C-H** π Interactions in the Novel Ni(II) Complex with Tetradentate Thiosemicarbazide Based Ligand

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 $[4-(2-diphenylphosphino-\alpha-ethoxy-benzyl-P)-3-methyl-1-acetyla$ cetone-isothiosemicarbazido-N1,N4,O]nickel(II), Ni(C₂₈H₃₀N₃O₂SP)],represents one of the rare examples of transition metal complexes withS-alkylisothiosemicarbazide-derived ligands where a phosphorus atomis involved in the coordination sphere of the metal atom. The Ni(II)atom in the [Ni(C₂₈H₃₀N₃O₂SP)] complex has a distorted squareplanar configuration formed by a thiosemicarbazide-based tetradentateligand with ONNP donor atoms. This complex molecule containsthree condensed chelate rings. The six-membered chelate ringcontaining the P atom adopts an unusual boat conformation, while theother two chelate rings are planar.

The crystal structure has been determined by a single-crystal Xray analysis and refined to a final R = 0.044 for 10824 reflections and 657 parameters. Two independent molecules with the same composition exist in the asymmetric unit. There are no hydrogen bonds in the crystal structure but crystal packing is stabilized by eight C-H… π and four π … π interactions. Some of the C-H… π interactions are with the H…Cg distance shorter than 2.70Å (Cg is the centroid of five- or six-membered ring with delocalized π bonds). Two of the C-H… π interactions are intramolecular and play a very significant role in the orientation of phenyl rings and -OCH₂CH₃ fragments.

Keywords: C-H··· π interaction, Ni(II) complex, thiosemicarbazide