SINGLE CRYSTAL X-RAY DIFFRACTION STUDY OF DIOXANE, PYRAZINE, AND PYRIDINE COMPLEXES OF 3-(1-AMINO-2,2,2-TRIFLUOROETHYLIDENE)-2-IMINO-1,1,4,5,6,7-HEXAFLUOROINDAN

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Single crystals of complexes of 3-(1-amino-2,2,2-trifluoroethylidene)-2-imino-1,1,4,5,6,7-hexafluoroindan (**1**) with 1,4-dioxane, pyrazine, and pyridine have been synthesized. Their structure was investigated by X-ray analysis. In crystals of the dioxane complex, compound **1** is present together with its tautomer — 2-amino-3-(1-imino-2,2,2-trifluoroethyl)-1,1,4,5,6,7-hexafluoroindene (**1a**), and these compounds are in an equilibrium ratio of ~60:40. Gas-phase quantum chemical calculations have been performed to examine the possibility of a tautomeric equilibrium of enaminoimine **1** in the corresponding complexes.

Keywords: polyfluorinated enaminoimines, indan, indene, synthesis, structure, X-ray diffraction analysis, tautomers, quantum chemical calculations.