The Sum of van der Waals Radii – A Pitfall in the Search for Bonding

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The most widely used criterion for the evaluation of chemical bonding, especially of weak bonding, are interatomic distances shorter than the sum of the van der Waals radii, $d(\mathrm{X}\cdots\mathrm{Y}) < \Sigma r(\mathrm{vdW})[\mathrm{X},\mathrm{Y}]$. The shortcomings of these radii are, however, so serious, that illicit conclusions are easily arrived at. It is proposed to discard the 'shorter than Σr(vdW)' criterion altogether and to rely on alternative criteria.

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