



FIG. 5: (Color online) Same as Fig. 3 except $\gamma = 90^\circ$. The two insets, (b) and (c), show the behavior of the potentials for $r = 1.4$ a.u. on two different magnification scales: Region (b) is the magnified version of (a), region (c) is magnified (b).

contribution is positive and C_4/R^4 is negative (see Eq. 1). Therefore, their sum combined with the short-range interaction produces a potential curve (for fixed r and γ near 90°) that has a pronounced minimum in PES-PS and just a should-like feature in the present PES (see inset (c) in Fig. 5). The curve is repulsive asymptotically. A possible reason for the above differences is the somewhat smaller basis set (d-aug-cc-PVTZ) used in calculation of PES-PS [11].

The numerical data available about PES-BT [19, 23] is given in Table I. Since the calcula-