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TERTIARY PHOSPHINE COMPLEXES OF THE f-BLOCK METALS; CRYSTAL STRUCTURE OF Yb{N(SiMe<sub>3</sub>)<sub>2</sub>}<sub>2</sub>{Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub> PMe<sub>2</sub>} AND EVIDENCE FOR A YTTERBIUM- $\gamma$ -CARBON INTERACTION

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### **Authors**

Tilley, T.D.  
Andersen, R.A.  
Zalkin, A.

### **Publication Date**

1982-02-01



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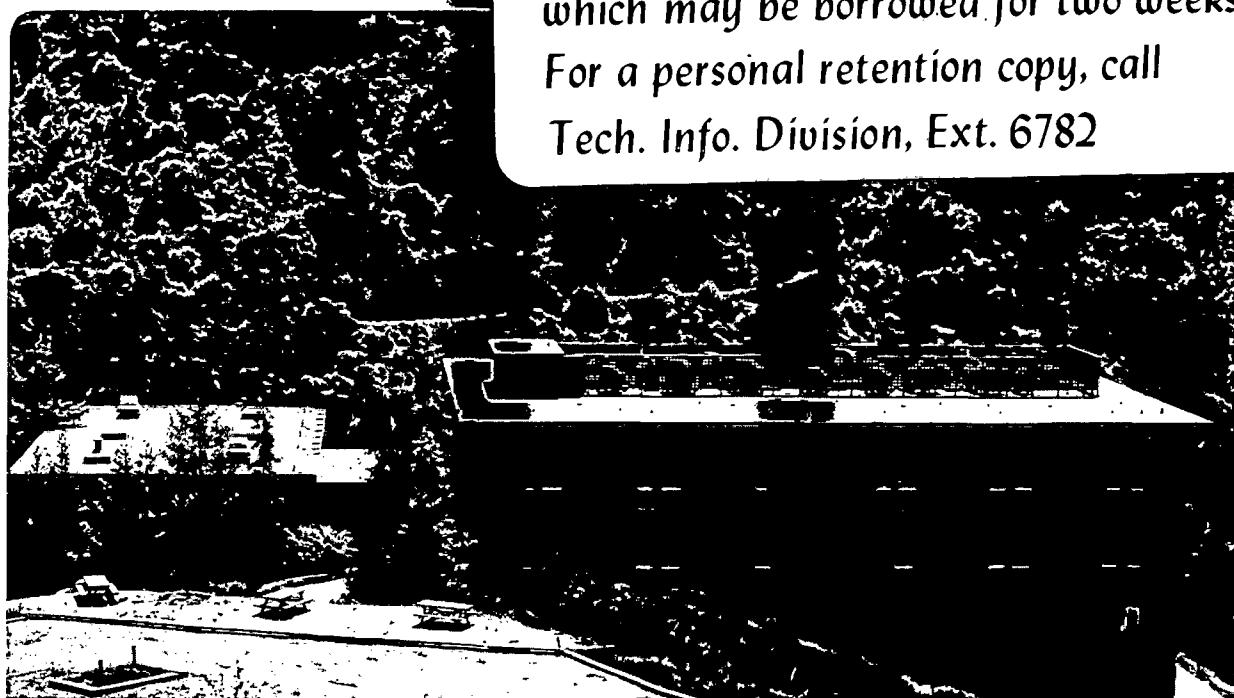
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CRYSTAL STRUCTURE OF Yb{N(SiMe<sub>3</sub>)<sub>2</sub>}<sub>2</sub>{Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>}  
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T. Don Tilley, Richard A. Andersen,  
and Allan Zalkin

February 1982

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Tertiary Phosphine Complexes of the f-Block Metals;  
Crystal Structure of Yb[N(SiMe<sub>3</sub>)<sub>2</sub>]<sub>2</sub>[Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>]  
And Evidence for a Ytterbium- $\gamma$ -Carbon Interaction

T. Don Tilley, Richard A. Andersen\*, and Allan Zalkin

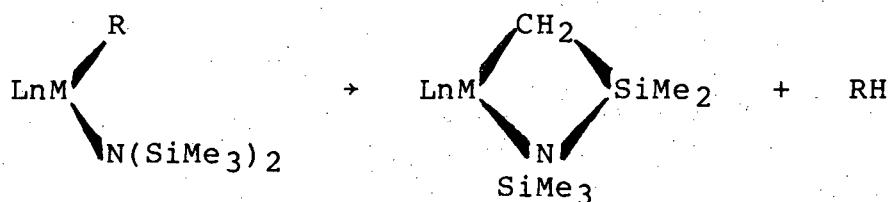
Chemistry Department and Materials and  
Molecular Research Division of Lawrence  
Berkeley Laboratory, University of California  
Berkeley, California 94720

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\* Address correspondence to this author at the Chemistry Department, University of California, Berkeley.  
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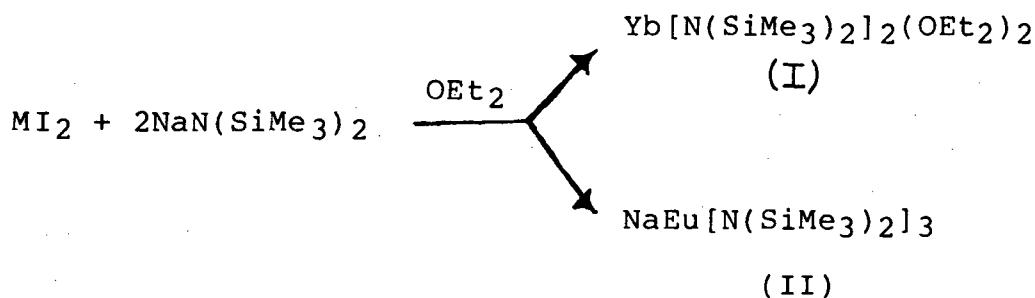
Abstract

The first lanthanide-tertiary phosphine complex,  $\text{Yb}[\text{N}(\text{SiMe}_3)_2]_2\text{-}[\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2]$  has been prepared and structurally characterized by X-ray methods. Of more importance, however, is the observation that a methyl group on each of the  $(\text{Me}_3\text{Si})_2\text{N}$  ligands is very close to the ytterbium atom (the  $\text{Yb-C(5)}$  contact is ca. 3 Å). This interaction is interpreted as being important in the hydrocarbon activation of the silylamine group in other metal (U, Th, Ti, Hf or Zr) complexes, leading to elimination of a  $\gamma$ -hydrogen atom to form the metallacycle shown below (R=alkyl, hydride).



The 4f-block metals have a rich coordination chemistry with nitrogen and oxygen ligands.<sup>1a</sup> In contrast only one example of a tertiary phosphine complex of a lanthanide metal  $Cp_3YbPPh_3$ , has been claimed.<sup>1b-e</sup> Lanthanide ions are generally thought to be the examples of class Al<sub>f</sub> or hard <sup>1g</sup> Lewis acids. Thus, the most thermodynamically stable complexes are formed between nitrogen and oxygen donors and lanthanide acceptors rather than between phosphorus and sulfur donors. The isolation of phosphine complexes of the actinide metals (thorium or uranium) of the type  $MX_4(dmpe)_2$ , where dmpe is bis-1,2-dimethylphosphinoethane and X is halide, alkyl, or phenoxide<sup>2a</sup> and  $U(Me_5C_5)_2H(dmpe)$ <sup>2b</sup> suggests that phosphine complexes of the lanthanide metals should be isolable. A synthetic route to such compounds would seem to require lanthanide complexes with empty coordination sites or ligands that are readily displaced by tertiary phosphines.

We have described a preparation of the divalent  $Eu[N(SiMe_3)_2]_2L_2$ , where L=tetrahydrofuran or 1,2-dimethoxyethane, which utilizes sodium naphthalene as a reducing agent.<sup>3</sup> This synthetic method is only applicable in relatively strong donor solvents, and was unsuccessful in the preparation of ytterbium(II) derivatives. A much improved synthetic scheme, which allows preparation of europium(II) and ytterbium(II) silylamides in the weaker donor solvent diethyl ether, is shown below.



The type of product isolated is metal-dependent. With ytterbium, crystallization from diethyl ether yields the bis-(diethyl ether) complex (I)<sup>4</sup>, whereas for europium, similar crystallization conditions give the anionic complex (II).<sup>5</sup> The different types of complexes can be explained by noting that in a given coordination number, the ionic radius of Eu(II) is ca. 0.1 Å greater than that of Yb(II).<sup>6</sup> Since two diethyl molecules are less sterically demanding than a silylamine group, the latter is more readily accommodated about the coordination sphere of the larger Eu(II) ion. The preparation of pentane-soluble complexes of  $M[N(SiMe_3)_2]_2$ , where M=Eu or Yb, with the relatively weak donor ligands  $[N(SiMe_3)_2]^-$  or  $OEt_2$  are suitable reagents for preparation of phosphine complexes of  $M[N(SiMe_3)_2]_2$  by way of displacement reactions.

