

**Table 3.9:**  $(\text{H}_3\text{O}^+)(\text{H}_2\text{O})$ 

| method                | $D_e^{\text{cpc}}$ | BSSE | $D_0^{\text{h}}$   | $r_{\text{O}\cdots\text{O}}$ | $\Delta r_{\text{O-H}}(\text{d})$ | $\Delta\omega(\text{d})$ |
|-----------------------|--------------------|------|--------------------|------------------------------|-----------------------------------|--------------------------|
| HF <sup>a</sup>       | 125.53             | 0.73 | 119.52             | 2.4325                       | 0.0886                            | −1705                    |
| MP2                   | 137.70             | 8.63 | 135.12             | 2.3909                       | 0.2205                            | −2856                    |
| B3LYP                 | 150.02             | 1.72 | 146.34             | 2.4060                       | 0.2242                            | −2700                    |
| B97-1                 | 150.93             | 1.67 | 146.85             | 2.4003                       | 0.2233                            | −2681                    |
| PBE0                  | 154.66             | 1.64 | 150.14             | 2.3927                       | 0.2208                            | −2633                    |
| HCTH                  | 139.52             | 2.04 | 134.43             | 2.4133                       | 0.2293                            | −2580                    |
| HCTH38                | 150.02             | 2.07 | 145.09             | 2.4114                       | 0.2275                            | −2562                    |
| BLYP                  | 150.82             | 2.11 | 146.08             | 2.4336                       | 0.2291                            | −2511                    |
| PBE                   | 159.15             | 2.09 | 153.43             | 2.4222                       | 0.2251                            | −2402                    |
| LDA                   | 188.02             | 1.90 | 181.26             | 2.3991                       | 0.2110                            | −2230                    |
| Best <i>ab initio</i> | 137.7 <sup>b</sup> |      | 134.5 <sup>b</sup> | 2.3861 <sup>c</sup>          |                                   | −2784 <sup>c</sup>       |

<sup>a</sup> $\text{C}_s$  geometry, see text.

<sup>b</sup>CCSD(T)/aug-cc-pV5Zf on O and cc-pVQZd on H, [46].

<sup>c</sup>CCSD(T)/TZ2Pf on O and TZ2P on H, [46].