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Erratum

Erratum to: 'Complete basis set and density functional determination of the enthalpy of formation of the controversial HO_3 radical. A discrepancy between theory and experiment' [Chem. Phys. Lett. 365 (2002) 440–449] ☆,☆☆

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We have recently published in this journal a report on the enthalpy of formation of the HO_3 radical [1]. Very recently, it has been brought to our attention that some of the numbers in the original Tables 3 and 5 are erroneous. We are including here the correct tables. These changes do not affect the conclusions reached in the paper.

Reference

[1] P.A. Denis, M. Kieninger, O.N. Ventura, R.E. Cachau, G.H.F. Diercksen, Chem. Phys. Lett. 365 (2002) 440.

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Table 3
Enthalpy of formation of HOOOH, obtained in this work from the reaction of atomization HOOOH → 2H + 3O, in kcal/mol

Method	Basis Set	$\Delta_f H^0(298)$
HF	cc-pVDZ	185.4
	cc-pVTZ	174.3
	cc-pVQZ	173.9
CCSD	cc-pVDZ	31.3
	cc-pVTZ	7.2
	cc-pVQZ	−0.1
CCSD(T)	cc-pVDZ	22.0
	cc-pCVDZ	8.4
	cc-pVTZ	−6.7
	cc-pCVTZ	−7.1
CCSD(T,Full)	cc-pCVTZ	−7.6
CCSD(T) extrapolated		−21.6
G3		−19.9
CBS-QB3		−23.5
CBS-APNO		−21.1
B3LYP	6-311++G(3df,2pd)	−27.7
B3PW91	6-311++G(3df,2pd)	−26.1

Table 5
Enthalpy of reaction of the isodesmic reaction (3) and enthalpy of formation of the HO_3 radical derived from the isodesmic reaction and from the atomization reaction

Method	Reaction (1)		Reaction (3)	Reaction (4)	Reaction (5)
	$\Delta_r H^0(298)$	$\Delta_f H^0(298)$	$\Delta_f H^0(298)$	$\Delta_f H^0(298)$	$\Delta_f H^0(298)$
HF/cc-pVDZ	19.0	27.1	191.0		
HF/cc-pVTZ	20.4	25.7	181.4		
HF/cc-pVQZ	21.6	24.6	180.5		
MP2/cc-pVDZ	29.9	16.2			
MP2/cc-pVTZ	32.2	12.9			
MP2/cc-pVQZ	33.5	12.6			
B3LYP/cc-pVDZ	41.8	4.3			
B3LYP/6-311++G(3df,2pd)	39.7	6.3	−2.1	8.6	3.1
B3PW91/6-311++G(3df,2pd)	40.5	5.6	−2.0	8.4	6.3
CCSD/cc-pVDZ	31.4	14.7	54.8		
CCSD(T)/cc-pVDZ	33.5	12.6	44.3		
CCSD(T)/cc-pCVDZ			43.9		
CCSD(T,Full)/cc-pCVDZ			43.4		
CCSD/cc-pVTZ	32.8	13.3	35.7		
CCSD(T)/cc-pVTZ	35.3	10.8	21.1		
CCSD(T)/cc-pCVTZ			20.8		
CCSD(T,Full)/cc-pCVTZ			20.1		
CCSD/cc-pVQZ	33.9	12.2	29.6		
CCSD(T)/cc-pVQZ			14.0		
CCSD(T)/∞	37.3	8.8	7.9		
G3	37.6	8.5	8.4		
CBS-QB3	38.1	8.0	5.3	7.2	7.7
CBS-APNO	39.3	6.8	6.3	5.9	6.1

All values in kcal/mol.