The coordinated diethyl ether in (I) is displaced by 1,2-dimethylphosphinoethane (dmpe) giving purple, diamagnetic  $Yb[N(SiMe_3)_2]_2(dmpe)$ .<sup>7</sup> An ORTEP drawing is shown in Figure 1.<sup>9</sup> As this is the first lanthanide phosphine complex to be structurally characterized, no bond length data are available for comparison. However, a value for the Yb-P bond length can be estimated from the value of  $3.104 \pm 0.006$  Å found in the eight coordinate  $U(OPh)_4(dmpe)_2$ .<sup>2a</sup> The ionic radius of four coordinate Yb(II) is estimated to be ca. 0.1 Å less than that of eight coordinate U(IV).<sup>6</sup> Thus, the estimated Yb-P bond length of 3.0 Å is close to the actual value of  $3.012(4)$  Å.

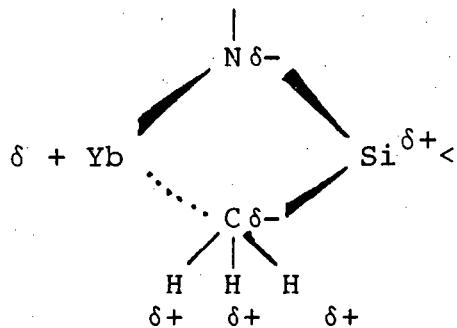
Inspection of the bond distances and angles (Figure 2) in the  $N(SiMe_3)_2$  ligands, which are related by two-fold molecular symmetry, reveals distortions that result from an inter-

action between the C(5) methyl group and the ytterbium atom as shown in Figure II. The Yb-N-Si(1) bond angle of  $108.5(6)^\circ$  is less than the Yb-N-Si(2) angle of  $121.0(7)^\circ$ . The latter angle is normal since it lies in the range found for other metal silylamides ( $121.5 \pm 4.5^\circ$ ).<sup>10</sup> In addition the N-Si(1)-C(5) angle of  $106.3(7)^\circ$  is smaller than the other N-Si(1)-C(4,6) and N-Si(2)-C(7,8,9) angles which average to  $115.4 \pm 0.8^\circ$  and  $112.1 \pm 1.5^\circ$ , respectively. This is accompanied by an opening of the Si(1)-N-Si(2) angle to  $130.5(8)^\circ$  which is larger than is observed in metal-silylamides which average to  $119.5 \pm 3.6^\circ$ .<sup>10</sup> The Yb-C(5) interaction appears to lengthen the bond distances within the incipient metallacyclic ring [YbNSi(1)C(5)] relative to the normal YbNSiC(Me) group, though these bond distances are not statistically significant. Thus, the N-Si(1) distance of  $1.691(13)\text{\AA}$  is equal to that of the N-Si(2) distance of  $1.667(13)\text{\AA}$ . Further, the Si(1)-C(5) distance of  $1.896(20)\text{\AA}$  is not significantly different from the other two Si(1)-C(Me) distances of  $1.861(20)$  and  $1.872(16)\text{\AA}$ .

The Yb-C(5) separation is less than the sum of the van der Waals radius of a methyl group ( $2.0\text{ \AA}$ ) and the divalent metallic radius of ytterbium ( $1.7\text{ \AA}$ ),<sup>11</sup> but longer than the Yb(III)-C(methyl) distances of  $2.57\text{ \AA}$  in  $[\text{Cp}_2\text{Yb}(\mu-\text{Me})]_2$ .<sup>12a</sup> Thus, the C(5) carbon atom, and two of the three hydrogen atoms bonded to it, are closer than expected to the metal atom. These three hydrogens were located and refined isotropically to reasonable tetrahedral positions about C(5) and no distortion due to presence of the ytterbium was observed. The Yb-H distances refined to  $2.76(8)$ ,  $2.85(6)$  and  $3.18(1)\text{ \AA}$ , and the H-C(5)-H bond angles are  $110$ ,  $105$  and  $113^\circ$  as

shown in Figure II.

Geometrically, the ytterbium-C(5) methyl interaction resembles the situation observed for compounds in which a methyl group bridges two metals, *i.e.*  $[Cp_2Y(\mu\text{-Me})]_2$ ,<sup>12a</sup>  $[Cp_2Yb(\mu\text{-Me})]_2$ ,<sup>12a</sup>  $[Cp_2Yb(\mu\text{-Me})_2AlMe_2]$ ,<sup>12b</sup> and  $[AlMe_3]_2$ .<sup>12c</sup> In  $[Cp_2Y(\mu\text{-Me})]_2$  and  $[AlMe_3]_2$  the hydrogen atoms on the methyl groups were located and they point away from the metal atoms, ruling out a direct metal-hydrogen interaction. The M-( $\mu$ C)-M angles in these alkyls are 87° in  $[Cp_2Yb(\mu\text{-Me})]_2$ , 88° in  $[Cp_2Y(\mu\text{-Me})]_2$ , 83 and 78° in  $[Cp_2Yb(\mu\text{-Me})_2AlMe_2]$ , and 76° in  $[AlMe_3]_2$ . The Yb...C(5)Si(1) angle is 79.9(7)° in  $Yb[N(SiMe_3)_2]_2$  (dmpe). It is therefore appealing to the view Yb-methyl group as semi-bridging the electropositive ytterbium atom. The postulate that the interaction is primarily due to a metal-carbon rather than a metal-hydrogen interaction is consistent with the expected charge distribution (on the basis of relative electronegativity values) shown below.



This is in contrast to the situation found in transition metals in which M...HC interactions are observed.<sup>13</sup>

This model for the metal-carbon interaction in  $Yb[N(SiMe_3)_2]_2$ -

(dmpe) is important in defining the role of the metal atom in  $[(\text{Me}_3\text{Si})_2\text{N}]_3\text{MMe}$  ( $\text{M}=\text{Th}, \text{U}$ ) compounds in activating the  $\gamma$ -Hydrogen atoms on the silylamide ligands.<sup>14</sup> The  $\text{M} \dots \text{CH}_3$  interaction should increase the acidity of the hydrogen atom on the methyl group, promoting alkane elimination through a four-center transition state, as previously described. Therefore, a  $\text{M} \dots \text{CH}_3\text{Si}$  interaction may be important in metallacycle formation, and an oxidative addition process, which is doubtless endothermic for these tetravalent metals, is not required.

The anionic europium complex, II, also undergoes reaction with dmpe, giving an orange, paramagnetic complex of empirical formula  $\text{Eu}[\text{N}(\text{SiMe}_3)_2]_2(\text{dmpe})_{1.5}$ .<sup>15</sup> The europium complex, II, and the ytterbium complex, I, yield 2:1 complexes with tri-n-butylphosphine of composition  $\text{M}[\text{N}(\text{SiMe}_3)_2]_2(\text{PBu}_3^n)_2$ , where M is Eu<sup>16</sup> or Yb.<sup>17</sup>

Acknowledgement. This work is supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under contract number W-7405-Eng-48. We also thank Dr. F. L. Hollander, staff crystallographer of the U.C. Berkeley X-ray facility (CHEXRAY) for collecting the X-ray data.

Supplementary Material. Positional and thermal parameters and structure factors with their estimated standard deviations (10 pages). Ordering information is given on any current mast head page.

