

LIST OF TABLES

Table		Page
1	Binding energy of ethylene, benzene and ethylbenzene on the Brønsted proton of faujasite zeolites (binding energy in kcal/mol)	59
2	The optimized geometric parameters of isolated zeolite clusters (20T and ONIOM model), ethylene adsorption complex, transition state (TS1), and alkoxide intermediate of steps (1) and (2) on FAU using ONIOM3 (distances are in angstroms and angles are in degrees)	65
3	The optimized geometric parameters of benzene–alkoxide adsorption complex, transition state (TS2), and product ethylbenzene adsorption of step (3) on FAU using ONIOM3 (distances are in angstroms and angles are in degrees)	70
4	The optimized geometric parameters of the ethylene-alkoxide adsorption complex, second transition state (TS2) and product butoxide of step 3 on faujasite (FAU) using the ONIOM3. Distances are in angstroms and angles are in degrees	74
5	The optimized geometric parameters of isolated molecule, co-adsorption complex, transition state (TS), and product of concerted reaction of benzene alkylation on FAU using ONIOM3 (distances are in angstroms and angles are in degrees)	78
6	The optimized geometric parameters of the isolated molecule, co-adsorption complex, transition state (TS) and product butoxide of concerted reaction of dimerization of ethylene on faujasite (FAU) using the ONIOM3.	82
7	The optimized geometric parameters of the zeolite 5T and 46T clusters calculated at B3LYP/ 6-31G(d,p) and ONIOM(B3LYP/6-31G(d,p):UFF) levels	86

LIST OF TABLES (continued)

Table		Page
8	The relevant parameters for the propene oxide, propanal, and propanone adsorbed on 5T and 46T H-ZSM-5 zeolite clusters	88
9	The calculated relative energies (kcal/mol) of reactant, first-transition state (TS1), intermediate, second-transition state (TS2), product, first activation energy barrier (ΔE_{a1}), and second activation energy barrier (ΔE_{a2}) for the isomerization reaction of propene oxide over 5T and 46T clusters of H-ZSM-5 calculated at B3LYP/6-31G(d,p) and ONIOM (B3LYP/6-31G(d,p): UFF) levels	93
10	The relative and activation barrier energies regarding the N ₂ O decomposition on the bare perfect and the defective SWNTs and the Chloride anion doped perfect and the defective SWNTs	107
11	The charge gained on N ₂ O of all stationary points of N ₂ O decomposition on the bare perfect site (pSWNT), the defective site (dSWNT) and the Chloride anion doped perfect site (Cl ⁻ @pSWNT), the defective site (Cl ⁻ @dSWNT) of (5,5) SWNT	107