of Chemistry College Station, Texas 77843	1
Dr. C. Quicksall Georgetown University Department of Chemistry 37th & O Streets Washington, D.C. 20007	1

TECHNICAL REPORT DISTRIBUTION LIST

	No. Copies
Dr. D. B. Brown University of Vermont Department of Chemistry Burlington, Vermont 05401	1
Dr. W. B. Fox Naval Research Laboratory Chemistry Division Code 6130 Washington, D.C. 20375	1
Dr. J. Adcock University of Tennessee Department of Chemistry Knoxville, Tennessee 37916	1
Dr. A. Cowley University of Texas Department of Chemistry Austin, Texas 78712	1
Dr. W. Hatfield University of North Carolina Department of Chemistry Chapel Hill, North Carolina 27514	1
Dr. D. Seyferth Massachusetts Institute of Technology Department of Chemistry Cambridge, Massachusetts 02139	1
Dr. M. H. Chisholm Princeton University Department of Chemistry Princeton, New Jersey 08540	1
Dr. B. Foxman Brandeis University Department of Chemistry Waltham, Massachusetts 02154	1
Dr. T. Marks Northwestern University Department of Chemistry Evanston, Illinois 60201	1
Dr. J. Zuckerman University of Oklahoma Department of Chemistry Norman, Oklahoma 73019	1
Dr. G. Geoffrey Pennsylvania State University Department of Chemistry University Park, Pennsylvania 16802	1

SUPPLEMENTAL MATERIAL

Structure factor amplitudes for 2,3-Di-η-cyclopentadienyl-10-carba-(2,3)-(Nickelacobalta)-decaborane(8)

The table lists the values of h, k, ℓ, cFo and cFc for each observed reflection. The value of c is 2.914.

H	L	FO	FC
****	K = 0	****	
0	-26	88	84
0	2	87	77
0	4	849	999
0	6	196	193
0	8	323	310
0	10	170	164
0	12	321	315
0	14	164	160
0	16	250	256
0	18	181	183
0	20	136	142
0	22	123	122
0	24	48	43
0	28	25	16
2	-28	24	22
2	-26	76	69
2	-22	143	140
2	-20	42	43
2	-18	214	207
2	-16	76	78
2	-14	241	239
2	-12	98	96
2	-10	264	281
2	-8	94	96
2	-6	128	123
2	-4	332	319
2	-2	176	157
2	0	389	379
2	2	252	250
2	4	107	101
2	8	208	211
2	10	67	72
2	12	178	182
2	14	48	36
2	16	124	124
2	18	31	26
2	20	91	88
2	22	20	26
2	24	27	25
4	-28	24	3
4	-24	18	4
4	-20	26	4
4	-18	47	44
4	-14	66	63
4	-12	68	64
4	-10	56	52
4	-8	67	66
4	-6	275	273
4	-2	298	301
4	0	247	244
4	2	172	183
4	4	210	210
4	6	163	160
4	8	91	93
4	10	104	98
4	12	151	150
4	14	65	68
4	16	127	127
4	18	35	32
4	20	72	69
4	22	37	20
4	24	66	59
6	-28	77	71
6	-26	65	53
6	-24	96	94
6	-22	110	105
6	-20	135	134
6	-18	174	175
6	-16	213	214
6	-14	228	227
6	-12	203	201
6	-10	383	393
6	-8	133	136
6	-6	478	472
6	-4	83	81
6	-2	336	326
6	0	65	66
6	2	481	481
6	4	122	126
6	6	414	431
6	8	210	215
6	10	241	244
6	12	218	220
6	14	181	175
6	16	130	129
6	18	132	124
6	20	96	92
6	22	71	73
6	24	85	79
8	-28	94	95
8	-24	112	117
8	-22	34	43
8	-20	150	158
8	-18	45	50
8	-16	222	220
8	-14	94	93
8	-12	244	242
8	-10	245	238
8	-8	253	248
8	-6	267	265
8	-4	171	165
8	-2	223	213
8	0	113	112
8	2	306	304
8	4	105	102
8	6	219	222
8	8	31	21
8	10	141	145
8	12	19	20
8	14	99	104
8	16	25	17
8	18	58	64
8	20	35	26
8	22	42	45
10	-22	32	18
10	-14	41	45
10	-10	40	42
10	-8	41	40
10	-6	65	67
10	-4	136	139
10	-2	74	76
10	0	111	111
10	2	50	48
10	6	50	54
10	12	40	38
10	14	38	39
10	16	49	48
10	18	49	48
10	20	21	16
12	-26	59	59
12	-24	64	71
12	-22	84	78
12	-20	101	103
12	-18	92	84
12	-16	113	118
12	-14	76	74
12	-12	125	122
12	-10	22	14
12	-8	166	174
12	-4	238	252
12	-2	24	25
12	0	190	198
12	4	131	138
12	6	58	60
12	8	132	137
12	10	79	76
12	12	117	123
12	14	83	78
12	16	83	83
14	-22	118	115
14	-20	53	53
14	-18	136	138
14	-16	87	83
14	-14	132	133
14	-12	100	102
14	-10	99	101
14	-8	148	149
14	-6	100	103
14	-4	167	166
14	-2	93	100
14	0	121	121
14	2	42	43
14	4	124	121
14	8	118	123
14	12	87	87
16	-20	25	14
16	-18	28	17
16	-16	20	9
16	-14	25	19
16	-10	25	26
16	-8	20	22
16	-6	35	39
16	-4	20	21
16	-2	21	15
16	0	23	6
16	3	26	0
16	4	7	3
16	8	29	17
18	-14	75	84
18	-10	96	97
18	-6	84	87
18	-2	84	87
****	K = 1	****	
1	-28	65	68
1	-27	71	62
1	-24	70	90
1	-23	33	58
1	-22	35	54
1	-20	117	148
1	-19	30	106
1	-18	103	118
1	-16	178	189
1	-15	106	177
1	-14	156	173
1	-13	82	86
1	-12	226	225
1	-11	208	208
1	-10	191	195
1	-9	101	101
1	-8	200	197
1	-7	283	283
1	-6	214	209
1	-5	26	21
1	-4	81	79
1	-3	463	485
1	-2	550	564
1	-1	186	179
1	0	188	190
1	1	322	329
1	2	452	461
1	3	340	349
1	4	89	89
1	5	172	170
1	6	211	198
1	7	170	171
1	8	80	79
1	9	165	168
1	10	240	237
1	11	124	123
1	12	72	73
1	13	126	129
1	14	191	196
1	15	107	110
1	16	68	71
1	17	62	64
1	18	131	136
1	19	63	69
1	20	66	68
1	22	51	60
1	23	64	60
1	24	57	54
3	-28	21	19
3	-25	32	33
3	-24	49	38
3	-23	23	20
3	-20	70	73
3	-19	44	44
3	-18	19	18
3	-17	17	12
3	-16	58	60
3	-15	42	48
3	-14	45	40
3	-13	86	87
3	-12	71	72
3	-11	61	62
3	-10	18	22
3	-9	68	72
3	-8	43	41
3	-7	23	4
3	-6	41	34
3	-5	70	70
3	-4	17	11
3	-3	334	338
3	-2	141	128
3	0	137	134
3	1	345	356
3	2	15	9
3	3	73	72
3	4	17	11
3	5	31	30
3	6	21	19
3	7	63	63
3	8	19	17
3	9	24	12
3	10	20	17
3	11	81	81
3	13	19	9
3	14	18	28
3	18	20	11
3	19	28	32
3	20	30	13
3	23	25	4
3	24	20	16
5	-28	35	31
5	-26	25	27
5	-25	55	48
5	-24	43	45
5	-22	36	34
5	-21	98	94
5	-20	87	80
5	-18	80	80
5	-17	94	96
5	-16	137	139
5	-15	63	64
5	-14	82	88

