

*Erratum*Correlated One-Center Wavefunctions
for Two-Electron MoleculesII. Configuration-Interaction Functions and Application to HeH^+

F. GREEN and T.-J. TSENG

Theoret. chim. Acta (Berl.) 12, 57—65 (1968)

Received September 8, 1969

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_1	$-E_1^0$	$-E_1^\alpha$	ΔE_1	$-\Delta E_1/E_1^0$ %
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