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Todd C. Thompson and Donald G. Truhlar

Citation: J. Chem. Phys. 77, 3777 (1982); doi: 10.1063/1.444461

View online: <http://dx.doi.org/10.1063/1.444461>

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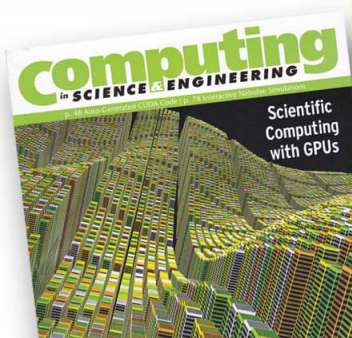
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<sup>5</sup>See, e.g., W. H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973), pp. 238–246.

<sup>6</sup>E. T. Jaynes, *IEEE Proc.* **51**, 89 (1963).

<sup>7</sup>J. P. Davis (unpublished work).

<sup>8</sup>See, e.g., Ref. 6 or R. J. Glauber, *Phys. Rev.* **131**, 2766 (1963).

<sup>9</sup>K. Wodkiewicz, in *Foundations of Radiation Theory and Quantum*

*Electrodynamics*, edited by A. O. Barut (Plenum, New York, 1980).

<sup>10</sup>W. H. Miller, *Adv. Chem. Phys.* **25**, 69 (1974); **30**, 77 (1975).

<sup>11</sup>K. C. Kulander and A. E. Orel, *J. Chem. Phys.* **75**, 675 (1981).

<sup>12</sup>E. J. Heller, *J. Chem. Phys.* **75**, 2923 (1981).

## ERRATA

### Erratum: Stabilization calculations of resonance energies for chemical reactions [*J. Chem. Phys.* **76**, 1790 (1982)]

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In Eq. (4), the exponent should be  $-1/4$ . In Table III, H + FH should read H + H<sub>2</sub>.

TABLE I(E). Corrections to Table I.

$E_i^{CI}$	$\delta E$	$N$	$ S_{if} ^2$	$n_{1f}$	$n_{2f}$	$E_f^{SCF}$
H + FH						
6.31	0.007	11	0.896	0	0	6.74
			0.079	1	2	20.60
			0.017	0	2	12.86
15.41	0.24	9	0.624	1	0	14.57
			0.421	0	2	12.96
			0.059	2	2	25.52
18.43	0.40	10	0.429	0	3	16.35
			0.389	1	1	16.82
			0.012	3	1	32.44
H + MuH						
14.41	0.03	11	0.903	0	0	15.45
			0.029	1	2	43.81
			0.018	2	0	27.25

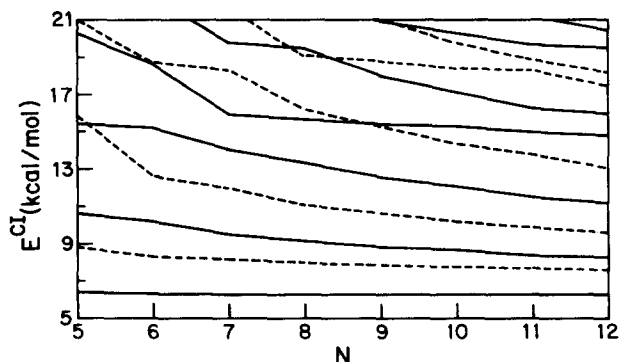


FIG. 1(E). Corrected version of Fig. 1.

There was an error in the computer program such that all results for H + FH and H + MuH were numerically wrong. The correct results are given here in Figs. 1(E) and 3(E) and Tables I(E), II(E), and III(E). The originally reported calculations for H + H<sub>2</sub> are all correct.

The changes in the conclusions are as follows: The

TABLE II(E). Comparison of SCF and CI stabilization energies (kcal/mol) calculated with quartic force field to those for full potential surface for H + FH.<sup>a</sup>

$n_{1f}$	$n_{2f}$	$E_f^{SCF}$		$E_i^{CI}$	
		Quartic	Full	Quartic	Full
0	0	6.89	6.75	6.74	6.32
1	0	14.88	14.57	16.31	15.29
0	2	15.33	12.96		
0	3	21.84	16.35	17.74	18.42
1	1	18.75	16.82		

<sup>a</sup> $N = 10$ ,  $\alpha_1 = \alpha_2 = 1.0$ .

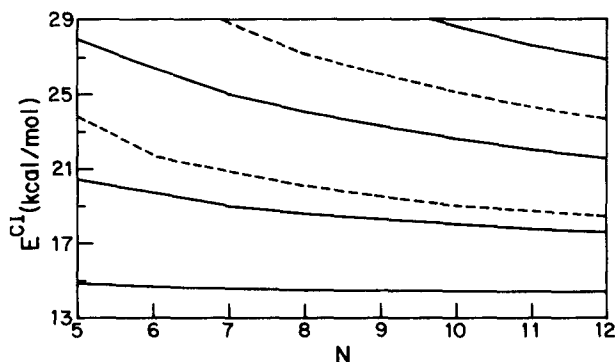


FIG. 3(E). Corrected version of Fig. 3.

TABLE III(E). Corrections to Table III for H + MuH.

$\alpha_1$	$\alpha_2$	$E_t^{\text{CI}}$	$\Delta E$	$N$	$ S_{ty} ^2$	$n_{1y}$	$n_{2y}$	$E^{\text{SCF}}$
0.8	0.8	14.36	0.04	11	0.861	0	0	15.45
					0.050	1	2	41.84
					0.026	2	0	27.16

natural-collision-coordinate vibrationally adiabatic assignment of the third resonance in H + FH does not provide the dominant contribution to the stabilized CI wave function. This resonance is better interpreted as

a Fermi resonance of the natural-collision-coordinate assignment of (1, 1) and the hyperspherical-coordinate-type assignment of (0, 3). The errors in the CI stabilization resonance energies in Table I(E) are  $\pm 0.1$ ,  $< 0.1$ , 0.0, 0.6, and 0.1 kcal/mol, respectively. In all cases the SCF calculations have larger errors, namely, 0.4, 0.8, 1.0, and 1.15 kcal/mol, respectively. The errors in the CI stabilization energies are sometimes smaller than the resonance widths. For all five resonances considered in the original paper the corrected average error in the CI stabilization resonance energies is only 0.2 kcal/mol, and the corrected average error in the SCF resonance energies is 1.1 kcal/mol.

## Erratum: Raman spectroscopy of supercooled water [J. Chem. Phys. 76, 2221 (1982)]

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The labeling of Fig. 1, p. 2222 is incorrect. The  $\Delta$  wave number scale should read from 2000 to 3024  $\text{cm}^{-1}$  at intervals of 204.8  $\text{cm}^{-1}$  instead of 2200 to 2750  $\text{cm}^{-1}$ .