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- (4) Orange crystals from diethyl ether (-70°C), mp 69-71°C.  
 $^1\text{H}$  NMR (26°C, PhH-d<sub>6</sub>): δ 0.41s, 36H, N(SiMe<sub>3</sub>)<sub>2</sub>; 1.06t (J=7Hz), 12H, OCH<sub>2</sub>CH<sub>3</sub>; 3.51q (J=7Hz), 8H, OCH<sub>2</sub>CH<sub>3</sub>.  $^{13}\text{C}\{\text{H}\}$  NMR (26°C, PhH-d<sub>6</sub>): δ 5.57, N(SiMe<sub>3</sub>)<sub>2</sub>; 14.7 (OCH<sub>2</sub>CH<sub>3</sub>); 65.2 (OCH<sub>2</sub>CH<sub>3</sub>).
- (5) Yellow needles from diethyl ether (-70°C), mp 152-153°C. The crystal structure of this complex has been completed and will be described later, Zalkin, A., unpublished results.
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- (7) Purple prisms from pentane (-10°C), mp 195-197°C.  $^1\text{H}$  NMR (26°C, PhH-d<sub>6</sub>): δ 0.46, s, 36H, N(SiMe<sub>3</sub>)<sub>2</sub>; 0.86, apparent singlet, 12H, PMe<sub>2</sub>; 1.04, a three line pattern, with the separation of the outer-most lines being 13 Hz,<sup>8</sup> 4H, PCH<sub>2</sub>.  $^{13}\text{C}\{\text{H}\}$  NMR (26°C, PhH-d<sub>6</sub>): δ 5.75, N(SiMe<sub>3</sub>)<sub>2</sub>; 11.6, apparent singlet, PMe<sub>2</sub>; 25.8, apparent three-line pattern with a separation between the outer-most lines of 8 Hz. The spin system of dmpe in the  $^1\text{H}$  NMR spectrum is X<sub>6</sub>AY<sub>2</sub>Y'Y''<sub>2</sub>A'Y'\_6 and in the  $^{13}\text{C}\{\text{H}\}$  NMR spectrum is ABX. Accordingly, a first order analysis is inappropriate.<sup>8</sup>  $^{31}\text{P}\{\text{H}\}$  NMR (26°C, PhH-d<sub>6</sub>): δ-40.9. The coordination chemical shift, defined as the chemical shift of the complex less that of the free ligand, is 8.5 p.p.m.
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- (9) The compound crystallizes in the orthorhombic space group

$F2dd(C_{2V}^{19})$  with cell dimensions  $a=11.353(2)$ ,  $b=18.704(5)$ , and  $c=31.084(8)\text{\AA}$  with  $Z=8$  and  $d_{\text{calc}}=1.296 \text{ gcm}^{-3}$ . The data were collected on a Nonius CAD-4 automated diffractometer using MoK $\alpha$  X-rays ( $\lambda = 0.70930 \text{ \AA}$ ). The data were corrected for absorption ( $\mu = 22.6 \text{ cm}^{-1}$ ). The structure was solved from Patterson and electron density maps and refined by full-matrix least-squares to a conventional R factor of 0.050 using 1916 data where  $F^2 > \sigma(F^2)$ .

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(14) Simpson, S. J.; Turner, H. W.; Andersen, R. A. J. Am. Chem. Soc. 1979, 101, 7728-7729; Inorg. Chem. 1981, 20, 2991-2995.

(15) Orange prisms from pentane (-10°C). Anal. Calcd for C<sub>21</sub>H<sub>60</sub>N<sub>2</sub>EuP<sub>3</sub>Si<sub>4</sub>: C, 36.1; H, 8.67; N, 4.01; P, 13.3. Found: C, 35.4; H, 8.34; N, 3.80; P, 13.0. The <sup>1</sup>H NMR spectrum of a benzene extract of a solution of the complex which had been hydrolyzed with D<sub>2</sub>O showed resonances due to DN(SiMe<sub>3</sub>)<sub>2</sub> and dmpe in area ratio 2:1.5.

(16) Orange crystals from pentane (-70°C), mp 48-49°C. Anal. Calcd for C<sub>36</sub>H<sub>90</sub>N<sub>2</sub>EuP<sub>2</sub>Si<sub>4</sub>: C, 49.3; H, 10.3; N, 3.19; P, 7.06. Found: C, 49.0; H, 10.2; N, 2.79; P, 6.82. The paramagnetic complex,  $\mu_B = 7.4$  B.M. (Evans' method, 30°C, PhH), was hydrolyzed with water and the <sup>1</sup>H NMR of an aliquot in benzene gave resonances due to (Me<sub>3</sub>Si)<sub>2</sub>NH and PBu<sub>3</sub><sup>n</sup> in a 1:1 molar ratio.

(17) Brown-red prisms from pentane (-70°C), mp 46-48°C. Anal. Calcd for C<sub>36</sub>H<sub>90</sub>N<sub>2</sub>P<sub>2</sub>Si<sub>4</sub>Yb: C, 48.1; H, 10.1; N, 3.12, P, 6.89. Found: 48.8; H, 10.0; N, 2.87; P, 7.47. <sup>1</sup>H NMR (26°C, PhH-d<sub>6</sub>): δ 0.48, s, 36H, N(SiMe<sub>3</sub>)<sub>2</sub>; 1.00, an apparent triplet with the separation between the outermost lines being 12 Hz, 18H, P(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>)<sub>3</sub>; 1.49 an apparent singlet, 36H, P(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>)<sub>3</sub>. <sup>13</sup>C{<sup>1</sup>H} NMR (26°C, PHH-d<sub>6</sub>): δ 6.27, s, N(SiMe<sub>3</sub>)<sub>2</sub>; 14.0, an apparent singlet due to the γ-C of PBu<sub>3</sub><sup>n</sup>; three apparent doublets at 24.9 (separation of 10 Hz), 26.9 (separation of 10 Hz)

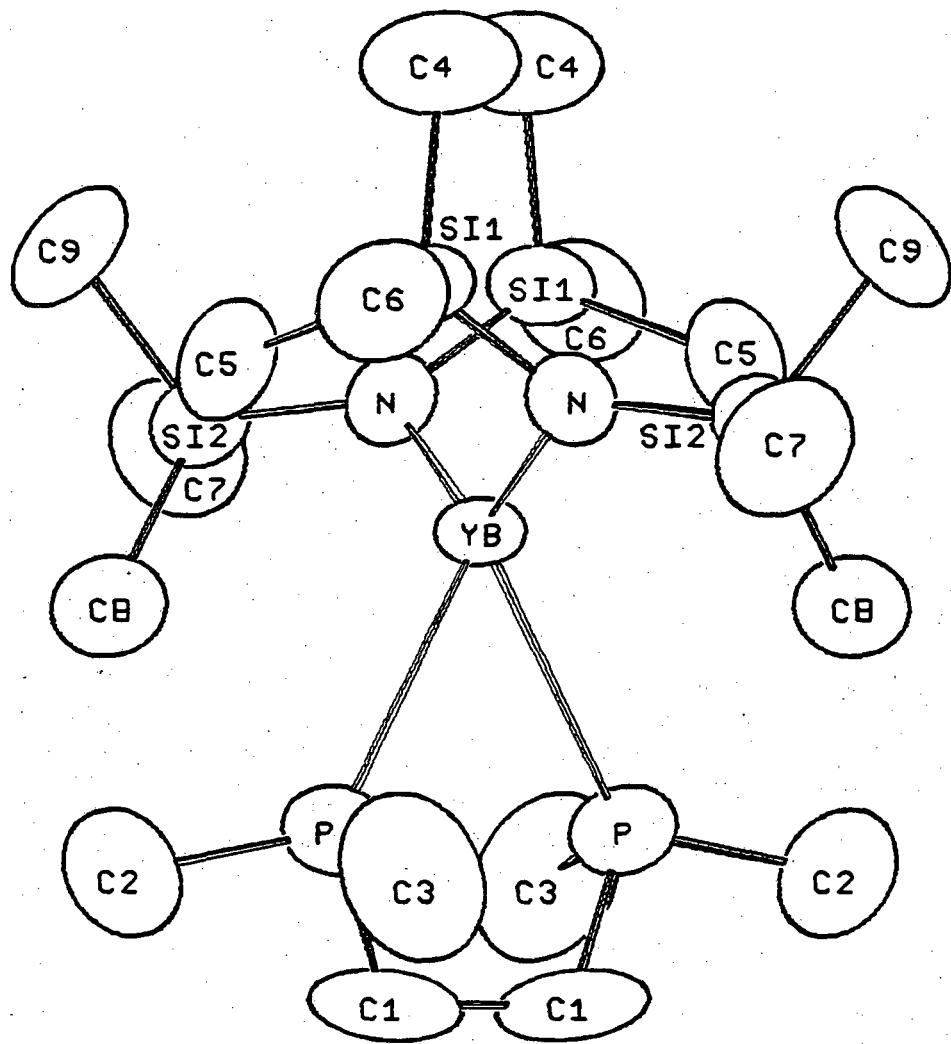
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and 28.3 (separation of 11 Hz) due to the other three carbon atoms.  $^{31}\text{P}\{\text{H}\}$  NMR ( $26^\circ\text{C}$ ,  $\text{PhH-d}_6$ ),  $\delta$  -29.6. The coordination chemical shift is zero.

