INORGANIC CHEMISTRY

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Time Required: 15 Mint

Pentakis (arylisocyanide) cobalt (I) Complexes

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ACS Division Member?

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Plan ACS\_\_\_nonACS\_X publication. Where? Zeitschrift für Naturforschung No\_\_\_Uncertain\_

Presentation requires projector: 2x2" (35 mm) X 3½ x4" (standard) Overhead Vu-Graph Film: 8 mm Sound Other equipment (specify)

ABSTRACT. 200 words or equivalent. TITLE OF PAPER, Authors' Names, Addresses with Zip Code, One-Line Space, Abstract. Single-space typing. Use full width of ruled area below.

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SOLUTION STRUCTURE OF MONO- AND DISUBSTITUTED PENTAKIS (ARYLISOCYANIDE) - COBALT (I) COMPLEXES. Clifford A.L. Becker, Department of Chemistry, the American University of Beirut, Beirut, LEBANON; and George C. Papavassiliou, Physical Chemistry Institute, the National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 501, GREECE.

The v(-N≡C) for twenty-eight mono- and disubstituted pentakis(arylisocyanide)cobalt(I) complexes are investigated by IR and Raman spectroscopy in CH2Cl2-solution at 25 Co. Inverse application of Angular-Overlap approximation is made to help identify the proposed structures. The  $[Co(CNR)_4L]X$ ,  $L = P(OPh)_3$ ,  $P(OC_6H_4Cl-p)_3$ ;  $X = ClO_4$ ,  $BF_4$ ; are interpreted as C<sub>3v</sub> axially-substituted trigonal bipyramidal, but increase of the ∠PCoC (equatorial) and Co-C(axial) bond length are suggested. The  $[Co(CNR)_3L_2]X$ ,  $L = P(OMe)_3$ , P(OEt)<sub>3</sub>, P(OPr-i)<sub>3</sub>; are interpreted as  $C_{2v}$ -distorted axially-disubstituted trigonal bipyramidal, in which one equatorial ∠CCoC is diminished to allow increased d<sub>m</sub>+π\*-acceptance through Co  $3d_{x^2-v^2}$ . The ZPCoP is probably linear but the unique Co-C(equatorial) bond could be shortened. The [Co(CNR)3 (PPh3)2]X are also interpreted as C2v-distorted trigonal bipyramidal, but with larger distortions as befits decreasing  $d_{11} \rightarrow \pi^*$  accepting ability: RNC > P(OMe)<sub>3</sub> > PPh<sub>3</sub>. The [Co(CNR)<sub>4</sub>PPh<sub>3</sub>]X are interpreted as  $C_{5}$ -distorted axially-substituted trigonal bipyramidal through spectra analogy with PPh3-disubstituted complexes and dissimilarity with  $C_{3v}$  [Co(CNR)<sub>4</sub>L]X. The [Co(CNPh)<sub>3</sub>L<sub>2</sub>]X, L = P(OPh)<sub>3</sub>, P(CC6H4Cl-p)3; are different in solution than crystalline state, but clearly not D3h axially-disubstituted trigonal bipyramidal. A Cs axial-equatorial disubstituted trigonal bipyramidal solution-structure is tentatively suggested.

