

**Cryospectroscopic and *ab initio* studies of noncovalent interactions
between volatile anesthetics (enflurane, isoflurane) and dimethyl ether.
Spectroscopic evidence of trimer formation**

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Volatile halogenated hydrocarbons and ethers reveal strong analgesic and anesthetic effects. Among these compounds, enflurane and isoflurane belong to isomers which often used for purposes of invasive surgery. These halogenated compounds possess two CH groups which can act as weak CH donor in interactions with targets of acceptor property [1-3]. One of the simplest acceptors including O atom with lone electron pair is dimethyl ether (DME). The attention focuses on the features of noncovalent interactions between these isomers (particularly isoflurane) and DME. As an experimental tool effective in detection of weak complex formation, the FTIR spectroscopy of cryosolutions has been chosen.

Cryospectroscopic measurements, performed with isoflurane dissolved in liquefied Kr and Xe, have shown that the basic features of the temperature changes in the region of CH stretching bands are defined by two largely populated rotamers [4]. However, at T~118 – 130 K only one the most stable conformer lettered by *a*, with two CH groups contrarily oriented, possess c.a. 90 % of the whole population. Thus, it contributes predominantly to the IR spectrum registered in liquefied Kr.

In the case of enflurane, the FCICH and CHF₂ groups act as CH donors of somewhat different strength when interacting with dimethyl ether ((CD₃)₂O). It is worth noting that the complexes formed are stabilized by so called blue-shifting H-bonds predominantly. In the case of isoflurane one can expect that both CH groups will interact with molecular acceptors in a similar way. Somewhat stronger complexes are expected to be formed when H atom of CHFCl-group is engaged in H-bonding type interactions. In this report, the results on the cryospectroscopic temperature studies of isoflurane + dimethyl ether (DME) mixtures dissolved in liquefied Kr are presented at a wide range of concentrations. *Ab initio* calculations were made to obtain geometric and spectroscopic parameters of stable forms of dimers and trimer, and to interpret temperature and concentration changes revealed in the IR spectrum of the system studied. To avoid the overlapping effect in the region of CH stretching vibrations the wholly deuterium substituted form of DME was used.

The calculations have been performed using the computer resources of the Resource Centre of SPbGU (<http://cc.spbu.ru>). The spectroscopic measurements were partly performed on the apparatus of the Resource Center Geomodel of SPbGU.

References:

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