H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
5	-13	92	93	7	12	152	152	11	10	76	78	15	9	29	25
5	-12	168	166	7	13	69	77	11	11	71	70	15	10	29	25
5	-11	108	113	7	14	71	76	11	12	61	60	17	-17	39	33
5	-10	35	36	7	15	35	34	11	14	63	65	17	-15	31	27
5	-9	130	129	7	16	104	104	11	15	52	53	17	-14	22	4
5	-8	221	217	7	17	85	87	11	16	62	60	17	-13	48	40
5	-7	84	86	7	18	47	47	11	17	24	10	17	-12	41	36
5	-6	106	103	7	19	36	33	11	18	25	30	17	-11	37	30
5	-5	156	148	7	20	56	59	13	-24	78	75	17	-9	35	34
5	-4	129	121	7	21	72	73	13	-23	65	59	17	-8	50	41
5	-3	155	149	7	22	38	37	13	-22	53	56	17	-7	34	29
5	-2	22	22	7	23	22	10	13	-21	21	18	17	-6	28	8
5	-1	97	89	9	-27	26	22	13	-20	91	92	17	-5	33	27
5	0	118	116	9	-26	51	48	13	-19	99	103	17	-4	48	46
5	1	177	170	9	-25	45	47	13	-18	84	84	17	-3	35	33
5	2	17	6	9	-23	38	34	13	-17	25	1				
5	3	23	13	9	-22	55	59	13	-16	93	95	****	K =	2	****
5	4	276	277	9	-21	31	37	13	-15	128	127	0	-25	126	122
5	5	199	206	9	-18	95	87	13	-14	86	91	0	0	140	153
5	6	61	60	9	-17	40	41	13	-13	26	28	0	1	303	293
5	7	29	29	9	-16	20	10	13	-12	77	82	0	2	69	73
5	8	180	178	9	-14	88	89	13	-11	122	123	0	3	172	167
5	9	195	194	9	-13	62	54	13	-10	111	113	0	4	66	69
5	10	160	163	9	-12	44	50	13	-9	42	38	0	5	398	390
5	12	103	103	9	-11	27	24	13	-8	53	58	0	6	25	35
5	13	139	138	9	-10	108	108	13	-7	100	99	0	7	213	205
5	14	166	165	9	-9	47	42	13	-6	186	188	0	8	23	27
5	15	35	32	9	-8	64	61	13	-5	44	37	0	9	330	325
5	16	76	77	9	-7	32	41	13	-4	61	61	0	10	120	122
5	17	116	112	9	-6	119	114	13	-3	80	79	0	11	138	144
5	18	94	93	9	-5	29	27	13	-2	183	186	0	12	27	36
5	19	22	30	9	-4	41	36	13	-1	59	63	0	13	300	288
5	20	39	47	9	-2	44	41	13	0	30	29	0	14	42	43
5	21	89	89	9	-1	36	28	13	1	83	83	0	15	69	72
5	22	70	68	9	0	97	94	13	2	129	131	0	17	215	214
7	-27	24	22	9	1	26	30	13	3	76	80	0	19	23	15
7	-26	83	77	9	2	47	46	13	4	24	19	0	20	29	36
7	-25	95	99	9	4	75	79	13	5	76	79	0	21	137	134
7	-24	49	46	9	5	40	39	13	6	122	122	0	23	26	27
7	-23	32	28	9	6	27	32	13	7	90	91	2	-27	64	58
7	-22	96	104	9	8	44	40	13	8	25	35	2	-25	75	77
7	-21	114	118	9	9	30	33	13	9	52	54	2	-23	63	62
7	-20	78	85	9	12	30	30	13	10	109	107	2	-21	90	92
7	-19	25	26	11	-26	28	20	13	11	86	82	2	-19	35	29
7	-18	158	164	11	-22	49	52	13	12	32	38	2	-17	178	176
7	-17	120	125	11	-19	38	42	13	13	26	19	2	-16	36	32
7	-16	110	112	11	-18	67	62	13	14	78	74	2	-15	40	42
7	-14	173	173	11	-17	22	19	13	15	49	50	2	-13	223	222
7	-13	211	209	11	-15	78	77	15	-20	59	61	2	-12	33	27
7	-12	192	185	11	-14	63	63	15	-19	59	54	2	-10	35	30
7	-11	17	8	11	-13	43	41	15	-17	26	23	2	-9	225	231
7	-10	142	133	11	-12	18	18	15	-16	67	74	2	-7	75	81
7	-9	269	267	11	-11	98	98	15	-15	65	65	2	-6	24	27
7	-8	355	347	11	-10	71	72	15	-13	29	22	2	-5	183	178
7	-7	94	92	11	-9	80	83	15	-12	83	77	2	-4	61	63
7	-6	149	149	11	-8	22	24	15	-11	72	74	2	-3	38	33
7	-5	208	200	11	-7	83	84	15	-10	26	33	2	-2	82	82
7	-4	346	350	11	-6	143	143	15	-9	23	16	2	-1	37	33
7	-3	127	123	11	-5	93	91	15	-8	78	76	2	0	152	151
7	-2	93	92	11	-4	49	45	15	-7	72	70	2	1	15	4
7	-1	217	205	11	-3	56	56	15	-6	68	68	2	2	52	52
7	0	357	359	11	-2	170	169	15	-4	67	74	2	3	152	146
7	1	123	123	11	-1	119	119	15	-3	55	56	2	4	43	44
7	2	63	63	11	0	25	26	15	-2	61	62	2	7	164	169
7	3	203	204	11	1	37	41	15	-1	29	6	2	9	78	80
7	4	331	327	11	2	90	88	15	0	30	31	2	10	47	47
7	5	180	175	11	3	128	129	15	1	43	45	2	11	96	93
7	7	122	122	11	4	47	45	15	2	59	52	2	13	100	98
7	8	205	206	11	5	25	16	15	4	24	8	2	14	43	45
7	9	129	128	11	6	68	67	15	5	35	34	2	15	70	75
7	10	78	77	11	7	95	97	15	6	40	43	2	17	44	43
7	11	58	55	11	8	55	54	15	7	19	9	2	19	22	20

