

**Table 3. Electrostatic Contribution to the Catalytic Effects of Specific Enzymes<sup>a</sup>**

system	$(\Delta\Delta g_{\text{tot}}^{\ddagger})_{\text{calc}}$	$(\Delta\Delta g_{\text{elect}}^{\ddagger})_{\text{calc}}$	$(\Delta\Delta g_{\text{cage}}^{\ddagger})_{\text{calc}}$	$\Delta\Delta g_{\text{obs}}^{\ddagger}$	ref
DhlA	11.6	8 <sup>b</sup> (8)	2.3	11.7	95, 96
CM	10.3	8 (14)	0.0	9.1	90
ODCase	19.0	17 <sup>c</sup>		23.0	36
ribosome	8.0	− (8)	0.0	6.0	97

<sup>a</sup> The table compares the total calculated catalytic effect and the corresponding electrostatic contribution. All energies are given in kcal/mol. <sup>b</sup> Obtained by taking the calculated catalytic effect of ref 95 and multiplying it by the percent contribution obtained in ref 96. The values within parentheses were obtained by the LRA approach. <sup>c</sup> Obtained by FEP calculations of the binding energy of the RS and TS.