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Separation of Trimethoxybenzene Isomers by Bile Acids

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Molecular selectivity by host-guest procedures is an increasing method to help in the separation of enantiomers. In this study, two similar bile acids, cholic acid (CA) and deoxycholic acid (DCA), were used as hosts to separate the mixtures of several isomer guests. The different compounds prepared were analyzed by single crystal X-Ray diffraction. Our first guest mixtures were the isomers of trimethoxybenzene (TMB) whose normal boiling points range from 241 to 255°C. We prepared equimolar mixtures of the three isomers in pairs and dissolved the CA/DCA host in them, such that the total guest to host ratio was 5. The selectivity preference is CA: TMB135 > TMB123 ≈ TMB124, while it is reversed for DCA: TMB123 > TMB124 > TMB135. Some of the crystal structures with CA as host suffered from partial disorder, while the DCA structures were grown from pairs of equimolar guest mixtures, and all contained both guests in different proportions. Packing analysis revealed the importance of layering of the hydrophilic and lipophilic regions of the structures with the TMB guests accommodated in the lipophilic layers. Further analytical measurements carried out by NMR are in agreement with the structural results.

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