H	L	FO	FC
2	20	26	2
2	21	37	31
2	-23	35	36
2	-19	65	63
2	-18	21	4
2	-16	55	56
2	-15	47	44
2	-14	23	22
2	-13	85	82
2	-12	55	60
2	-11	64	64
2	-10	57	60
2	-9	98	98
2	-8	83	82
2	-7	82	81
2	-6	93	87
2	-3	23	14
2	-2	115	113
2	-1	26	18
2	0	101	100
2	1	21	14
2	2	80	79
2	3	54	53
2	4	37	34
2	5	19	24
2	6	86	86
2	7	185	187
2	8	40	43
2	9	25	31
2	10	29	31
2	11	151	152
2	12	37	42
2	13	24	16
2	14	30	28
2	15	87	89
2	16	22	13
2	17	71	70
2	19	95	93
2	21	49	46
2	22	21	12
2	23	70	69
6	-27	87	85
6	-24	22	2
6	-23	146	147
6	-21	22	24
6	-19	159	162
6	-17	38	36
6	-16	34	44
6	-15	201	211
6	-13	146	147
6	-12	26	19
6	-11	308	299
6	-10	40	34
6	-9	192	195
6	-8	65	64
6	-7	283	274
6	-6	112	107
6	-5	213	214
6	-4	27	28
6	-3	205	202
6	-2	139	128
6	-1	204	198
6	0	26	23
6	1	228	222
6	2	112	111
6	3	275	268
6	4	54	56
6	5	197	203
6	6	33	35
6	7	317	308
6	8	26	27
6	9	146	147
6	10	24	17
6	11	214	215
6	12	32	35
6	13	48	44
6	14	31	19
6	15	164	158
6	19	154	146
6	23	99	88
8	-27	73	73
8	-25	56	55
8	-24	22	8
8	-23	113	116
8	-21	60	57
8	-20	34	34
8	-19	120	124
8	-18	20	7
8	-16	52	41
8	-15	172	177
8	-11	253	253
8	-10	34	3
8	-9	50	41
8	-8	21	23
8	-7	299	284
8	-6	23	5
8	-5	29	23
8	-4	36	32
8	-3	332	317
8	-2	25	20
8	-1	110	109
8	0	16	10
8	1	238	229
8	2	19	11
8	3	144	145
8	4	21	4
8	5	160	160
8	6	19	11
8	7	84	83
8	8	19	12
8	9	116	119
8	10	36	31
8	11	37	36
8	12	30	30
8	13	62	65
8	14	25	25
8	15	66	67
8	17	38	41
8	19	62	62
8	20	26	7
8	21	30	27
10	-24	26	7
10	-13	35	35
10	-11	50	46
10	-9	21	25
10	-8	19	15
10	-7	85	83
10	-5	30	24
10	-3	67	68
10	-2	17	13
10	-1	27	22
10	1	89	90
10	3	27	19
10	4	31	29
10	5	78	80
10	8	23	11
10	9	66	68
10	10	24	18
10	11	26	9
10	12	26	13
10	13	53	56
10	14	25	23
10	16	19	6
10	17	30	26
10	18	21	5
10	19	29	27
12	-25	69	65
12	-22	28	13
12	-21	107	100
12	-20	36	28
12	-19	37	30
12	-17	137	135
12	-16	34	28
12	-15	64	58
12	-14	22	25
12	-13	149	151
12	-11	87	86
12	-10	39	36
12	-9	169	177
12	-8	46	33
12	-7	107	106
12	-6	39	19
12	-5	153	160
12	-4	70	66
12	-3	148	149
12	-1	117	115
12	0	41	32
12	1	174	175
12	2	22	17
12	3	93	93
12	4	24	14
12	5	156	159
12	6	29	18
12	7	65	67
12	8	22	24
12	9	148	148
12	11	35	37
12	12	28	25
12	13	117	115
14	-23	39	43
14	-21	94	96
14	-19	43	51
14	-18	31	10
14	-17	126	131
14	-15	33	41
14	-14	28	19
14	-13	147	152
14	-9	170	170
14	-8	25	20
14	-6	30	21
14	-5	161	162
14	-4	33	38
14	-3	52	56
14	-1	145	147
14	0	30	27
14	1	74	77
14	2	22	4
14	3	110	115
14	4	29	17
14	5	79	81
14	7	70	73
14	9	75	76
14	11	51	44
14	12	27	10
16	-18	20	9
16	-16	29	3
16	-15	23	11
16	-14	26	10
16	-12	23	12
16	-8	23	13
16	-7	29	2
16	-3	22	2
16	-2	36	7
16	0	20	5
16	2	32	8
16	3	32	26
16	6	25	4
16	7	28	22
18	-12	20	1
18	-11	94	94
18	-9	51	47
18	-7	77	83
18	-5	75	74
18	-3	53	61
18	-2	29	14

**** K = 3 ****

H	L	FO	FC
1	-26	24	31
1	-25	57	55
1	-24	55	56
1	-23	111	104
1	-22	32	42
1	-21	31	34
1	-20	76	81
1	-19	130	126
1	-18	51	47
1	-16	125	131
1	-15	198	201
1	-14	101	108
1	-13	49	46
1	-12	147	149
1	-11	264	258
1	-10	165	167
1	-9	31	25
1	-8	125	126
1	-7	359	373
1	-6	202	195
1	-5	117	120
1	-4	57	61
1	-3	332	327
1	-2	214	201
1	-1	111	114
1	0	55	54
1	1	232	231
1	2	194	193
1	3	235	234
1	4	51	50
1	5	277	282
1	6	205	208
1	7	204	217
1	8	19	16
1	9	141	139
1	10	175	172
1	11	177	171
1	12	62	64
1	13	69	73
1	14	112	113
1	15	139	141
1	16	61	63
1	17	55	54
1	18	55	54
1	19	83	88
1	20	34	35
1	22	44	43
1	23	88	83
1	24	21	25
3	-27	23	28
3	-26	25	2
3	-25	35	36
3	-24	31	23
3	-22	30	5
3	-21	21	22
3	-20	31	27
3	-19	31	40
3	-17	38	39
3	-16	28	37
3	-15	65	67
3	-14	21	2

