NON-PLANAR STRUCTURES OF THE HIGH-ENERGY ROTATIONAL CONFORMERS OF 2-METHYLBUTA-1,3-DIENE (ISOPRENE) AND 2,3-DIMETHYLBUTA-1,3-DIENE

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Optimization of the geometrical parameters and determination of the force fields for rotamers of the title molecules were performed at the MP2(FC)/aug-cc-pVDZ//MP2(FC)/aug-cc-pVDZ computational level. The vibrational analyses of these conformers were carried out using scaled quantum-mechanical force field methodology. Recent experimental wavenumbers for these conformers and their deuteroisomers were incorporated into these analyses. The theoretical non-planar structures of the high-energy conformers of 2-methylbuta-1,3-diene (isoprene) and 2,3-dimethylbuta-1,3-diene were corroborated by good agreement between the experimental and theoretical wavenumbers of the molecules under investigation. The dihedral angles of the non-planar high-energy conformers for rotation around the =C–C= bond are as follows: 41.6° for 2-methylbuta-1,3-diene (isoprene)[a] and 47.0° for 2,3-dimethylbuta-1,3-diene[b]. Previous studies performed at the HF/6-31G level gave 41.0° and 48.5° for the first and second compounds, respectively.

[a] Yu. N. Panchenko, Ch. W. Bock, J. D. Larkin, A. V. Abramenkov, F. Kühnemann, *Struct. Chem.* 19, 421 (2008).
[b] Yu. N. Panchenko, Ch. W. Bock, J. D. Larkin, A. V. Abramenkov, *Struct. Chem.* 19, 793 (2008).