The ITER Project

Thomas H. Stix *et al.* take issue with the present course of the International Thermonuclear Experimental Reactor (ITER) initiative (Letters, 16 Feb., p. 891). ITER is a fusion research facility based on the highly successful "tokamak" approach to plasma confinement, now being designed under an international agreement executed in 1992 by the European Union, Japan, the Russian Federation, and the United States.

ITER seeks to achieve, for the first time ever in controlled fusion research, a self-heated "burning" deuterium-tritium plasma. Plasma burn has been widely endorsed as a critically important and appropriate next step for fusion.

Stix *et al.* question combining this step with three other "giant steps": large size, long pulse, and superconducting magnets. The size of the ITER plasma is dictated by the requirement to provide sufficient energy confinement to reach the burning state; this is determined from size-scaling relationships derived from experiments on tokamaks with plasma volumes spanning two orders of magnitude; the largest of these tokamaks already operate at plasma densities and temperatures similar to those expected in ITER. Confinement in a tokamak is determined primarily by the magnitude of the plasma current: ITER's plasma current is about four times larger than that in the Joint European Torus. The step in pulse length is derived from the additional physics requirement to sustain the burn over times long compared with those characteristic of the evolution of plasma profiles. The step from copper to superconducting magnets has been found to be the most practical way of achieving the required pulse lengths. Superconducting magnets have already been used in tokamaks, including one of the size of Princeton's successful Tokamak Fusion Test Reactor. The long pulse and the superconducting magnets are also essential for ITER to advance fusion engineering objectives. The engineering features of ITER are generic to any fusion reactor; in ITER, they can be tested together in an integrated facility, made possible only by international partnership.

Stix *et al.* also question the capability of the ITER design to achieve its stated technical objectives. Recognizing the need for broad technical consensus, a Technical Advisory Committee (TAC) was formed which, on a continuing basis, reports to the ruling ITER Council on the adequacy of the ITER design and its physics basis. The TAC's 16 members are drawn equally from all four partners, but they serve as individuals, independent of both the design team and their respective governmental agencies. Last July, the TAC completed a review of the "Interim Design" and, with unanimity, concluded that the design can fully meet ITER's mission and technical objectives.

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The letters from Stix *et al.*, Ernesto Mazzucato, and William E. Parkins (16 Feb., p. 891) have two common themes, namely, that we should postpone or even cancel the ITER project and that we do not know how to make an attractive fusion reactor.

Stix *et al.* and Mazzucato correctly note the tremendous progress that has been made in fusion research and that we are in a period where our expectations of continued progress are high. This is used as an argument to suggest that a commitment to

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 $Re(CH_3)_6$ reported recently by Valerie Pfennig 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

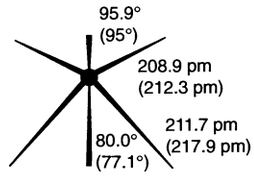

Fig. 1. Schematic representation of the C_{3v} equilibrium structure for $W(CH_3)_6$. Average bond lengths (in picometers) and angles are shown for the VALBOND-computed structure (upper numbers) and for the crystallographic structure (lower numbers, in parentheses).

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 Pfennig and Seppelt, and ab initio results recently communicated to us by M. Kaupp (*4*).

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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*).