**Figure Captions**

**Figure I.** An ORTEP diagram of  $\text{Yb}[\text{N}(\text{SiMe}_3)_2]_2$  (dmpe). Some bond lengths and bond angles are:  $\text{Yb-N} = 2.331(13)\text{\AA}$ ;  $\text{Yb-P} = 3.012(4)\text{\AA}$ ;  $\text{N-Yb-N} = 123.6(6)^\circ$ ;  $\text{P-Yb-P} = 68.4(2)^\circ$ ;  $\text{N-Yb-P} = 101.2(3)^\circ$ .

**Figure II.** A line drawing showing the  $\text{Yb-C}(5)$  interaction. The bond angles are in degrees and the bond lengths are in angstroms.



XBL 8110-7070

Figure 1.

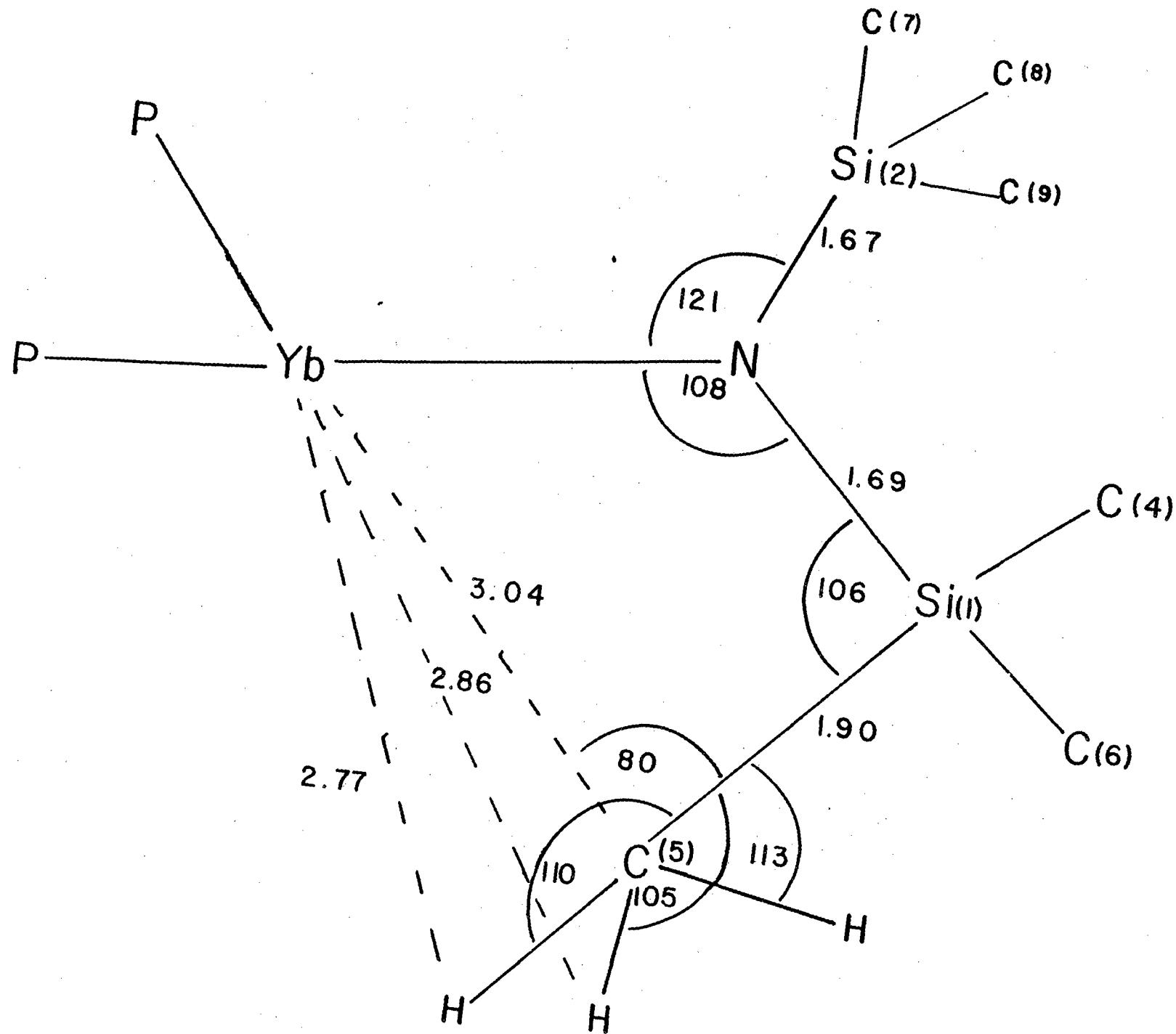


Figure II

XBL 822-8074

## Supplementary Material for

Tertiary Phosphine Complexes of the f-Block Metals; Crystal  
Structure of  $\text{YbN}(\text{SiMe}_3)_2(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)$ : Evidence for a  
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Table A: Positional Parameters for  $[(\text{Me}_3\text{Si})_2\text{N}]_2\text{Yb}(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PM}_2)^*$ 

ATOM	X	Y	Z
YB	0	0	0
P	.2194(4)	.0053(2)	.05440(14)
N	-.097(1)	.1031(7)	.0226(4)
SI(1)	-.1801(4)	.0827(2)	.06602(12)
SI(2)	-.0807(4)	.1802(2)	-.00380(12)
C(1)	.349(2)	-.016(1)	.0217(8)
C(2)	.251(2)	-.048(1)	.1010(7)
C(3)	.252(3)	.092(1)	.0745(8)
C(4)	-.341(2)	.075(1)	.0548(8)
C(5)	-.125(2)	-.007(1)	.0863(8)
C(6)	-.171(2)	.1458(8)	.1127(6)
C(7)	-.059(3)	.2596(9)	.0317(8)
C(8)	.053(2)	.175(1)	-.0384(5)
C(9)	-.208(2)	.200(1)	-.0409(6)
H(12)	-.047(7)	-.006(3)	.090(2)
H(13)	-.149(8)	-.038(5)	.067(3)
H(14)	-.153(9)	-.019(5)	.117(3)
H(1)	.3518	-.0667	.018
H(2)	.4169	0	.0363
H(3)	.3229	-.0324	.1134
H(4)	.2555	-.0963	.0933
H(5)	.1889	-.0412	.1216
H(6)	.2622	.124	.0512
H(7)	.3228	.0899	.091
H(8)	.1894	.1077	.0923
H(9)	-.3527	.0380	.0339
H(10)	-.369	.1187	.0437
H(11)	-.3809	.0629	.0804
H(15)	-.1946	.1922	.1036
H(16)	-.0911	.143	.1224
H(17)	-.2198	.1297	.1351
H(18)	.0105	.2528	.0484
H(19)	-.1246	.2649	.0499
H(20)	-.0499	.301	.0142
H(21)	.0438	.1368	-.0584
H(22)	.1199	.1665	-.0210
H(23)	.062	.2186	-.0535
H(24)	-.2787	.2028	-.0245
H(25)	-.2149	.1626	-.0615
H(26)	-.1947	.2440	-.0551

\* Estimated standard deviations are in parenthesis, Hydrogen atoms H(1) through H(26) were estimated but are not refined in the least-squares procedure.

Table B. Thermal parameters in the  $[(\text{Me}_3\text{Si})_2\text{N}]_2\text{Yb}(\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2)$  structures\*

ATOM	B11	B22	B33	B12	B13	B23	EEQ
YB	2.26(3)	3.57(3)	5.29(3)	0	0	-0.24(5)	3.71(2)
P	4.2(2)	6.3(2)	6.2(2)	-0.5(1)	-1.3(2)	-0.3(2)	5.5(1)
N	4.5(6)	5.6(7)	5.5(5)	-0.7(5)	-1.1(5)	.5(5)	5.3(3)
SI(1)	3.3(1)	5.5(2)	6.2(2)	-0.3(2)	.2(1)	-0.7(2)	5.0(1)
SI(2)	4.6(2)	4.3(2)	6.9(2)	0.7(1)	-0.1(2)	.1(2)	5.3(1)
C(1)	4.2(8)	10.1(14)	10.9(13)	0.1(8)	-2.3(8)	-0.9(11)	8.4(7)
C(2)	7.3(10)	9.7(13)	10.4(12)	-0.2(11)	-3.7(10)	1.3(11)	9.1(7)
C(3)	15.8(22)	10.3(15)	12.0(15)	-4.4(16)	-8.0(16)	-0.5(13)	12.7(10)
C(4)	4.9(9)	13.0(17)	11.1(13)	-0.5(11)	.4(9)	-1.8(12)	9.7(8)
C(5)	5.5(10)	6.8(10)	8.4(11)	-0.1(8)	2.1(9)	.4(8)	6.9(6)
C(6)	8.5(11)	6.2(8)	7.8(8)	-0.7(9)	.3(9)	-1.8(7)	7.5(5)
C(7)	10.4(16)	5.3(9)	10.0(13)	-1.2(9)	1.4(11)	-1.4(8)	8.6(8)
C(8)	5.4(8)	7.6(10)	8.2(9)	1.5(7)	.3(7)	.5(7)	7.1(5)
C(9)	6.5(11)	6.7(10)	11.2(12)	2.3(8)	-2.1(9)	1.3(8)	8.1(6)
H(12)	-0.6(8)						
H(13)	.4896						
H(14)	1.8343						
H(1)	12.000						
H(2)	12.000						
H(3)	12.000						
H(4)	12.000						
H(5)	12.000						
H(6)	12.000						
H(7)	12.000						
H(8)	12.000						
H(9)	12.000						
H(10)	12.000						
H(11)	12.000						
H(15)	12.000						
H(16)	12.000						
H(17)	12.000						
H(18)	12.000						
H(19)	12.000						
H(20)	12.000						
H(21)	12.000						
H(22)	12.000						
H(23)	12.000						
H(24)	12.000						
H(25)	12.000						
H(26)	12.000						

