ERRATA

Erratum: Symmetry-adapted perturbation theory of nonadditive three-body interactions in van der Waals molecules. I. General theory [J. Chem. Phys. 103, 8058 (1995)]

Robert Moszynski
Institute of Theoretical Chemistry, Nijmegen-SON Research Center, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands and Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

Paul E. S. Wormer
Institute of Theoretical Chemistry, Nijmegen-SON Research Center, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

Bogumil Jeziorski
Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

Ad van der Avoird
Institute of Theoretical Chemistry, Nijmegen-SON Research Center, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

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In Ref. 1 we criticized the expression for the third-order induction nonadditivity used by Piecuch.[2] Actually, Eq. (15) of Ref. 2 is correct and equivalent to Eqs. (51) and (53) of Ref. 1, provided that the wave functions used in Ref. 2 are real, which was tacitly assumed by Piecuch.[2] Therefore, the criticism of the numerical results reported in Ref. 3 is not correct. The fact that our criticism of the work of Piecuch is unwarranted has also been pointed out in Refs. 4 and 5. We thank P. Piecuch and K. Szalewicz for a useful correspondence on this subject.

In the expression for the induction-dispersion nonadditivity, Eq. (48) of Ref. 1, the quadratic response function $\Pi^{\nu_2\nu\nu_1}_{\mu_2\mu\mu_1}(-i\omega,0)$ should be replaced by $\Pi^{\nu_1\nu_2\nu}_{\mu_1\mu_2\mu}(-i\omega,0)$. In translating this expression to the orbital basis in the random phase approximation (RPA) we overlooked contributions from the RPA amplitudes $(\bar{V}_n)^a_r = d^{aa_1}_{rr_1}(V_n)^{r_1}_{a_1}$, defined via the $(V_n)^a_r$ amplitudes of Ref. 1, where $d^{aa_1}_{rr_1} = d^{rr_1}_{aa_1} = 4[(\mathbf{A}-\mathbf{B})^{-1}]_{ra,r_1a_1}$, and the matrices $\mathbf{A}$ and $\mathbf{B}$ are defined as in Ref. 6. The final expression for $E^{(210)}_{ind-disp}$ in the random-phase approximation, Eq. (A10) of Ref. 1, should read:

$$
\begin{aligned}
E^{(210)}_{ind-disp} = & -32\sum_n (V_n)^a_r \sum_m (C_C)^b_s (n|m)[v^{rs}_{as'}(V_m)^{s'}_b - v^{rb'}_{ab}(V_m)^s_{b'}]/(\omega_n+\omega_m) \\
& + 32\Bigg[\sum_n \sum_{mm'} (C_C)^b_s (n|m)(n|m') \\
& \times (g^{sb_1}_{s's_1}(V_m)^{s_1}_{b_1}(V_{m'})^{s'}_b + g^{ss_1}_{s'b_1}(V_m)^{b_1}_{s_1}(V_{m'})^{s'}_b - g^{b's_1}_{bb_1}(V_m)^{b_1}_{s_1}(V_{m'})^s_{b'} - g^{b'b_1}_{bs_1}(V_m)^{s_1}_{b_1}(V_{m'})^s_{b'})I_{mm'n}\Bigg] + m \leftrightarrow m' \\
& + 8\Bigg[\sum_n \sum_{mm'} (C_C)^b_s (n|m)(n|m')(g^{sb_1}_{s's_1}(\bar{V}_m)^{s_1}_{b_1}(\bar{V}_{m'})^{s'}_b - g^{ss_1}_{s'b_1}(\bar{V}_m)^{b_1}_{s_1}(\bar{V}_{m'})^{s'}_b - g^{b'b_1}_{bs_1}(\bar{V}_m)^{s_1}_{b_1}(\bar{V}_{m'})^s_{b'} \\
& + g^{b's_1}_{bb_1}(\bar{V}_m)^{b_1}_{s_1}(\bar{V}_{m'})^s_{b'})J_{mm'n}\omega_m\omega_{m'}\omega_n\Bigg] + m \leftrightarrow m' + 32\sum_n \sum_{mm'} (n|m)(n|m')(V_m)^b_s[(f_C)^s_{s'}(V_{m'})^{s'}_b \\
& - (f_C)^{b'}_b (V_{m'})^s_{b'}]I_{mm'n} - 8\sum_n \sum_{mm'} (n|m)(n|m')[(f_C)^{s'}_s(\bar{V}_m)^b_{s'}(\bar{V}_{m'})^s_b \\
& - (f_C)^{b'}_b (\bar{V}_m)^b_s (\bar{V}_{m'})^s_{b'}]J_{mm'n}\omega_m\omega_{m'}\omega_n ,
\end{aligned}
\tag{1}
$$

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where for convenience we introduced the RPA integrals $(n|m)=(V_n)^a_r v^{rs}_{ab}(V_m)^b_s$, and the energy denominators $J_{jj'n}=[(\omega_j+\omega_n)(\omega_{j'}+\omega_n)(\omega_j+\omega_{j'})]^{-1}$ and $I_{jj'n}=\{[(\omega_n+\omega_j)(\omega_n+\omega_{j'})]^{-1}+[(\omega_n+\omega_j)(\omega_j+\omega_{j'})]^{-1}+[(\omega_n+\omega_{j'})(\omega_j+\omega_{j'})]^{-1}\}/2$.

Finally, we want to note that the second and fourth terms in Eq. (A11) of Ref. 1 should have reversed signs, and that the last four terms of Eq. (B3) should be multiplied by two, rather than by four. We thank K. Szalewicz for pointing out to us the latter error.

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