

Erratum: The role of single-particle density in chemistry [Rev. Mod. Phys. 53, 95 (1981)]

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Please note the following corrections:

Page 101, end of paragraph 2: Figures 1 and 2 were inadvertently omitted and are reprinted here. Note that the earlier Figs. 1, 2, and 3 are now Figs. 3, 4, and 5, respectively.

Page 103, line 5 after Eq. (2.68): Read D^1 instead of D^2 .

Page 126, reference to Rajagopal (1980): Read Vol. 41 instead of Vol. 61.

We apologize to our readers for these errors.

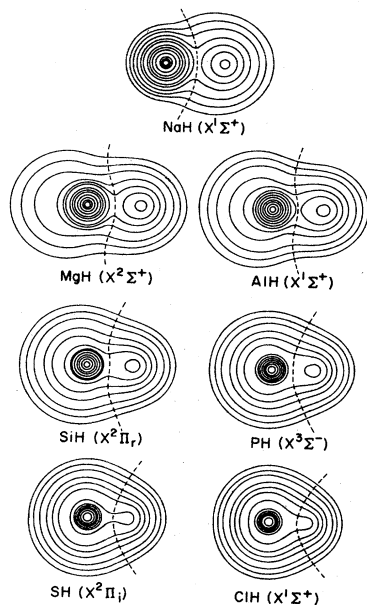


FIG. 1. Contour maps of electron densities for neutral ground-state hydrides of second-row atoms, using Hartree-Fock wave functions. The virial partitioning surfaces defining atomlike fragments are indicated by dashed lines. Contours (in a.u.) increase in value from the outermost contour inwards in steps of 2×10^{-2} , 4×10^{-2} , 8×10^{-2} . The smallest contour value is 0.002 with n increasing in steps of unity to yield the highest contour value of 20. (Reproduced from Fig. 2 of Bader and Messer, 1974. Courtesy, the National Research Council of Canada.)

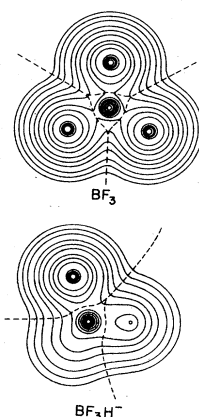


FIG. 2. Contour maps of electron densities in (top) the molecular plane of $\text{BF}_3[X(^1A_1')]$ and (bottom) a plane containing boron, a fluorine and hydrogen nuclei in $\text{BF}_3\text{H}^- [X(^1A_1)]$. The dashed lines indicate intersections of the zero-flux partitioning surfaces with these planes. The contours (in a.u.) increase in value from the outermost contour inwards in steps of 2×10^{-2} , 4×10^{-2} , 8×10^{-2} . The smallest contour value is 0.002 with n increasing in steps of unity to yield the highest contour value of 20. The atomlike fragment populations are $\text{BF}_3 : N(\text{B}) = 2.41$, $N(\text{F}) = 9.86$; $\text{BF}_3\text{H}^- : N(\text{B}) = 2.50$, $N(\text{F}) = 9.91$, $N(\text{H}) = 1.76$. (Reproduced from Fig. 1 of Bader, 1975. Courtesy, the American Chemical Society.)