\* The anisotropic temperature factor has the form  $\exp(-0.25(B_{11}h^2a^*{}^2 + 2B_{12}hka^*b^* + \dots))$ . The isotropic temperature factor has the form  $\exp(-B(\sin\theta)/\lambda)^2$ .

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 6.0)  
 YB (((CH<sub>3</sub>)<sub>3</sub>SI)2N)2 ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>) F(0,0,0) = 3956

F<sub>OB</sub> AND F<sub>CA</sub> ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.

SG = ESTIMATED STANDARD DEVIATION OF FCB. DEL = |F<sub>OB</sub>| - |F<sub>CA</sub>|.

\* INDICATES ZERO WEIGHTED DATA.

L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL			
H, K = -12, 0	10	232	9	-3	17	208	8	-7	20	35	10	-15	3	148	6	2		
0 295 12 4	14	222	8	-7	19	135	6	-12	22	230	9	-4	5	348	14	-7		
4 259 10 -13	16	39	10	1	21	127	6	-7	H, K = -9,	7	0	528	20	44	7	357	13	12
H, K = -12, 2	18	194	8	-18	H, K =				H, K = -8,	4			9	367	14	-6		
2 205 8 -10	H, K = -10,	6			1	314	12	5	2	102	5	0	11	372	14	3		
4 64 7 2	0	277	10	-16	3	216	9	-4	4	399	15	45	13	226	8	8		
H, K = -11, 1	4	280	10	-21	5	231	9	-19	6	93	6	-6	15	203	8	22		
1 214 8 -10	8	262	10	-17	7	119	8	-16	8	329	12	14	17	157	6	18		
3 226 8 -3	12	240	9	-3	9	143	6	-9	10	93	5	8	19	98	9	13		
5 188 7 -11	16	211	9	-11	11	158	6	-6	12	326	12	6	21	138	7	-5		
7 193 7 -6	H, K = -10,	8			13	200	8	-1	16	279	11	-6	23	144	6	-2		
9 192 7 -4	2	240	10	-18	15	184	7	3	18	49	12	3	25	123	5	-9		
11 182 7 -12	6	222	8	-3	17	189	7	-4	20	211	8	-3	27	125	6	-0		
13 185 8 -15	10	209	8	2	19	116	7	1	24	146	6	-8	H, K =	-7,	3			
H, K = -11, 3	H, K = -10,	10			H, K =	-9,	9		H, K = -8,	6			1	330	12	16		
1 137 6 -6	0	265	10	-28	1	240	9	-11	2	403	15	38	3	480	18	22		
3 139 6 -20	4	219	8	-21	3	252	9	-18	4	38	19	12	5	312	12	8		
5 187 7 -2	6	32	30	18	5	160	6	-1	6	256	9	23	7	415	15	-4		
7 180 8 -9	8	187	7	-0	7	156	6	-12	10	256	10	-5	9	472	17	1		
9 162 6 -4	H, K =	-9,	1		9	153	6	-5	14	296	11	-14	11	249	9	-4		
11 176 7 4	1	349	13	39	11	134	6	7	18	204	8	-6	13	399	15	21		
13 122 6 -12	3	307	12	41	13	158	7	-2	22	122	5	-14	15	196	7	13		
H, K = -11, 5	5	303	11	37	15	130	7	-6	H, K =	-8,	8		17	136	6	10		
1 107 6 -17	7	245	9	14	H, K =	-9,	11		0	471	18	38	19	203	8	1		
3 171 7 -12	9	182	8	15	1	185	7	-24	2	40	44	18*	21	139	6	1		
5 195 8 -9	11	193	8	-4	3	154	6	-15	4	372	14	10	23	171	7	11		
7 245 9 -13	13	137	7	-6	5	164	7	-31	8	284	11	-1	25	173	7	-2		
9 230 9 -3	15	162	6	-2	7	147	6	-7	10	64	10	6	H, K =	-7,	5			
11 194 8 -8	17	178	7	-4	9	122	5	-15	12	296	11	-7	1	203	8	-2		
H, K = -11, 7	19	165	6	4	11	136	6	-13	16	266	10	4	3	192	7	-11		
1 108 9 -10	21	150	6	-6	13	87	8	-18	18	38	9	10	5	286	11	6		
3 120 6 -8	H, K =	-9,	3		H, K =	-9,	13		20	196	8	8	7	241	9	1		
5 193 8 -11	1	346	13	46	1	160	7	-2	H, K =	-8,	10		9	267	10	3		
7 205 8 -3	3	357	13	43	3	140	7	-6	2	257	10	-5	11	326	12	9		
H, K = -10, 0	5	199	8	28	5	152	8	-11	4	34	41	-10*	13	193	7	-2		
2 398 15 -13	7	222	9	15	H, K =	-8,	0		6	274	10	-28	15	164	6	-0		
6 308 12 -7	9	188	8	3	0	271	10	14	10	244	9	-27	17	150	7	-3		
10 264 10 -2	11	157	8	17	4	379	14	4	12	63	6	7	19	73	8	-12		
14 288 11 -19	13	188	7	-6	8	470	17	5	14	169	7	-11	21	183	5	3		
18 224 8 -29	15	195	7	0	12	310	11	15	16	33	12	1	23	125	5	8		
H, K = -10, 2	17	173	7	7	16	156	8	5	18	146	6	1	25	91	12	-4		
0 324 12 -4	19	207	8	-3	20	215	8	-3	H, K =	-8,	12		H, K =	-7,	7			
2 70 30 6	21	132	6	-1	24	179	7	-14	0	184	7	-4	1	258	10	-15		
4 298 12 -7	H, K =	-9,	5		H, K =	-8,	2		4	228	9	-20	3	221	8	-7		
8 273 10 14	1	323	12	19	2	539	20	41	8	255	10	-29	5	281	10	13		
10 61 6 10	3	256	10	13	4	85	6	3	12	177	7	-17	7	312	12	9		
12 240 9 -2	5	226	10	-6	6	462	18	15	H, K =	-8,	14		9	259	10	27		
16 220 8 -18	7	151	8	-10	8	61	6	-4	2	236	9	0	11	331	12	21		
H, K = -10, 4	9	140	6	-16	10	417	15	22	4	37	16	-10	13	177	8	15		
2 277 10 -11	11	176	7	-8	12	77	11	4	6	232	9	-13	15	205	8	-3		
4 82 10 9	13	170	7	-8	14	254	9	21	H, K =	-7,	1		17	153	6	3		
6 250 9 -17	15	183	7	-8	18	246	9	7	1	219	8	16	19	102	5	-7		

