

ERRATUM

R.J. Bartlett, J.D. Watts, S.A. Kucharski and J. Noga, Non-iterative fifth-order triple and quadruple excitation energy corrections in correlated methods, Chem. Phys. Letters 165 (1990) 513.

Further study has indicated that some T_4 results in our recent paper were affected by a minor error. The changes are in the microhartree to tens of microhartree range, but as these results are likely to be used to check out future T_4 programs, the corrected values are shown below (energies in mhartree). The last digits of the previously reported values are given in parentheses.

In table 1, the modified values are

	HF		H ₂ O	
	1.5R _c	R _c	1.5R _c	2.0R _c
Q*[T(CCSD)]	-0.393(2)			2.782(812)
Q[T(CCSD)]		-0.441(2)	-1.525(7)	0.430(3)
Q*[T(QCISD)]			-1.587(5)	0.336(65)
Q[T(QCISD)]		-0.443(4)	-1.591(3)	0.994(0)

As these numbers are added to CC results, some of the values in table 2 that measure differences with full CI change accordingly.

	HF		H ₂ O	
	1.5R _c	R _c	1.5R _c	2.0R _c
CCSD+TQ*(CCSD)	0.563(4)			1.989(59)
QCISD+TQ*(QCISD)			-0.136(4)	-1.109(080)
CCSD+TQ(CCSD)		0.186(5)	0.109(7)	-4.341(38)
QCISD+TQ(QCISD)		-0.084(3)	-0.140(2)	-2.432(6)

Corrected average errors compared to full CI may be obtained from the above. None of the conclusions of the paper are affected by these slight changes. Also, in eq. (23) there is a typo and obviously missing fourth-order term. It should read:

$$\Delta E = \Delta E_{\text{CCSD}} + \Delta E_{\dagger b}^{[4]} + \Delta E_{\dagger \dagger}^{[5]} + \Delta E_{\dagger B}^{[5]} + \Delta E_{\ddagger}^{[5]} + \Delta E_{\ddagger \dagger}^{[5]}. \quad (23)$$
