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Erratum

Correlated One-Center Wavefunctions for Two-Electron Molecules

II. Configuration-Interaction Functions and Application to HeH^+

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A computer programming mistake was found. Tables 2, 3, 4, and 5 have been recalculated and are reproduced in full for the sake of completeness. The variation of α was performed uniformly in steps of 0.01, the variation of the orbital exponents (Tables 3 and 5) in steps of 0.01 or less.

Table 2. *Ground state energies (in a.u.) of* HeH^+, *obtained for fixed orbital exponents at* $R = 1.4$ *a.u.*

m	α_I	$-E_I^0$	$-E_I^\alpha$	ΔE_I	$-\Delta E_I/E_I^0$ %
1	0.40	2.76506	2.84792	0.08286	3.00
3	0.36	2.80045	2.85002	0.04957	1.77
6	0.29	2.82832	2.85338	0.02506	0.89
7	0.30	2.85734	2.88414	0.02680	0.94
8	0.27	2.89073	2.91394	0.02321	0.80
9	0.25	2.89811	2.91768	0.01937	0.68
10	0.25	2.91563	2.93570	0.02007	0.69
11	0.23	2.92515	2.94243	0.01728	0.59
12	0.23	2.93313	2.95055	0.01742	0.59
13	0.23	2.93786	2.95415	0.01629	0.55
14	0.22	2.94083	2.95419	0.01336	0.45
15	0.15	2.95069	2.95478	0.00409	0.14
17	0.14	2.95266	2.95522	0.00256	0.09
18	0.14	2.95650	2.95917	0.00267	0.09
19	0.18	2.95931	2.96343	0.00412	0.14
20	0.17	2.96013	2.96364	0.00351	0.12

Table 3. *Ground state energies (in a.u.) of* HeH^+, *obtained for optimized orbital exponents at* $R = 1.4$ *a.u.*

m	$-E_{II}^0$	$-E_{II}^{\alpha^*}$	$-E_{II}^\alpha$	ΔE_{II}	$-\frac{\Delta E_{II}}{E_{II}^0}$ %	$E_{II}^{\alpha^*}-E_{II}^\alpha$	$-\frac{E_{II}^{\alpha^*}-E_{II}^\alpha}{E_{II}^{\alpha^*}}$ %
1	2.80735	2.83065	2.84852	0.04117	1.47	0.01787	0.63
3	2.82657	2.84693	2.85293	0.02636	0.93	0.00600	0.21
6	2.82851	2.85234	2.85358	0.02507	0.89	0.00124	0.04
7	2.89469	2.91243	2.91484	0.02015	0.70	0.00241	0.08
8	2.89769	2.91678	2.91765	0.01996	0.69	0.00087	0.03