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and

100th Anniversary of Bray-Liebhafsky reaction

N-03-P
THEORETICAL STUDY OF GEOMETRIES AND ENERGIES OF THE Pt···H INTERACTIONS

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Geometries and energies of Pt···H interactions were studied using analysis of crystallographic data and quantum chemical calculations. Cambridge Structural Database (CSD) was searched for all crystal structures containing X-Pt···H-OH interactions. Analysis of geometrical parameters in crystal structures showed that in majority of crystal structures X-Pt···H interactions do not have tendency for linear arrangement. Based on the results of analysis of geometrical parameters, model systems for quantum chemical calculations were made. Results of quantum chemical calculations showed that in case of linear X-Pt···H arrangement (angle X-Pt-H = 180°) between PtS molecule and water calculated intermolecular interactions are repulsive, while in case of X-Pt···H interaction with the X-Pt-H angle value of 90° the interaction is attractive (ΔE = -2.42 kcal/mol). These results of quantum chemical calculations are in good agreement with the results of the analysis of crystallographic data.

N-04-P
SYNERGISM IN THE EXTRACTION OF CATECHOL AND HYDROQUINONE FROM AQUEOUS SOLUTIONS BY THE DIETHYL ETHER/1-BUTANOL MIXTURES

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Synergic effect in the extraction of catechol and hydroquinone from aqueous solutions by the diethyl ether/1-butanol solvent mixtures was investigated. Higher distribution ratios for both catechol and hydroquinone were obtained in the whole composition range of the diethyl ether/1-butanol binary mixture in comparison to extraction with pure solvents. For the same organic phases distribution ratios for catechol were higher than for hydroquinone, but the values of synergic coefficients were higher for hydroquinone.