## STRUCTURE FACTORS CONTINUED FCF

YB ((CH<sub>3</sub>)<sub>3</sub>Si)2N<sub>2</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL
21	138	6	3	12	510	19	12	14	243	9	5	21	169	7	3	17	198	7	5
23	129	6	7	14	73	8	-3	18	158	6	-14	23	139	6	-1	19	119	6	-16
H,K=	-7,	9		16	395	15	-2					25	83	5	-9	21	124	5	10
1	208	8	20	18	41	7	-10	0	352	13	-26	27	77	5	3	H,K=	-5,	15	
3	293	12	9	20	222	8	4	4	308	11	-8	29	42	8	-3	1	216	8	-1
5	217	8	22	24	194	7	2	8	289	11	5		H,K=	-5,	7	3	271	10	16
7	292	11	5	28	174	7	2	10	53	7	9	1	356	13	-21	5	161	6	-6
9	331	12	10	H,K=	-6,	4		12	259	10	3	3	306	11	-11	7	182	7	7
11	195	8	7	2	527	19	-5	16	209	8	-3	5	355	13	-20	9	158	6	3
13	258	10	-8	4	98	5	-10	H,K=	-6,	16		7	361	13	-12	11	128	6	-3
15	176	7	2	6	620	23	6	2	136	6	-21	9	245	9	-10	13	159	6	7
17	110	5	-3	8	98	4	1	6	184	7	0	11	308	12	13	15	142	7	7
19	165	6	2	10	528	19	17	10	174	7	-8	13	179	7	2	17	130	6	-7
21	101	5	-8	12	157	6	1	H,K=	-5,	1		15	253	9	20	H,K=	-5,	17	
H,K=	-7,	11		14	366	13	-6	1	644	23	50	17	225	8	15	1	116	5	1
1	108	15	-8	16	33	9	-9	3	395	14	8	19	223	8	7	3	99	5	-5
3	76	23	-6	18	228	8	1	5	351	13	15	21	155	7	-5	5	142	6	3
5	191	8	-12	22	213	8	6	7	353	13	25	23	156	7	-4	7	100	5	-8
7	169	9	-22	26	166	6	1	9	169	6	10	25	91	5	-4	9	108	5	7
9	197	7	-15	28	38	10	-3	11	273	10	8	27	86	5	-2	11	94	5	-2
11	188	7	-15	H,K=	-6,	6		13	270	10	1	H,K=	-5,	9		H,K=	-4,	0	
13	138	7	1	0	335	13	-55	15	349	13	-9	1	358	13	-25	0	625	22	60
15	116	5	1	4	349	13	-15	17	372	14	-15	3	409	15	-36	4	584	21	40
17	106	5	6	8	541	20	8	19	225	8	-3	5	266	10	-23	8	413	15	6
19	57	10	-3	12	315	12	19	21	208	8	21	7	282	11	-9	12	350	13	-9
H,K=	-7,	13		14	48	9	-5	23	103	5	1	9	281	11	15	1	396	15	2
1	196	7	-9	16	155	6	-3	25	94	5	-6	11	184	7	7	20	392	15	10
3	155	6	-9	18	27	32	6*	27	94	5	-2	13	274	11	19	24	207	8	3
5	229	9	-8	20	156	6	-5	29	93	5	-2	15	275	10	19	28	133	5	-15
7	206	8	-8	24	160	6	3	H,K=	-5,	3		17	233	6	2	H,K=	-4,	2	
9	207	8	-3	H,K=	-6,	8		1	559	20	10	19	242	9	-5	2	697	25	41
11	210	8	9	2	435	16	-50	3	723	26	34	21	172	7	-8	4	114	7	1
13	130	6	-14	4	75	5	-4	5	396	14	-9	23	133	6	-8	6	614	22	-11
15	132	6	7	6	524	19	-15	7	518	19	-2	25	115	5	-1	8	151	6	4
H,K=	-7,	15		8	37	13	8	9	373	14	15	H,K=	-5,	11		10	549	20	-18
1	113	5	-6	10	513	19	22	11	302	11	-15	1	249	9	-16	12	101	4	-1
3	181	7	3	12	128	5	-1	13	419	15	-3	3	206	8	2	14	483	18	-15
5	128	6	-3	14	322	12	25	15	356	13	-13	5	170	6	24	1	65	7	3
7	155	7	-4	18	254	10	-11	17	299	11	-23	7	156	6	26	1	468	17	-7
9	191	7	5	20	50	23	6	19	317	12	14	9	145	6	48	20	113	5	-2
11	118	5	-13	22	216	8	-5	21	209	8	-2	11	162	6	24	22	293	11	18
H,K=	-6,	0		H,K=	-6,	10		23	150	6	1	13	166	6	19	2	174	7	-9
2	448	16	11	0	295	11	-10	25	143	6	-1	15	197	10	0	30	122	5	-9
6	278	10	6	2	91	5	-3	27	90	5	3	17	207	8	6	H,K=	-4,	4	
10	309	12	12	4	285	11	3	29	96	5	3	19	131	5	1	0	807	29	38
14	397	15	-6	6	113	6	-7	H,K=	-5,	5		21	117	5	-5	2	77	6	-11
18	260	10	7	8	281	10	31	1	395	14	12	23	77	6	-1	4	690	25	-4
22	111	5	-8	10	37	9	6	3	377	14	-11	H,K=	-5,	13		8	98	4	0
26	144	6	-3	12	285	11	13	5	447	16	1	1	331	12	22	2	545	20	-15
H,K=	-6,	2		16	223	8	-8	7	255	9	-1	3	271	10	5	10	140	5	-8
0	795	29	47	18	55	6	-2	9	226	9	-7	5	240	9	22	12	365	13	-12
2	160	6	4	20	163	6	-8	11	294	11	34	7	166	6	8	14	110	5	-2
4	694	25	21	H,K=	-6,	12		13	114	5	6	9	147	10	3	1	456	17	21
6	49	5	-2	2	255	10	-12	15	200	7	10	11	190	8	4	18	34	8	9
8	548	20	22	6	198	8	1	17	216	8	12	13	191	7	-6	20	339	13	13
10	94	5	3	10	234	9	5	19	187	7	9	15	193	7	2	22	60	8	7

STRUCTURE FACTORS CONTINUED FCF  
 YB ((CH<sub>3</sub>)<sub>3</sub>Si)2N<sub>2</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL				
24	191	8	-8	6	351	13	24	11	390	14	-7	H, K=	-3,	13	16	299	11	-29	
26	59	5	1	10	260	10	-8	13	377	14	-5	1	180	7	8	18	107	5	1
28	130	5	2	14	242	9	-5	15	312	12	8	3	202	8	-3	20	258	10	-34
H, K=	-4,	6	18	206	8	1	17	334	12	24	5	317	12	30	24	266	10	22	
2	617	22	-3	H, K=	-4,	16	19	187	7	22	7	285	11	12	26	73	12	-8	
4	63	4	-2	0	285	11	16	21	163	6	17	9	273	11	15	28	187	7	4
6	474	17	-17	2	55	14	26	23	111	5	14	11	200	8	13	32	101	5	-1
8	60	4	6	4	248	10	11	25	144	7	-4	13	159	8	-8	H, K=	-2,	4	
10	238	10	-13	8	187	7	1	27	119	6	-1	15	139	8	-5	2	560	20	-24
12	49	5	-1	12	149	6	-2	29	131	6	-5	17	99	5	3	4	153	8	-9
14	430	16	28	16	167	7	6	31	102	5	7	19	141	6	5	6	596	21	1
16	81	4	5	H, K=	-4,	18	H, K=	-3,	7	21	126	7	6	8	45	17	14		
18	382	14	29	2	204	8	8	1	425	16	-12	23	131	6	4	10	674	24	-5
20	28	20	14	4	36	12	24	3	391	14	-8	H, K=	-3,	15	12	243	9	2	
22	208	8	4	6	161	8	-12	5	442	16	1	1	175	9	6	14	504	18	-14
26	117	5	-10	10	137	6	-11	7	369	14	-17	3	210	9	28	1E	109	4	3
H, K=	-4,	8	H, K=	-3,	1	9	374	14	-13	5	225	11	3	18	284	11	-28		
0	540	20	-35	1	588	21	70	11	252	9	-13	7	205	12	-2	20	78	4	-8
2	76	4	-3	3	418	15	18	13	417	15	-17	9	192	11	-2	22	215	8	13
4	561	20	-23	5	918	33	28	15	205	8	-5	11	196	7	-8	2E	230	9	2
6	133	5	-9	7	462	17	-3	17	273	10	19	13	150	6	-1	30	171	7	7
8	451	16	-43	9	655	24	6	19	119	5	8	15	139	6	-1	H, K=	-2,	6	
10	125	5	12	11	354	13	-20	21	146	6	12	17	116	5	5	0	700	25	-2
12	384	14	-19	13	303	11	-3	23	109	9	-1	19	124	7	6	2	195	8	11
14	78	4	5	15	223	8	-8	25	134	5	-4	H, K=	-3,	17	4	620	22	9	
16	421	16	15	17	174	6	15	27	115	5	-7	1	190	7	2	6	145	6	15
18	33	10	-14	19	247	9	-14	29	129	6	2	3	158	6	5	8	679	24	34
20	302	11	4	21	199	8	4	H, K=	-3,	9	5	150	6	2	10	103	4	0	
24	186	7	-9	23	253	9	10	1	256	10	-9	7	142	8	12	12	686	25	-5
28	120	5	-4	25	158	7	5	3	297	11	-5	9	129	6	-8	14	40	7	9
H, K=	-4,	10	27	146	6	-2	5	386	14	-13	11	144	6	9	1E	422	15	-10	
2	433	16	-11	29	92	5	-4	7	369	14	-10	13	107	5	-2	18	41	6	-4
4	128	5	-4	31	92	5	2	9	386	14	-8	15	148	6	8	20	255	9	19
6	360	13	-3	H, K=	-3,	3	11	384	14	-18	H, K=	-3,	19	22	28	12	1		
10	264	10	11	1	519	19	1	13	239	9	-9	1	124	6	-2	24	241	9	13
12	84	5	-2	3	458	17	26	15	233	9	9	3	109	6	-18	28	214	8	5
14	315	12	38	5	617	22	-28	17	206	8	0	5	109	8	-9	H, K=	-2,	8	
16	49	7	-10	7	636	23	-9	19	138	6	20	7	108	6	-6	2	456	17	-28
18	295	11	14	9	562	20	-17	21	167	7	0	H, K=	-2,	0	4	149	6	-4	
20	78	11	-2	11	486	18	-20	23	112	5	-6	2	786	28	62	6	446	16	-3
22	194	7	0	13	309	11	-17	25	135	6	2	61371	50	1E	2	109	5	10	
24	25	19	16	15	305	11	-14	27	127	5	-3	10	905	32	-21	10	487	18	-10
26	130	6	-1	17	214	8	-4	H, K=	-3,	11	14	465	17	-12	12	95	4	-3	
H, K=	-4,	12	19	233	9	1	1	275	10	20	18	236	9	-1E	14	359	13	-38	
0	345	13	6	21	163	6	0	3	315	12	19	22	348	13	-8	1E	95	4	3
2	74	6	3	23	157	6	3	5	308	12	15	26	276	10	17	18	225	8	-13
4	349	13	20	25	131	7	-3	7	413	15	1	30	156	6	2	20	69	5	1
8	261	10	37	27	170	7	-5	9	334	13	8	H, K=	-2,	2	22	165	7	1	
10	31	12	-8	29	109	5	-3	11	259	10	6	0	86	12	-21	24	35	25	-1
12	217	8	18	31	68	6	-13	13	180	7	17	2	294	11	-7	2E	167	6	-7
16	246	9	3	H, K=	-3,	5	15	156	6	33	4	651	23	4	30	137	6	-1	
20	201	8	8	1	403	15	-23	17	146	8	21	6	153	9	5	H, K=	-2,	10	
22	35	11	18	3	484	17	-14	19	167	7	10	8	855	31	-5	0	331	13	-8
24	139	7	9	5	480	17	4	21	128	5	3	10	135	7	5	2	110	5	-7
H, K=	-4,	14	7	373	14	-14	23	160	6	10	12	568	20	-25	4	435	16	17	
2	386	14	33	9	465	17	-13	25	127	6	5	14	78	4	-5	6	100	4	8

