

MOE Exercises Chpts. 4, 6, 11, 12

Name _____

4.1

Contribution	camphor (kcal/mol)	Comparison (kcal/mol)	difference (kcal/mol)	avored conformer
bond <u>str</u> energy				
<u>angle</u> energy				
<u>torsional</u> energy				
<u>Van der Waals</u>				
<u>electrostatic</u>				
total				

Does this comparison bare out the expectation that camphor is a highly strained molecule?

Which term in the force field shows the strain best?

Structure:

6.1. (a) Enthalpy of formation from bond energy tables:

(b) Reaction you used to calculate the enthalpy of formation from the experimental enthalpy of combustion:

Enthalpy of formation for solid camphor from the enthalpy of combustion _____

Enthalpy of formation for camphor (gas) from the enthalpy of combustion _____

(c) MM3 steric energy _____ MM3 bond energy _____

MM3 enthalpy of formation _____

6.3

compound	Literature $\Delta_f H^\circ(g)$ kcal/mol	Calculated $\Delta_f H^\circ MM3$	Δ kcal/ mol	torsional increments		Calculated $\Delta_f H^\circ MM3$ + total increment	new Δ kcal/ mol	% improv- ment
				# free rotations	total increment kcal/mol			
n-pentane	-35.00							
1-pentene	-5.00							
<i>cis</i> -2-pentene	-6.71							
<i>trans</i> -2-pentene								
2-methyl-1-butene								

11.1 The cavity diameter increased/decreased by _____% with waters present.

12.1

Potential energy terms in kcal mol⁻¹:

term	complex	CD	naphthol	difference	favors
stretch					
angle					
str-bend					
torsion					
oop					
electrostatic					
Van der Waals					
total (kcal/mol)					

Final binding energy result= _____kcal/mol.

The dominant term in the gas phase is the favorable/unfavorable _____ interaction.