H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
3	-13	16	24	7	-27	27	36	9	5	20	23	13	10	69	65
3	-12	52	53	7	-26	64	57	9	6	32	16	13	11	78	78
3	-11	19	15	7	-25	88	86	9	7	49	49	13	12	32	35
3	-10	38	35	7	-24	34	32	9	8	24	14	13	13	28	26
3	-9	70	68	7	-23	56	62	9	11	26	20	15	-20	26	39
3	-8	40	44	7	-22	78	73	9	12	20	23	15	-19	52	43
3	-7	49	47	7	-21	113	114	9	15	21	13	15	-18	27	0
3	-6	95	96	7	-20	67	70	9	18	22	14	15	-17	46	43
3	-5	27	32	7	-19	36	38	9	19	35	19	15	-16	52	52
3	-3	99	100	7	-18	63	65	11	-23	32	30	15	-15	47	49
3	-2	46	51	7	-17	138	143	11	-19	65	61	15	-12	47	53
3	0	29	38	7	-16	88	91	11	-18	26	31	15	-11	64	65
3	1	83	83	7	-15	47	52	11	-17	27	27	15	-10	42	34
3	2	25	30	7	-14	66	74	11	-15	65	70	15	-8	50	46
3	3	36	34	7	-13	221	230	11	-14	49	48	15	-7	72	62
3	4	75	74	7	-12	138	138	11	-13	38	36	15	-6	44	43
3	5	15	0	7	-11	30	28	11	-12	23	14	15	-4	43	44
3	6	31	27	7	-10	114	105	11	-11	85	81	15	-3	70	62
3	7	95	96	7	-9	277	270	11	-10	72	72	15	-2	47	40
3	9	45	42	7	-8	214	215	11	-9	58	60	15	0	32	33
3	10	21	24	7	-6	120	116	11	-8	31	26	15	1	52	59
3	12	33	31	7	-5	280	266	11	-7	105	106	15	2	40	38
3	14	18	11	7	-4	267	262	11	-6	76	83	15	3	25	8
3	16	28	18	7	-3	120	119	11	-5	87	84	15	4	21	11
3	18	26	23	7	-2	75	70	11	-4	24	22	15	5	29	32
3	19	26	19	7	-1	224	214	11	-3	56	50	15	6	36	28
3	21	37	37	7	0	272	266	11	-2	83	84	15	7	25	25
3	22	24	19	7	1	201	202	11	-1	119	118	17	-14	24	8
3	-26	31	26	7	2	23	13	11	2	76	76	17	-13	27	31
3	-25	61	61	7	3	114	112	11	3	108	105	17	-12	36	25
3	-24	37	34	7	4	221	218	11	4	25	24	17	-9	26	26
3	-22	39	36	7	5	202	208	11	5	24	11	17	-8	35	36
3	-21	81	82	7	6	20	17	11	6	61	60	17	-7	28	24
3	-20	56	57	7	7	145	147	11	7	101	99	17	-4	37	39
3	-18	36	34	7	8	137	136	11	8	27	25	17	-3	37	37
3	-17	58	60	7	9	138	141	11	10	48	50	17	-2	21	22
3	-16	88	85	7	11	113	110	11	11	98	99				
3	-15	77	81	7	12	93	90	11	12	33	26	****	K =	4	****
3	-13	129	127	7	13	110	109	11	14	40	36	0	0	475	488
3	-12	109	114	7	14	26	21	11	15	65	59	0	1	92	94
3	-11	164	164	7	15	21	20	11	16	27	29	0	3	61	55
3	-9	215	215	7	16	76	74	13	-23	70	72	0	4	417	425
3	-8	91	90	7	17	112	111	13	-22	38	29	0	5	150	149
3	-7	177	170	7	18	36	41	13	-21	22	19	0	6	123	125
3	-5	146	141	7	20	40	35	13	-20	55	58	0	7	65	59
3	-4	40	36	7	21	75	70	13	-19	112	107	0	8	331	319
3	-3	204	194	9	-25	38	41	13	-18	58	50	0	9	90	92
3	-1	127	122	9	-23	61	54	13	-17	25	7	0	10	210	208
3	0	37	37	9	-22	55	50	13	-16	53	53	0	11	17	3
3	1	234	231	9	-21	41	47	13	-15	127	126	0	12	235	236
3	2	22	16	9	-19	40	38	13	-14	71	65	0	13	75	70
3	3	69	71	9	-18	55	47	13	-13	24	26	0	14	157	155
3	4	111	110	9	-17	68	69	13	-12	34	40	0	16	146	150
3	5	293	297	9	-16	31	31	13	-11	146	146	0	17	47	47
3	6	41	40	9	-15	30	21	13	-10	72	71	0	18	90	94
3	7	63	62	9	-14	37	33	13	-9	53	49	0	20	100	98
3	8	124	121	9	-13	99	99	13	-8	34	36	0	21	29	32
3	9	225	228	9	-12	19	10	13	-7	144	149	0	22	84	76
3	10	78	80	9	-11	58	55	13	-6	92	89	0	23	35	41
3	11	58	63	9	-10	61	61	13	-5	63	63	0	24	56	52
3	12	77	79	9	-9	53	54	13	-4	29	27	2	-26	66	63
3	13	112	109	9	-7	50	50	13	-3	122	121	2	-23	36	37
3	14	80	81	9	-6	109	113	13	-2	101	96	2	-22	83	77
3	15	22	18	9	-5	37	37	13	-1	89	86	2	-20	34	26
3	16	52	52	9	-4	55	57	13	1	118	119	2	-18	109	113
3	17	96	100	9	-2	54	57	13	2	90	91	2	-17	38	40
3	18	74	70	9	-1	27	24	13	3	85	87	2	-16	57	54
3	19	44	46	9	0	105	105	13	5	89	89	2	-15	29	38
3	20	28	25	9	1	21	18	13	6	87	86	2	-14	171	171
3	21	84	89	9	2	20	25	13	7	89	91	2	-13	54	56
3	22	54	52	9	3	28	23	13	8	39	32	2	-12	101	101
3	23	37	31	9	4	49	49	13	9	54	50	2	-11	24	29

