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Participation of Aliphatic C-H hydrogen Bonding in anion Recognition

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Abstract

Enthalpically and entropically favorable anion receptors **1** and **2** are developed. The receptor **1** and **2** utilize 4 hydrogen bonds to bind halide anions. Receptor **1** utilizes two imidazolium (C-H)⁺---A⁻ hydrogen bonds, one aliphatic methine C-H---A⁻ hydrogen bond and one aromatic C-H---A⁻ hydrogen bond for anion binding, while receptor **2** utilizes one aliphatic methine C-H---A⁻ hydrogen bond and one aromatic C-H---A⁻ hydrogen bond and two aliphatic(methyl) C-H----A⁻ hydrogen bonds instead of imidazolium (C-H)⁺---A⁻ hydrogen bond for anion binding. By comparing anion affinity for these anion receptors it has been found that aliphatic C-H---A⁻ hydrogen bonds are comparable in strength to their imidazolium (C-H)⁺---A⁻ counterparts and well designed aliphatic C-H hydrogen bond could be a viable hydrogen bond interaction motif for anion host design.

Key words: hydrogen bond, C-H hydrogen bond, anion receptor

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