

**Table II.** Intrinsic Binding Energies (kcal mol<sup>-1</sup>)

| no. | group                          | energy | range <sup>a</sup> |
|-----|--------------------------------|--------|--------------------|
| 1   | DOF <sup>b</sup>               | -0.7   | -0.7--1.0          |
| 2   | C(sp <sup>2</sup> )            | 0.7    | 0.6-0.8            |
| 3   | C(sp <sup>3</sup> )            | 0.8    | 0.1-1.0            |
| 4   | N <sup>+</sup>                 | 11.5   | 10.4-15.0          |
| 5   | N                              | 1.2    | 0.8-1.8            |
| 6   | CO <sub>2</sub> <sup>-</sup>   | 8.2    | 7.3-10.3           |
| 7   | OPO <sub>3</sub> <sup>2-</sup> | 10.0   | 7.7-10.6           |
| 8   | OH                             | 2.5    | 2.5-4.0            |
| 9   | C=O                            | 3.4    | 3.2-4.0            |
| 10  | O,S                            | 1.1    | 0.7-2.0            |
| 11  | halogen                        | 1.3    | 0.2-2.0            |

<sup>a</sup> Range of energies for six random 100-compound data sets.

<sup>b</sup> Degrees of internal conformational freedom.