within the cement matrix could be reliably identified using powder diffraction and structural data bases. The search-match procedure was based only on experimental diffraction data from selected areas or selected crystals of the samples and qualitative information about their chemical composition. No other knowledge about mineral composition of the samples was required. The results were substantiated by crystal structure refinement against collected in situ intensity data. Some software issues and developments for routine operation will be presented. The future application of the developments is to identify newly formed mineral species in the chemically disturbed zone at the cement-Opalinus clay interface with micro-scale resolution.

Keywords: identification; cements; microdiffraction

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Biphenyls in Crystals: Conformations and Intermolecular Contacts. Olga V. Grineva. *Moscow M.V. Lomonosov State University, Chemistry Department, Moscow, Russia.*
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It is known that dihedral angle between phenyl planes in biphenyl molecule (φ) in gas phase is about 45° while in three solid phases it does not exceed 10°. There are several papers with statistical data concerning this parameter in substituted biphenyls (e. g. [1-3]) however they do not illuminate connections between preferential conformations of molecules and types of substituents or intermolecular contacts.
In this work, a comprehensive analysis of crystals containing biphenyls with small substituents (namely halogen atoms, OH, COOH, NH_2, NO_2, CN, CH_3, CF_3 and similar groups) was made on the basis of the Cambridge Structural Database. Structures with some other biphenyls were considered for comparison. Values of φ were investigated in relation to types and number of substituents, their positions, intermolecular contacts and supramolecular motifs.
For example, it was found [4] that as one could expect a fraction of planar and almost planar molecules (φ was in the interval from 0 to 5°) was higher (37 %) for 4,4'-biphenyls with small substituents than for biphenyls with arbitrary substituents in the 3,3',4,4',5,5'-positions (26 %) but besides this fraction was considerably higher for 4,4'-biphenyls having at least one OH-group (48 %). Specific intermolecular contacts (hydrogen bonds, halogen...halogen contacts and others) often lead to formation of infinite molecular chains or their fragments (trimers, dimers) in the crystals with 4,4'-biphenyls, connecting chemically different molecules in heteromolecular crystals.
It was revealed that position of a peak in φ distribution for biphenyls with one small ortho-substituent was almost the same (50°) as for biphenyls with one arbitrary ortho-substituent [3] though the range of the angle was narrower (from 38 to 70°). In case of biphenyls with four small ortho-substituents the angle changed from 70 (mainly from 80) to 90° with a peak at 85° except the biphenyls with four ortho-fluorine atoms having φ between 50 and 61°.

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