## STRUCTURE FACTORS CONTINUED FCF

YB ((CH<sub>3</sub>)<sub>3</sub>Si)2N<sub>2</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	FOB	SG	DEL	L	FCB	SG	DEL	L	FOB	SG	DEL	L	FCB	SG	DEL	L	FCB	SG	DEL
8	650	23	16	21	204	8	-26	29	82	7	-3	19	77	8	-2	28	96	5	-9
10	78	10	-4	23	168	6	7	H,K=	-1,	9		21	118	6	-9	32	105	5	1
12	440	16	-15	25	190	7	11	1	343	13	-36	H,K=	-1,	17		H,K=	0,	6	
14	29	14	-7	27	128	6	12	3	239	9	-34	1	195	8	-14	2	718	26	-117
16	234	9	12	29	137	6	4	5	350	13	-16	3	193	8	-6	4	236	10	-5
18	36	13	-10	31	100	6	2	7	196	7	-14	5	199	8	-4	6	758	27	-87
20	204	8	2	33	76	5	-10	9	239	9	20	7	189	7	4	8	99	7	-1
24	184	7	-3	H,K=	-1,	3		11	376	14	-30	9	202	8	8	10	624	23	-59
26	57	6	8	1	587	21	-39	13	152	6	-9	11	165	7	5	12	186	7	-12
28	146	6	7	3	181	8	-53	15	234	9	-19	13	158	6	-0	14	365	13	-38
H,K=	-2,	12		5	450	16	-8	17	234	9	-18	15	144	6	3	18	473	17	-28
2	353	13	-5	7	206	9	-7	19	128	6	4	17	103	6	-4	22	419	15	23
6	498	18	-4	9	338	12	-8	21	172	7	1	H,K=	-1,	19		26	195	8	-9
8	42	11	-3	11	367	13	-9	23	99	9	-13	1	112	6	-3	30	81	6	-7
10	446	16	17	13	308	12	-17	25	75	5	-7	3	131	7	-13	H,K=	0,	8	
14	220	8	36	15	308	11	-13	27	94	6	-3	5	93	9	-3	8	531	19	-37
18	170	8	2	17	311	12	-37	29	41	10	-1	7	106	6	1	2	180	7	-8
20	43	8	13	19	154	6	-21	H,K=	-1,	11		9	99	7	-4	4	405	15	-38
22	205	8	1	21	254	9	-17	1	432	16	-12	H,K=	0,	0		6	141	5	-1
24	34	12	-6	23	147	6	6	3	544	20	-17	41	170	42	-68	8	328	12	-45
26	162	6	7	25	94	5	16	5	297	11	-4	8	344	13	-9	10	83	5	-6
H,K=	-2,	14		27	126	9	-2	7	337	12	-5	12	471	17	-41	12	237	9	-21
0	161	6	-2	29	71	6	4	9	333	12	-4	16	615	22	-60	14	68	5	4
2	88	8	3	31	67	5	-6	11	256	10	-6	20	419	15	-19	16	254	10	-15
4	256	10	-6	H,K=	-1,	5		13	333	12	-6	24	181	7	1	18	115	5	-4
6	79	5	3	1	563	20	-57	15	209	8	12	28	177	7	-2	20	247	9	19
8	328	12	21	3	633	23	-28	17	221	8	15	32	156	6	4	24	156	7	-2
10	46	11	4	5	384	14	2	19	197	8	5	H,K=	0,	2		28	56	6	-4
12	258	10	0	7	487	18	-19	21	149	8	-8	2	891	32	-99	H,K=	0,	10	
16	159	6	-8	9	572	21	16	23	137	6	-4	4	299	11	-27	2	752	27	-27
20	139	6	-12	11	434	16	-2	25	120	6	1	6	111	6	-1	4	111	5	-12
H,K=	-2,	16		13	389	14	-2	27	93	5	3	8	119	10	-25	6	395	14	-35
2	271	12	2	15	371	14	-30	H,K=	-1,	13		10	432	16	-38	8	63	18	-23
6	273	11	1	17	299	11	-18	1	242	18	-21	12	189	7	-14	10	292	11	-19
10	272	10	-3	19	338	12	-13	3	202	8	-12	14	536	19	-56	12	85	4	5
12	55	9	16	21	261	10	-3	5	150	6	-21	16	42	9	5	14	429	16	-13
14	214	8	4	23	252	9	9	7	206	8	-4	18	429	16	-19	18	316	12	25
16	30	14	11	25	212	9	16	9	144	6	-0	20	105	4	5	22	210	9	-8
18	142	6	-8	27	128	6	3	11	199	8	25	22	215	8	-5	24	49	14	2
H,K=	-2,	18		29	118	5	7	12	182	7	14	24	65	5	-2	26	96	6	-11
0	210	8	-18	31	100	5	1	15	183	8	6	26	85	8	1	H,K=	0,	12	
4	192	8	-3	H,K=	-1,	7		17	150	9	-3	28	45	11	-12	0	756	27	0
6	50	9	9	1	473	17	-53	19	134	6	-8	30	107	5	-8	2	88	5	62
8	190	7	6	3	528	19	-54	21	120	5	-10	H,K=	0,	4		4	484	18	-17
12	177	7	3	5	254	10	8	23	76	11	-9	0	829	30	-93	8	208	8	-17
H,K=	-1,	1		7	486	18	-6	25	99	5	-2	2	260	10	-7	12	350	13	12
1	780	28	14	9	475	17	18	H,K=	-1,	15		4	734	26	-85	16	379	14	31
3	809	29	13	11	305	11	-1	1	197	9	-1	6	636	23	-27	18	48	14	18
5	454	16	-9	13	320	12	-13	3	157	6	7	8	441	16	-30	20	232	9	-6
7	414	15	-2	15	272	10	-23	5	181	7	2	10	62	8	-21	24	127	5	-5
9	459	17	-17	17	206	8	-20	7	153	7	0	12	380	14	-42	H,K=	0,	14	
11	490	18	-24	19	271	10	-10	9	149	8	3	14	68	4	2	2	262	10	-8
13	430	16	-26	21	175	7	14	11	173	9	-3	16	344	13	-34	4	110	5	6
15	356	13	-16	23	199	8	20	13	135	6	-6	18	117	5	6	6	114	6	11
17	325	12	-13	25	134	7	-1	15	128	6	-8	20	402	15	-25	8	28	30	17*
19	311	12	-18	27	101	5	-0	17	155	6	-9	24	242	9	15	10	146	6	11

