# Locating structure directing agent and Al in CHA: Combined study of structure determination of X-ray powder diffraction and classical lattice energy calculation

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Locating the structure directing agent and Al in zeolite CHA has been performed using structure determination of X ray powder diffraction combined with General Utility Lattice Program (GULP) calculation. Trimethyladamantylammonium ion ($TMAdaOH^+$) and benzyltrimethyl ammonium ion ($BTMAOH^+$) respectively have been found to fit in the pore, resulting in the formation of zeolite CHA which shows the superior catalytic performance in abatement of NOx using $NH_3$ in the exhaust gas stream of mobile car. The intimate interaction between the corresponding structure directing agent (SDA) and the counter ion due to the Al substitution in the framework has been characterized using the lattice energy calculation. The difference in the lattice energy of the zeolite CHA prepared with TMAdaOH was large compared to that of the zeolite CHA prepared with BTMAOH, which can be attributed probably to the molecule's size. Thereby, the SDA in the zeolite pore has been located readily and the resulting information can be useful for increasing the understanding in the zeolite formation mechanism and designing novel zeolite.