H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
2	-10	185	186	6	-20	105	110	8	15	35	30	14	-6	52	53
2	-9	73	75	6	-19	35	34	8	16	27	26	14	-5	35	30
2	-8	146	140	6	-18	117	118	8	18	61	60	14	-4	106	99
2	-6	113	108	6	-16	106	104	10	-20	22	14	14	-3	23	4
2	-5	127	122	6	-15	38	35	10	-14	26	15	14	-2	69	70
2	-4	200	192	6	-14	146	150	10	-11	28	34	14	-1	43	35
2	-3	21	24	6	-13	53	52	10	-10	21	21	14	0	98	95
2	-2	85	83	6	-12	68	69	10	-9	27	4	14	2	43	45
2	-1	97	95	6	-11	96	96	10	-8	27	25	14	3	36	35
2	0	182	179	6	-10	231	235	10	-7	32	38	14	4	103	107
2	1	43	42	6	-8	52	53	10	-6	22	15	14	5	28	8
2	2	127	126	6	-7	115	115	10	-4	48	50	14	6	21	2
2	3	95	94	6	-6	327	330	10	-3	29	29	14	7	23	22
2	4	137	134	6	-4	38	39	10	-2	39	32	14	8	81	86
2	5	44	42	6	-3	89	88	10	-1	35	34	14	9	27	18
2	6	54	55	6	-2	353	353	10	0	40	42	16	-14	34	27
2	7	58	55	6	-1	91	80	10	1	25	15	16	-10	23	12
2	8	147	151	6	0	48	43	10	2	39	41	16	-3	20	3
2	9	24	27	6	1	29	4	10	3	26	22	16	0	26	3
2	10	22	12	6	2	329	337	10	4	22	15	16	1	24	4
2	11	30	27	6	3	114	114	10	5	24	14	16	2	26	4
2	12	126	127	6	4	58	59	10	6	47	48				
2	13	50	51	6	6	240	246	10	8	23	24	****	K =	5	****
2	15	27	31	6	7	98	99	10	10	46	45	1	-24	75	66
2	16	57	62	6	8	63	68	10	11	25	17	1	-23	51	47
2	18	27	19	6	9	53	51	10	12	25	28	1	-22	43	36
2	20	29	24	6	10	166	168	10	13	22	10	1	-21	26	24
2	22	28	17	6	11	47	47	10	14	33	35	1	-20	92	91
2	23	21	0	6	12	107	106	10	15	25	6	1	-19	71	65
2	24	23	13	6	14	136	134	10	16	24	18	1	-18	74	71
4	-22	27	33	6	15	41	40	12	-22	61	53	1	-17	21	18
4	-18	39	33	6	16	116	115	12	-20	76	80	1	-16	117	119
4	-16	19	9	6	17	22	24	12	-19	23	5	1	-15	58	55
4	-15	46	50	6	18	90	86	12	-18	69	62	1	-14	118	112
4	-14	35	30	6	19	50	46	12	-17	37	38	1	-13	28	9
4	-13	23	24	6	20	87	84	12	-16	108	110	1	-12	150	153
4	-11	19	10	6	21	21	8	12	-14	61	58	1	-11	64	60
4	-10	80	78	8	-25	21	29	12	-13	50	47	1	-10	146	146
4	-9	37	40	8	-24	98	101	12	-12	115	113	1	-8	125	126
4	-8	43	38	8	-23	26	23	12	-11	37	31	1	-7	85	79
4	-7	57	58	8	-22	27	26	12	-10	36	39	1	-6	190	190
4	-6	136	134	8	-21	49	53	12	-9	52	43	1	-5	58	60
4	-5	50	48	8	-20	142	143	12	-8	124	128	1	-4	52	47
4	-4	54	50	8	-18	50	52	12	-7	34	24	1	-3	111	113
4	-3	30	27	8	-17	29	35	12	-5	33	24	1	-2	259	257
4	-2	135	127	8	-16	141	140	12	-4	147	148	1	-1	80	83
4	-1	75	77	8	-15	56	62	12	-3	21	17	1	0	89	88
4	0	85	83	8	-14	65	72	12	-2	22	4	1	1	127	131
4	1	17	7	8	-12	125	125	12	-1	27	32	1	2	227	227
4	2	147	150	8	-11	87	85	12	0	122	123	1	3	57	55
4	3	66	65	8	-10	97	97	12	1	42	35	1	4	61	65
4	4	105	107	8	-9	33	29	12	2	19	15	1	5	77	74
4	5	52	51	8	-8	172	168	12	3	42	46	1	6	178	178
4	6	120	118	8	-7	30	30	12	4	118	116	1	7	48	46
4	7	67	69	8	-6	133	136	12	5	43	39	1	8	39	38
4	8	81	79	8	-5	18	11	12	6	51	44	1	9	37	31
4	10	46	50	8	-4	154	153	12	7	27	21	1	10	172	173
4	11	20	19	8	-2	185	187	12	8	118	118	1	11	29	27
4	12	73	73	8	-1	20	8	12	9	36	31	1	12	52	55
4	13	30	25	8	0	35	32	12	10	62	57	1	13	34	27
4	14	41	40	8	1	29	25	12	12	85	86	1	14	134	136
4	16	88	86	8	2	167	168	12	13	22	13	1	15	24	26
4	17	22	26	8	3	30	26	14	-19	22	8	1	16	51	47
4	18	36	41	8	4	24	7	14	-18	102	96	1	17	31	37
4	19	28	25	8	5	58	58	14	-17	28	27	1	18	88	83
4	20	79	79	8	6	107	112	14	-16	68	60	1	19	32	37
4	21	23	27	8	7	52	46	14	-14	97	95	1	20	40	41
6	-26	38	38	8	9	45	49	14	-13	44	41	1	21	25	33
6	-24	87	84	8	10	103	102	14	-12	94	92	1	22	46	44
6	-23	28	43	8	11	23	28	14	-10	64	62	1	23	28	24
6	-22	78	79	8	12	33	12	14	-9	47	48	3	-24	21	23
6	-21	27	32	8	14	98	98	14	-8	113	109	3	-23	25	16

