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## ABSTRACT BOOK

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# An experimental and theoretical study of one redox-active ligand

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The crystal and molecular structure of *bis*(2-isobutyrylamidophenyl)amine has been determined from single crystal X-ray diffraction data [1]. It crystallizes in the triclinic space group *P-1*, Z = 2 with *a* = 9.5377(9) Å, *b* = 10.9710(10) Å, *c* = 18.6693(15) Å, α = 76.644(6)°, β = 80.010(6)°, γ = 81.379(7)°, and $D_{calc}$ = 1.212 mg/m$^3$. The molecular structure, vibrational frequencies and infrared intensities of *bis*(2-isobutyrylamidophenyl) amine were calculated by ab initio Hartree-Fock and Density Functional Theory methods (BLYP, B3PW91 and B3LYP) using the 6-31G(d,p) basis set [2]. The calculated geometric parameters were compared to the corresponding X-ray structure of the title compound. The harmonic vibrations computed for this compound by the B3LYP/6-31G(d,p) method are in good agreement with the observed IR spectral data. Theoretical vibrational spectra of the title compound were interpreted by means of PEDs using the SQM 2.0 program. A general better performance of the investigated methods was calculated by PAVF 1.0 program.

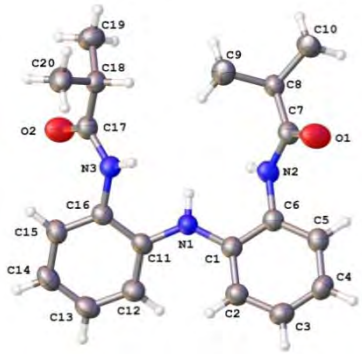


Figure 1. Molecular structure of *bis*(2-isobutyrylamidophenyl)amine.

***Keywords*:** Redox-active ligand, Ab-initio calculations, Infrared spectrum, DFT, B3LYP, BLYP, B3PW91.

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