

CORRIGENDA

Michael J. S. Dewar, Caoxian Jie and Jianguo Yu, SAM1; The first of a new series of general purpose quantum mechanical molecular models, *Tetrahedron* 1993, 49, 5003-5038.

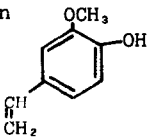
Table 1 compares with experiment the heats of formation calculated by SAM1, AM1, and PM3 for 402 molecules derived from C, H, O, N, and the halogens. In four cases, there are errors. The entries for these molecules that should have appeared in Table 1 are indicated below. Where there are differences, the original values are also listed, in parentheses, for comparison.

Molecule	ΔH_f obsd	ΔH_f SAM1	Error calculated by:		
			SAM1	AM1	PM3
Methyl iodide	3.5	0.3 (6.7)	-3.2 (3.2)	2.1	5.9
Isopropyl iodide	-9.9	-10.4 (-10.7)	-0.5 (-0.8)	4.2 (3.9)	4.6 (4.4)
Iodine monofluoride	-22.7	-12.7 (-13.0)	10.0 (9.7)	13.6 (13.8)	19.7 (14.9)
Iodine monochloride	4.3	-0.1	4.4 (-4.4)	-8.9	6.5

It seems unlikely that there can be any other errors of this kind. We have checked the SAM1 results quoted in all nine tables very carefully against the original computer output without finding any other discrepancies. Furthermore, Dr. Andrew P. Holder (Department of Chemistry, University of Missouri, Kansas City, MO 64110) has repeated the calculations for all 402 molecules in Table 1, using a different computer and a new version (AMPAC 4.5) of the AMPAC program, with identical results.

Yingfong Chen, Jian Liu, R. Stephen Davidson and Oliver W. Howarth, Isolation and structure of clematine, a new flavanone glycoside from *Clematis armandii* Franch, *Tetrahedron* 1993, 49, 5169-5176.

In scheme I, The fragment ion $m/z=179$ should be:

The fragment ion  is $m/z=150$.

