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LIST OF ABBREVIATION

B3LYP	=	Becke's three parameter hybrid functional using the LYP correlation functional
BR	=	Beckmann rearrangement
DFT	=	Density functional theory
FAU	=	Faujasite
FT-IR	=	Fourier Transform Infrared spectroscopy
GGA	=	Generalized gradient approximation
HF	=	Hartree Fock
H-ZSM-5	=	Proton-exchanged zeolite ZSM-5
H-FAU	=	Proton-exchanged zeolite FAU
LDA	=	Local density approximation
MAS-NMR	=	Magic-angle spinning Nuclear Magnetic Resonance
MP2	=	The second order Møller-Plesset perturbation theory
MOR	=	Mordenite
NMR	=	Nuclear Magnetic Resonance
SCREEP	=	Surface Charge Representation of the Electrostatic Embedding Potential
T	=	Tetrahedral
ZSM-5	=	Zeolite Scony Mobile-structure 5
6-31G(d,p)	=	Pople valence double zeta plus d and p polarization functions for heavy atom and hydrogen atoms
6-311G(d,p)	=	Pople valence triple zeta plus d and p polarization functions for heavy atom and hydrogen atoms