H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
3	-20	27	28	7	-16	84	82	11	-1	60	62	2	-19	21	17
3	-19	25	17	7	-14	114	119	11	0	24	11	2	-18	40	38
3	-16	49	54	7	-13	61	64	11	1	20	3	2	-17	99	95
3	-13	26	29	7	-12	111	113	11	2	78	78	2	-16	25	7
3	-12	71	76	7	-10	88	91	11	4	42	45	2	-15	27	14
3	-10	26	23	7	-9	66	63	11	6	65	68	2	-14	46	53
3	-9	45	41	7	-8	160	164	11	7	31	25	2	-13	100	99
3	-8	39	39	7	-6	106	109	11	8	74	72	2	-10	47	48
3	-7	31	24	7	-5	79	71	11	10	53	52	2	-9	94	93
3	-6	22	24	7	-4	196	193	11	11	50	41	2	-8	23	20
3	-5	38	37	7	-3	49	46	11	12	58	59	2	-7	21	23
3	-4	25	24	7	-2	56	57	13	-18	64	60	2	-5	106	106
3	-3	25	25	7	-1	59	56	13	-16	84	86	2	-4	67	67
3	-2	31	30	7	0	213	212	13	-15	50	44	2	-3	29	25
3	-1	25	32	7	1	55	55	13	-14	94	94	2	-2	26	24
3	0	20	17	7	3	40	39	13	-12	62	70	2	-1	116	117
3	1	26	16	7	4	183	180	13	-11	26	30	2	0	61	63
3	2	19	7	7	5	41	35	13	-10	125	129	2	1	24	27
3	3	41	42	7	7	34	31	13	-9	40	35	2	2	67	68
3	4	30	31	7	8	130	135	13	-8	44	33	2	3	97	98
3	5	23	8	7	9	46	44	13	-7	44	33	2	4	20	14
3	10	35	35	7	10	44	51	13	-6	145	149	2	5	23	24
3	11	32	27	7	11	39	39	13	-5	41	30	2	6	28	18
3	12	23	8	7	12	117	118	13	-4	52	49	2	7	62	60
3	18	37	33	7	13	47	50	13	-3	40	42	2	8	32	33
3	-24	27	36	7	14	59	65	13	-2	130	135	2	9	31	29
3	-23	26	6	7	15	36	32	13	-1	28	11	2	11	36	44
3	-22	40	43	7	16	92	88	13	0	52	53	2	12	34	36
3	-20	86	82	7	17	33	26	13	1	45	40	2	13	33	42
3	19	29	22	7	18	42	44	13	2	118	121	2	14	21	8
3	18	40	42	9	-23	28	4	13	5	33	33	2	15	40	39
3	17	41	33	9	-22	51	57	13	6	108	109	2	17	33	36
3	16	99	94	9	-21	25	26	13	7	35	26	2	18	31	1
3	15	21	27	9	-18	62	63	13	8	32	25	2	19	23	24
3	13	56	61	9	-17	44	44	13	9	23	16	4	-19	28	14
3	12	58	55	9	-14	59	60	15	-13	35	8	4	-18	24	25
3	11	41	42	9	-11	18	4	15	-12	56	55	4	-17	20	11
3	9	45	44	9	-10	69	71	15	-11	23	27	4	-15	24	14
3	8	159	157	9	-9	2	5	15	-10	33	27	4	-13	35	28
3	7	81	82	9	-8	50	58	15	-8	49	44	4	-11	22	27
3	6	22	9	9	-7	29	4	15	-7	28	19	4	-9	47	46
3	5	40	38	9	-6	76	72	15	-6	34	38	4	-7	27	32
3	4	207	209	9	-5	39	37	15	-5	19	5	4	-6	34	28
3	3	79	81	9	-4	48	43	15	-4	53	41	4	-5	46	47
3	2	48	47	9	-2	51	45	15	-2	41	32	4	-3	21	19
3	1	48	52	9	-1	52	48	15	1	21	19	4	-1	47	46
3	0	200	201	9	0	50	53	15	2	45	40	4	0	34	28
3	-1	80	81	9	1	21	3					4	1	23	13
3	-2	93	96	9	2	45	52	****	K =	6	****	4	2	21	6
3	-3	64	59	9	3	31	27	0	0	100	96	4	3	54	57
3	-4	168	165	9	4	38	41	0	1	159	159	4	4	38	31
3	-5	78	76	9	5	22	25	0	2	52	49	4	7	71	75
3	-6	60	63	9	6	25	36	0	3	131	133	4	8	25	13
3	-7	34	25	9	8	24	13	0	4	48	49	4	11	71	72
3	-8	105	106	9	14	26	5	0	5	147	147	4	12	42	42
3	-9	61	63	9	16	20	10	0	6	38	39	4	15	56	57
3	-10	75	79	11	-20	40	34	0	7	78	79	4	16	47	46
3	-12	90	88	11	-19	37	38	0	8	35	34	4	17	24	19
3	-13	54	59	11	-18	52	54	0	9	122	128	4	18	25	4
3	-14	110	112	11	-16	29	38	0	10	43	35	6	-22	25	27
3	-15	20	16	11	-15	36	31	0	11	42	42	6	-20	37	30
3	-16	80	78	11	-14	71	70	0	12	48	51	6	-19	96	88
3	-17	40	35	11	-11	41	41	0	13	125	124	6	-18	50	51
3	-18	96	95	11	-10	55	58	0	14	58	59	6	-17	29	30
3	-20	43	35	11	-9	21	9	0	15	50	37	6	-16	46	47
3	-24	39	32	11	-8	19	15	0	16	37	36	6	-15	123	119
3	-22	97	101	11	-7	52	54	0	17	127	119	6	-14	48	44
3	-21	39	41	11	-6	81	76	0	18	47	47	6	-13	68	65
3	-20	70	63	11	-5	57	59	0	19	31	21	6	-12	29	28
3	-19	26	11	11	-4	39	21	0	20	23	21	6	-11	129	132
3	-18	133	139	11	-3	42	37	0	21	91	86	6	-10	45	56
3	-17	70	71	11	-2	104	98	2	-21	73	65	6	-9	80	80

H	I	FO	PC	H	L	FO	PC	H	L	FO	PC	H	L	FO	PC
6	-8	33	22	10	12	25	14	3	2	27	29	9	7	33	22
6	-7	116	124	12	-16	32	20	3	4	24	8	11	-13	31	29
6	-6	82	83	12	-15	23	27	3	5	23	15	11	-11	29	33
6	-5	89	89	12	-14	30	38	3	6	20	19	11	-10	25	23
6	-4	29	23	12	-13	77	78	3	10	21	5	11	-9	51	46
6	-3	109	111	12	-12	38	38	3	17	28	4	11	-7	28	33
6	-2	79	80	12	-11	59	53	5	-17	60	59	11	-5	52	49
6	-1	116	109	12	-9	78	79	5	-15	35	40	11	-4	25	4
6	0	24	18	12	-8	69	61	5	-14	26	13	11	-3	42	31
6	1	95	93	12	-7	81	77	5	-13	75	75	11	-1	65	59
6	2	77	79	12	-6	23	15	5	-12	42	44	11	0	28	20
6	3	128	129	12	-5	84	86	5	-11	76	74	11	1	26	26
6	4	22	12	12	-4	92	82	5	-10	22	12	11	2	23	18
6	5	77	78	12	-3	80	85	5	-9	86	83	11	3	66	65
6	6	50	56	12	-1	84	85	5	-8	24	23				
6	7	136	139	12	0	73	70	5	-7	82	86	****	K =	8	****
6	8	28	18	12	1	77	82	5	-5	69	67	0	0	135	131
6	9	63	62	12	3	68	65	5	-3	96	101	0	1	73	77
6	10	37	38	12	4	45	44	5	-1	54	56	0	2	22	22
6	11	125	129	12	5	75	76	5	0	20	15	0	3	46	40
6	12	43	38	12	6	36	38	5	1	104	106	0	4	126	126
6	13	27	26	12	7	32	36	5	2	22	15	0	5	101	102
6	14	45	43	14	-10	26	34	5	3	43	42	0	6	44	36
6	15	94	93	14	-9	86	87	5	4	24	29	0	7	44	28
6	16	23	25	14	-6	25	34	5	5	122	121	0	8	99	103
8	-21	24	23	14	-5	82	87	5	6	30	6	0	9	86	87
8	-20	39	29	14	-4	41	43	5	7	34	34	0	10	30	34
8	-19	65	68	14	-3	20	25	5	8	39	48	0	11	27	14
8	-18	28	8	14	-2	20	24	5	9	117	120	0	12	76	75
8	-16	29	32	14	-1	82	79	5	10	21	11	0	13	64	68
8	-15	104	104	14	0	34	27	5	12	35	30	0	14	33	40
8	-13	28	13					5	13	83	86	0	15	24	6
8	-12	25	28	****	K =	7	****	5	14	23	14	2	-15	24	22
8	-11	124	124	1	-19	81	81	5	15	29	20	2	-14	51	47
8	-10	37	38	1	-18	33	22	7	-18	20	19	2	-13	46	42
8	-8	51	45	1	-15	125	125	7	-17	85	84	2	-12	29	36
8	-7	116	113	1	-14	45	41	7	-16	20	30	2	-11	35	30
8	-6	40	43	1	-11	145	145	7	-15	29	4	2	-10	45	45
8	-4	43	42	1	-10	54	55	7	-13	132	128	2	-9	51	53
8	-3	108	103	1	-8	38	31	7	-12	48	52	2	-8	49	53
8	-2	42	43	1	-7	155	156	7	-11	37	26	2	-7	30	28
8	-1	47	37	1	-6	57	52	7	-10	38	25	2	-6	46	53
8	0	21	23	1	-5	43	38	7	-9	141	143	2	-5	67	69
8	1	99	99	1	-4	63	53	7	-8	51	45	2	-4	59	61
8	2	63	62	1	-3	154	155	7	-7	43	46	2	-2	39	43
8	3	52	51	1	-2	21	19	7	-6	21	9	2	-1	48	57
8	4	24	20	1	-1	64	67	7	-5	129	129	2	0	62	65
8	5	88	89	1	1	125	127	7	-4	58	50	2	1	35	27
8	6	33	35	1	2	43	39	7	-3	68	66	2	2	25	21
8	7	56	53	1	3	100	104	7	-2	25	11	2	3	47	48
8	8	26	1	1	4	34	32	7	-1	119	122	2	4	57	58
8	9	60	60	1	5	103	107	7	0	54	54	2	5	36	37
8	11	40	43	1	6	60	61	7	1	80	78	2	7	41	35
8	12	22	2	1	7	102	104	7	3	104	108	2	8	38	38
8	13	24	28	1	9	75	77	7	4	61	56	2	9	32	29
8	14	31	21	1	10	39	38	7	5	96	95	2	11	35	23
8	15	34	28	1	11	105	101	7	7	83	81	2	12	33	32
10	-15	26	8	1	13	47	54	7	8	55	55	2	13	35	24
10	-11	24	14	1	14	36	28	7	9	81	85	4	-10	37	47
10	-9	23	5	1	15	88	88	7	11	35	38	4	-9	23	21
10	-7	21	5	1	16	24	2	7	12	30	22	4	-6	43	39
10	-6	28	35	1	17	38	33	7	13	63	63	4	-5	20	26
10	-3	38	29	1	18	36	17	9	-13	43	44	4	-2	37	33
10	-1	22	0	3	19	26	34	9	-9	55	51	4	-1	35	35
10	0	25	29	3	15	48	43	9	-8	35	25	4	0	27	22
10	1	27	27	3	13	25	24	9	-7	20	12	4	2	25	37
10	2	19	22	3	11	37	33	9	-5	55	47	4	3	41	38
10	5	27	20	3	10	23	23	9	-4	27	39	4	4	41	37
10	7	21	16	3	7	35	36	9	-2	31	30	4	6	44	45
10	9	36	31	3	3	27	36	9	-1	46	45	4	7	52	44
10	10	37	26	3	2	25	2	9	2	31	18	4	8	49	46
10	11	24	17	3	1	26	30	9	3	34	37	4	10	41	40

