

the construction of ITER be postponed. I would argue just the opposite. We need to build on our excellent progress and take advantage of the unique opportunity offered by participation in ITER to move forward with fusion science and energy development. Projects like ITER are always faced with the idealistic argument that we should wait for better results. Such logic would have postponed most major undertakings that have lead to significant scientific and technological progress.

The letters raise valid technical issues (including improved plasma confinement, control of disruptions, and engineering and materials development). These issues have been clearly recognized by fusion researchers, in general, and ITER, in particular. They are being responsibly addressed in the ITER research and development and base program activities.

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Structure of $W(CH_3)_6$

The exquisite solid-state structural characterizations of $W(CH_3)_6$ and $Re(CH_3)_6$ re-

ported recently by Valerie Pfenning and Konrad Seppelt (Reports, 2 Feb., p. 626) challenge our understanding of the forces controlling molecular structures. For metal complexes containing only alkyl or hydride ligands, the existence of structures that appear to violate valence shell electron pair repulsion (VSEPR) conventions is particularly intriguing. Application of the simple concept of orbital hybridization, first espoused by Linus Pauling 65 years ago (1) and recently revised by us (2), results in (i) the prediction of the observed C_{3v} -distorted trigonal prismatic geometry for $W(CH_3)_6$ and (ii) a robust model for rationalizing the shapes of homoleptic methyl compounds.

Transition metals form covalent, two-electron bonds with hydride and alkyl ligands. For complexes with a valence orbital electron count of 12 or fewer electrons [such as the 12-electron $W(CH_3)_6$], we have shown that the hybridization of the metal center can be described as sd^{n-1} , where n is the number of bonds plus lone pairs. Thus, $W(CH_3)_6$ exhibits sd^5 hybridization at the metal center. The shapes of sd^5 hybrids are such that orthogonality of hybrid orbital pairs occurs at angles of 63° and 117° . Four arrangements of the six ligands, two that have C_{3v} and two that have C_{5v} point group symmetry, are consistent with these angular preferences. For WH_6 , ab initio computations suggest that all four

of these structures are distinct minima of roughly equivalent energy. One might expect the intermethyl steric effects of $W(CH_3)_6$ to favor the most open (C_{3v}) geometry and to distort the bond angles to larger values. Using a valence bond theory-based molecular mechanics method (VALBOND), we computed (2) a C_{3v} equilibrium geometry for $W(CH_3)_6$ (Fig. 1). This

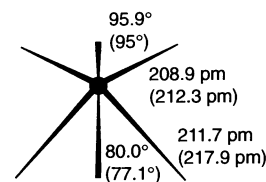


Fig. 1. Schematic representation of the C_{3v} equilibrium structure for $W(CH_3)_6$. Average bond lengths (in picometers) and angles are shown for the VALBOND-computed structure (upper numbers) and for the crystallographic structure (lower numbers, in parentheses).

structure exemplifies the essential attributes of the crystallographic structure, despite using only generic, rule-based parameters. Molecular dynamics simulations revealed a low energy motion corresponding to movement of the metal atom along the C_3 axis with a maximum of approximately 3.0 kilocalories per mole at the trigonal prismatic D_{3h} geometry. Our computational results are consistent with the gas-phase electron-diffraction data of Haaland and co-workers (3), the x-ray crystallographic results of Pfenning and Seppelt, and ab initio results recently communicated to us by M. Kaupp (4).

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References

1. L. Pauling, *J. Am. Chem. Soc.* **53**, 1367 (1931).
2. C. R. Landis, T. Cleveland, T. K. Firman, *ibid.* **117**, 1859 (1995).
3. A. Haaland, A. Hammel, K. Rypdal, H. V. Volden, *ibid.* **112**, 4547 (1990).
4. M. Kaupp, *ibid.*, in press.

Response: It is a pleasant surprise to learn that, with a simple model, the shape of the $W(CH_3)_6$ molecule [and also qualitatively that of $Re(CH_3)_6$] can be precisely predicted and that a similar model can predict an ab initio result (1). For skeptics, it may be stressed that these predictions were published (2) or submitted (1) before our *Science* paper appeared and that neither of the two scientists had previous knowledge about our crystallographic work.

I apologize to Landis for overlooking his recent theoretical publication on this subject (2).

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LETTERS

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1. M. Kaupp, *J. Am. Chem. Soc.*, in press.
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Strangelovian Concepts

Richard A. Kerr's article "A Strangelove ocean comes back to life" (Research News, 1 Dec., p. 1442) attributes the doomsday machine to Dr. Strangelove. I must strongly object! Strangelove was the originator of the "mine shaft" concept, in which extant shafts would be inhabited by *Homo sapiens* of a controversial gender ratio. The "mind shaft" strategy was developed as a countermeasure to assure homonid survival in case of inadvertent detonation of a doomsday machine.

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Note from the Editor-in-Chief

During our consideration of the report "Identification of a dual specificity kinase that activates the Jun kinases and p38-Mpk2" by A. Lin *et al.*, which was published in our issue of 14 April 1995 (p. 286), a name was removed by the corresponding author from the report's list of authors. A subsequent disagreement between some of the report's authors and the person whose name was omitted brought to light the fact that we had not obtained a signed statement from the report's corresponding author and the person whose name was omitted saying that they agreed to the authorship changes. We were remiss in not obtaining these statements and will do so in the future as a matter of policy.

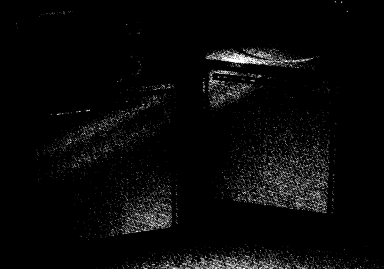
—FLOYD E. BLOOM

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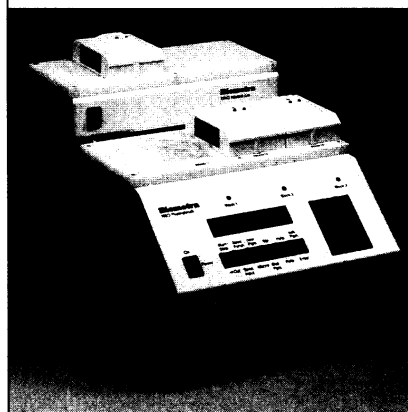
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