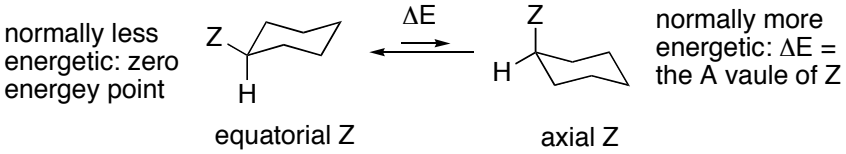
Table of A-Values

CHEM 330 handout

Conformational Free Energy Difference (ΔG, kcal/mol) for Common Substituents X in Cyclohexanes



X	A-value kcal/mol		X	A-value kcal/mol		X	A-value kcal/mol
F	**0.24**		**SMe**	**1.0**		**CH_3**	**1.8**
Cl	**0.4**		**SPh**	**1.2**		**CH_2CH_3**	**2.0**
Br	**0.2-0.7**		**S(O)Me**	**1.2**		**i-C_3H_7**	**2.2**
I	**0.4**		**$S(O)_2Me$**	**2.5**		**c-C_6H_{11}**	**2.2**
OH	**0.6 (0.9*)**		**NH_2**	**1.2 (1.8*)**		**t-C_4H_9**	**> 4.5**
OMe	**0.7**		**$NH_3^{(+)}$**	**1.9**		**ethynyl**	**0.2**
OEt	**0.9**		**NHMe**	**1.0**		**C_6H_5**	**3.0**
OAc	**0.7**		**NMe_2**	**2.1**		**COOH**	**1.2**
OTs	**0.7**		**$NMe_3^{(+)}$**	**2.4**		**$COO^{(-)}$**	**2.2**
OTMS	**0.7**		**NO_2**	**1.0**		**COOMe**	**1.1**
SH	**1.2**		**N_3**	**0.5**		**CN**	**0.2**

*** In H-bonding solvents**