TABLE 8 The Difference in Potential Energy Surface (PES) Between Protonated 3-(Diethyl-amino) propylamine and 1,3-Diaminopentane Structures

Model/Basis Set	ΔE (kJ·mol^{-1})	
	3-(Diethylamino) propylamine	1,3-Diaminopentane
HF/6-311G+(d,p)	64.91	-7.13
DFT/B3LYP/3-21G	5.72	-17.71
DFT/B3LYP/6-311G+(d,p)	14.93	-6.13
MP2/6-311G+(d,p)	21.00	-8.65