Name:_____

CHEMISTRY 5021/8021
MIDTERM EXAM — SPRING 2003

1. ENTHALPY (150 points)

A commonly tabulated molecular thermodynamic quantity is the 298 K heat of formation. Explain in as detailed a fashion as possible how this quantity is typically computed at the below levels of theory. In addition, comment on roughly how good or bad the given approach is for the calculation of this property and provide some reason for *why* it is particularly good or bad. You may find choosing a specific example or examples to helpful at various points, and you should feel free to use them, although they are not required.

a) Directly using the MMX force field (30 points).

(use back of next page if required)

b) Directly using AM1 (30 points).

(use back of next page if required)

c) Directly at the MP2/6-31+G(d) level (30 points).

(use back of next page if required)

d) Directly at the G3 level (30 points).

(use back of next page if required)

e) Using an isodesmic equation in conjunction with an arbitrarily chosen level (30 points).

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