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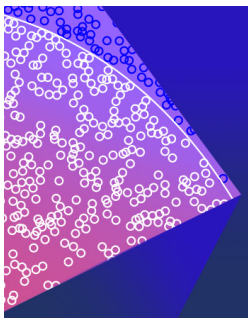

Erratum: Second-order Møller–Plesset perturbation theory as a configuration and orbital generator in multiconfiguration self-consistent-field calculations [J. Chem. Phys. 88, 3834 (1988)]

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The correlation part of the one-electron density matrix elements reported in the Appendix are in error by a factor of $\sqrt{2}$. The correct expressions read as follows:

$$D_{\alpha\beta} = 2\delta_{\alpha\beta} - \sum_{pq\gamma} \frac{(\alpha p|\gamma q)}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_p - \epsilon_q} \langle\langle p\beta|\gamma q\rangle\rangle, \tag{A1}$$

$$D_{mn} = \sum_{p\gamma\delta} \frac{(\gamma p|\delta n)}{\epsilon_\gamma + \epsilon_\delta - \epsilon_p - \epsilon_n} \langle\langle m\delta|\gamma p\rangle\rangle, \tag{A2}$$

$$D_{m\beta} = (\epsilon_\beta - \epsilon_m)^{-1} \Big\{ \sum_{pq\gamma} (mp|\gamma q)\langle\langle p\beta|\gamma q\rangle\rangle - \sum_{p\gamma\delta} (\gamma p|\delta\beta)\langle\langle m\delta|\gamma p\rangle\rangle \Big\}, \tag{A3}$$

where

$$\langle\langle m\alpha|\beta n\rangle\rangle = \frac{4(m\alpha|\beta n) - 2(m\beta|\alpha n)}{\epsilon_\alpha + \epsilon_\beta - \epsilon_n - \epsilon_m}.$$

The MP2 natural occupation numbers for H_2O and HCl reported in Tables II and III, respectively, have been recalculated using the corrected formulas. The corrected MP2 occupation numbers agree even better with the MCSCF natural occupation numbers. We have repeated the H_2O calculations and found that the step lengths change very little (orbital step lengths = 0.223, 6.74×10^{-2}, 7.81×10^{-3}, and 6.39×10^{-5}) compared to the previous values (orbital step lengths = 0.225, 6.58×10^{-2}, 1.38×10^{-2}, and 2.32×10^{-4}) reported in Table V. No conclusions stated in the article are affected by the error in the density matrix elements.

TABLE III. Natural orbital occupation numbers larger than 0.0001 in HCl calculations.

Orbital numbers	Irr. rep.	MP2 σ	MP2 π	CAS1[a] σ	CAS1[a] π	CAS1[b] σ	CAS1[b] π
1		1.9998	3.9972	2.0000	4.0000	2.0000	4.0000
2		1.9990	3.9802	2.0000	3.9799	2.0000	3.9968
3		1.9982	0.0173	2.0000	0.0199	2.0000	0.0029
4		1.9917	0.0023	1.9900		1.9991	
5		1.9825	0.0002	1.9741		1.9984	
6		0.0145		0.0243		0.0015	
7		0.0061		0.0074		0.0010	
8		0.0054		0.0071		0.0001	
9		0.0014					
10		0.0013					
11		0.0009					
12		0.0004					
13		0.0003					
14		0.0003					
15		0.0002					
16		0.0001					

[a] MP2 NOs were used as an initial guess for the orbitals.
[b] CHF orbitals were used as an initial guess for the orbitals.

TABLE II. Natural orbital occupation numbers larger than 0.0001 in H_2O calculations.

Orbital numbers	Irr. rep.	MP2 a_1	MP2 b_1	MP2 b_2	MP2 a_2	MCSCF(CAS1) a_1	MCSCF(CAS1) b_1	MCSCF(CAS1) b_2	MCSCF(CAS1) a_2	MCSCF(CAS2) a_1	MCSCF(CAS2) b_1	MCSCF(CAS2) b_2	MCSCF(CAS2) a_2
1		1.9994	1.9668	1.9648	0.0059	2.0000	1.9784	1.9755	0.0	2.000	1.9693	1.9673	0.0054
2		1.9850	0.0212	0.0250	0.0007	1.9879	0.0208	0.0242		1.9846	0.0207	0.0271	
3		1.9648	0.0053	0.0061	0.0002	1.9764				1.9672	0.0049	0.0052	
4		0.0235	0.0006	0.0009		0.0237				0.0253			
5		0.0118	0.0006	0.0008		0.0129				0.0127			
6		0.0062	0.0002	0.0004						0.0055			
7		0.0052	0.0001	0.0003						0.0049			
8		0.0010		0.0002									
9		0.0007		0.0001									
10		0.0005											
11		0.0004											
12		0.0003											
13		0.0002											

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