Erratum: Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules [J. Chem. Phys. 82, 2418 (1985)]

D. W. Schwenke and D. G. Truhlar

View Online   Export Citation

ARTICLES YOU MAY BE INTERESTED IN

$(C_2H_4)_2$, they concluded that $(C_2H_4)_2$ had no rotational structure. They apparently interpreted the statements of Liu et al.[2] to indicate rotational lines had been resolved, although this would not be possible at 0.9 cm^{-1} resolution. The confusion which has surfaced appears to be over the use of the term "rotational structure" which Fischer et al.[1] applies to resolvable rotational lines, while Liu et al.[2] used the term in the context of a rotational band contour. This appears to be the source of the discrepancy, as stated in the paper by Fischer et al.[1] To avoid further misunderstanding, we have adopted the definition of Fischer et al.[1] in all subse-

quent reports from our laboratory. There is now agreement[4] between the two groups that both homogeneous and inhomogeneous effects are important in determining the shape of the dimer spectrum.

[1]G. Fischer, R. E. Miller, P. F. Vohralik, and R. O. Watts, J. Chem. Phys. **83**, 1471 (1985).
[2]W.-L. Liu, K. Kolenbrander, and J. M. Lisy, Chem. Phys. Lett. **112**, 585 (1984).
[3]G. Fischer, R. E. Miller, and R. O. Watts, Chem. Phys. **80**, 147 (1983).
[4]R. E. Miller and R. O. Watts (private communication).

ERRATA

Erratum: Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules [J. Chem. Phys. 82, 2418 (1985)]

D. W. Schwenke and D. G. Truhlar
Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455

There are some transcription errors in the interaction energies given in Tables III, IV, and VII. These are corrected in Table I. There are also minor errors in the statistics quoted in Tables V and VI, and these are corrected in Table II. These corrections do not alter our conclusions or discussion in any way.

We would also like to take this opportunity to clarify a possible point of confusion about our basis sets. All of our basis sets are completely and correctly specified in Table I and its references. Thus our 6-311G** basis set involves six-function Cartesian d sets, whereas the "standard" choice is a five-function d set. Similarly, the specified exponential parameters we use for polarization and diffuse functions may differ from other values in the literature.

We are grateful to Dr. R. Zahradník and Dr. P. Hobza for pointing out one these errors.

TABLE I. Corrections to Tables III, IV, and VII.

Table	Basis number	Geometry	Correction(s)
III	2	2	$V = 0.67$
	3	1	$V = 15.7$, $V^{cc} = 18.2$
	5	2	$V = 0.07$
	7	2	$V^{cc} = 2.19$
	8	1	$V = 12.9$
	11	2	$V = 1.43$, $V^{cc} = 2.34$
	13	1	$V = 18.5$, $V^{cc} = 19.1$
	13	2	$V = 2.19$, $V^{cc} = 2.29$
	14	2	$V = 2.12$
	15	2	$V = 0.77$
	16	2	$V = 2.19$
	22	1	$V = 18.4$, $V^{cc} = 18.8$
	25	1	$V^{cc} = 18.1$
	26	1	$V^{cc} = 18.5$
	26	2	$V^{cc} = 2.19$
	31	1	$V^{cc} = 18.1$
	32	1	$V = 18.3$
IV	1	3	$V^{cc} = -0.404$
	2	3	$V = -7.18$
VII	3	1	$V^{pc} = 15.9$
	3	2	$V^{pc} = 0.30$

TABLE II. Corrections to Tables V and VI.

Table	Group	Geometry	Correction(s)
V	1	1	V:mean $= 15.5$, rms $= 2.2$; V^{cc}:mean $= 18.5$, rms $= 3.7$
	2	1	V:mean $= 17.1$, rms $= 1.8$
	2	2	V:mean $= 1.83$; $V^{cc} = 2.41$, rms $= 0.31$
	3	1	V:rms $= 0.28$; V^{cc}:mean $= 18.58$, rms $= 0.24$
	4	1	V:rms $= 0.23$; V^{cc}:mean $= 18.42$
VI	1	1	V:mean $= 15.6$, rms $= 2.3$; V^{cc}:mean $= 18.2$, rms $= 3.4$
	2	1	V:mean $= 17.9$ V^{cc}:mean $= 18.8$, rms $= 0.4$
	2	2	V:mean $= 1.91$, rms $= 0.46$
	3	2	V:rms $= 0.02$

0021-9606/86/074113-01$02.10