H	L	FO	FC	H	L	FO	FC	H	L	FO	FC	H	L	FO	FC
4	11	31	26	6	-1	58	55	8	-8	44	45	10	-4	32	23
4	12	35	36	6	1	41	38	8	-7	54	47	10	-2	28	13
6	-14	81	81	6	2	100	102	8	-6	57	51				
6	-12	29	35	6	3	65	66	8	-5	22	2	****	K =	9	****
6	-11	71	70	6	4	33	27	8	-4	23	31	1	-8	37	39
6	-10	106	108	6	5	34	29	8	-3	43	40	1	-6	74	68
6	-9	28	18	6	6	106	106	8	-2	49	48	1	-4	33	35
6	-8	35	31	6	7	68	66	8	0	29	21	1	-2	95	94
6	-7	65	72	6	8	29	33	8	1	40	41	3	-4	20	8
6	-6	102	102	8	-12	53	53	8	2	53	53	3	-3	31	16
6	-5	33	38	8	-11	61	59	8	3	22	12	5	-4	62	69
6	-3	49	55	8	-10	50	48	8	5	31	44	5	-3	28	25
6	-2	92	96	8	-9	23	11	8	6	50	53	5	-1	34	18

AD-A050 502 CALIFORNIA UNIV LOS ANGELES DEPT OF CHEMISTRY F/G 7/2
STRUCTURES OF METALLOCARBORANES. IX. CRYSTAL AND MOLECULAR STRU--ETC(U)
JAN 78 G E HARDY, K P CALLAHAN, M F HAWTHORNE N00014-76-C-0390

UNCLASSIFIED TR-100 NL

2 OF 2
AD
A050502

END
DATE
FILMED
7-78
DDC

SUPPLEMENTARY

INFORMATION

AD-A050 502

'ERSITY OF CALIFORNIA, LOS ANGELES

EY • DAVIS • IRVINE • LOS ANGELES • RIVERSIDE • SAN DIEGO • SAN FRANCISCO

SANTA BARBARA • SANTA CRUZ

DEPARTMENT OF CHEMISTRY
LOS ANGELES, CALIFORNIA 90024

February 24, 1978

TO: Technical Report Distribution List

FROM: M. F. Hawthorne

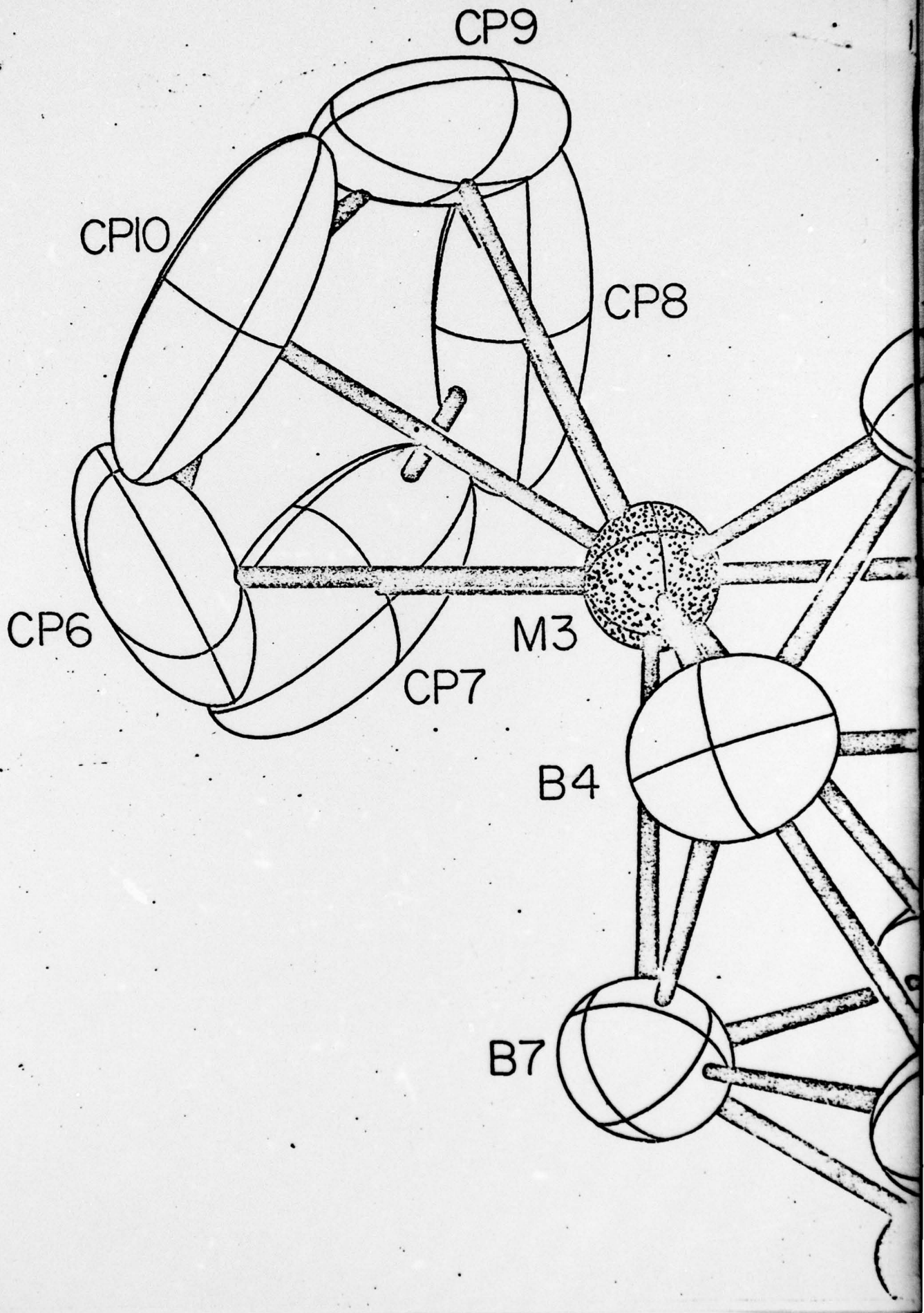
RE: TR's 100 and 101 - corrections, missing page, and missing figure

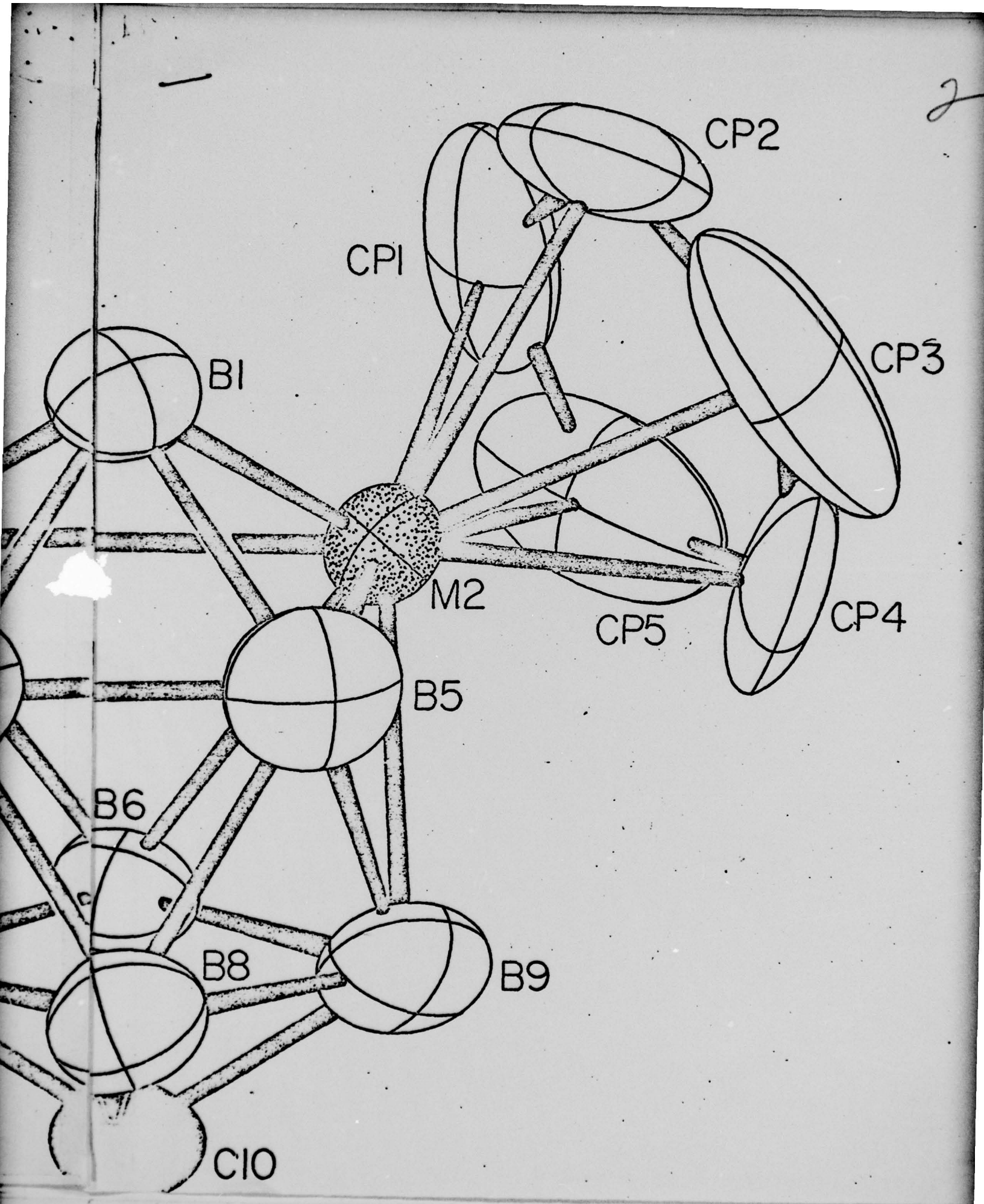
Please insert the enclosed corrected and missing pages to the technical reports we sent you recently:

The figure goes with TR 100, entitled "Structures of Metallocarboranes. IX. Crystal and Molecular Structure of the Ten-Vertex . . .," by G. E. Hardy, K. P. Callahan, and M. F. Hawthorne. It should be placed behind the last page of Table IV.

Page 15 goes with TR 101, entitled "Synthesis of Closo- and Nido-Metallocenes," by R. N. Leyden, B. P. Sullivan, R. T. Baker, and M. F. Hawthorne. Please replace the old page 15 with this newly corrected copy.

Page 25 also goes with TR 101. This reference page was missing from the copy we sent you.


CP9
CP10
CP8
CP6
M3
CP7
B4
B7


CP2
CP1
CP3
B1
M2
CP5
CP4
B5
B6
B8
B9
C10