## STRUCTURE FACTORS CONTINUED FCF

YB ((CH<sub>3</sub>)<sub>3</sub>Si)2N<sub>2</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	
12	82	13	-2	H, K=	1,	5		11	260	10	-25	18	237	9	-17	19	225	8	33	
14	225	8	2	1	571	21	-19	13	333	12	-15	22	345	13	2	20	62	8	-8	
18	205	8	-3	3	603	22	-35	15	212	8	5	26	276	10	9	22	162	6	7	
20	52	7	15	5	356	13	-55	17	222	8	17	30	161	6	-4	24	36	15	-0	
22	115	E	-3	7	452	16	-56	19	199	8	10	H, K=	2,	2		26	172	8	1	
	H, K=	0,	16	9	539	19	-63	21	151	6	-8	0	99	10	41	30	137	6	6	
0	341	13	1	11	419	15	-50	23	139	6	-4	2	324	12	24	H, K=	2,	10		
2	79	15	8	13	361	13	-44	25	119	5	1	4	661	24	47	0	346	13	-23	
4	317	12	-2	15	364	13	-20	27	92	5	-5	6	151	9	4	2	109	5	-8	
8	263	11	0	17	289	11	-11	H, K=	1,	13		8	822	29	-28	4	434	16	-3	
12	223	8	-7	19	333	12	-9	1	247	9	-9	10	129	7	2	6	95	4	2	
16	208	8	8	21	263	10	-9	3	199	8	8	12	549	20	-58	8	629	23	-9	
20	195	7	10	23	260	10	5	5	157	7	6	14	80	4	-2	10	57	19	-23	
	H, K=	0,	18	25	211	8	8	7	206	8	13	16	291	11	-6	12	432	16	-37	
2	211	9	-1	27	127	7	-10	9	147	6	-6	18	102	4	-4	14	45	6	11	
6	215	8	-6	29	117	5	1	11	201	8	12	20	260	10	4	16	233	9	11	
10	182	7	-7	31	103	5	8	13	183	7	12	22	36	8	7	18	53	6	6	
12	64	8	9	H, K=	1,	7		15	182	10	1	24	261	10	26	20	207	8	11	
14	127	E	-11	1	494	18	-1	17	155	6	6	26	63	19	-11	24	186	7	-0	
	H, K=	0,	20	3	515	19	-17	19	135	6	2	28	181	7	-1	26	57	9	11	
0	161	7	1	5	246	10	-23	21	122	5	2	32	105	5	4	28	145	6	4	
	H, K=	1,	1	7	471	17	-31	23	77	9	-2	H, K=	2,	4		H, K=	2,	12		
1	869	32	102	9	465	17	-46	25	94	5	-3	2	591	21	10	2	354	13	-29	
3	790	28	1	11	297	11	-32	H, K=	1,	15	4	154	10	-6	6	491	18	-10		
5	441	16	-18	13	306	11	-35	1	206	8	18	6	562	20	-32	8	39	21	-4	
7	403	15	-26	15	266	10	5	3	161	6	14	8	49	15	19	10	430	16	-11	
9	452	16	-34	17	203	8	-4	5	189	7	23	10	632	23	-55	14	216	8	3	
11	480	17	-41	19	274	10	8	7	158	8	1	12	239	9	-1	18	171	8	1	
13	420	15	-55	21	170	6	9	9	148	7	-4	14	479	17	-24	20	48	7	16	
15	345	13	-40	23	192	7	6	11	179	9	-2	16	105	4	1	22	207	8	7	
17	321	12	-18	25	135	6	-12	13	139	6	-4	18	283	11	3	24	43	9	2	
19	310	11	-5	27	102	5	-7	15	134	6	4	20	82	6	-2	26	161	6	3	
21	200	8	-9	29	81	5	-6	17	159	6	5	22	213	8	-6	H, K=	2,	14		
23	165	6	6	31	66	6	1	19	71	6	-6	26	233	9	-1	0	171	8	43	
25	190	7	15	H, K=	1,	9		21	123	5	5	30	167	6	5	2	101	6	15	
27	129	7	-8	1	359	13	8	H, K=	1,	17	H, K=	2,	6		4	261	10	40		
29	138	6	1	3	243	9	0	1	201	9	1	0	730	26	28	6	75	7	-1	
31	108	5	-0	5	347	13	-15	3	203	9	5	2	194	7	9	8	323	12	35	
33	82	8	-3	7	198	8	-15	5	204	8	-10	4	586	21	-24	10	50	16	6	
	H, K=	1,	3	9	237	9	-26	7	194	7	-3	6	134	8	3	12	255	10	6	
1	58	E	21	33	11	370	14	-31	9	204	8	-2	8	641	23	-58	16	157	6	4
3	167	7	27	13	152	6	-9	11	168	7	-7	10	96	4	-8	20	144	6	6	
5	410	15	-21	15	228	9	-9	13	158	6	-1	12	645	23	-67	H, K=	2,	16		
7	194	9	5	17	234	9	9	15	139	10	-2	16	407	15	-23	2	276	11	3	
9	320	12	-28	19	125	5	23	17	109	6	9	20	253	9	-6	6	279	11	-6	
11	354	13	-42	21	175	7	12	H, K=	1,	19	24	241	9	-10	10	271	10	-17		
13	305	11	-34	23	102	10	-6	1	117	6	14	28	217	8	6	14	216	8	1	
15	295	11	-25	25	85	5	-6	3	140	6	5	H, K=	2,	8		18	140	6	-9	
17	305	11	-6	27	95	5	0	5	91	6	-9	2	455	17	-4	H, K=	2,	18		
19	150	6	2	29	47	7	-5	7	112	6	2	4	143	5	-10	0	216	9	-1	
21	249	9	-4	H, K=	1,	11		9	96	7	-14	6	428	16	-8	4	190	7	-7	
23	148	6	5	1	456	17	2	H, K=	2,	0	8	100	4	0	8	191	8	-5		
25	93	7	-2	3	549	20	-14	2	857	31	27	10	471	17	-21	12	180	7	2	
27	130	7	-1	5	302	11	-5	6	1398	51	29	12	92	5	-4	H, K=	3,	1		
29	63	6	-14	7	342	13	-12	10	903	32	-62	14	347	13	-9	1	640	23	52	
31	68	5	-8	9	325	12	-18	14	464	17	-44	16	94	4	-1	3	454	17	43	

## STRUCTURE FACTORS CONTINUED FCF

YB (((CH<sub>3</sub>)<sub>3</sub>Si)<sub>2</sub>N)<sub>2</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	994	36	112	15	207	8	-6	11	194	8	5	26	57	6	0	H, K=	4,	16	
7	476	17	14	17	264	10	-7	13	142	6	-12	28	128	6	4	0	297	11	3
9	657	24	13	19	125	5	10	15	133	6	-2	H, K=	4,	6	4	251	10	3	
11	355	13	-32	21	150	6	5	17	111	5	1	2	702	25	46	8	177	7	-6
13	300	11	-13	23	105	10	-9	19	122	6	-6	4	61	4	-4	12	147	6	-11
15	228	9	-9	25	132	6	3	H, K=	3,	17	6	492	18	23	14	39	33	33	
17	176	7	-12	27	124	5	5	1	197	8	-8	8	52	5	-1	16	176	7	1
19	244	9	-23	29	127	6	4	3	165	7	5	10	239	9	-8	H, K=	4,	18	
21	195	7	-22	H, K=	3,	9	5	5	145	8	-15	14	427	16	-38	2	210	9	3
23	256	10	7	1	268	10	-4	7	132	7	-0	16	77	5	-8	6	160	7	1
25	155	8	11	3	298	11	-14	9	126	7	-12	18	381	15	-6	10	133	7	-6
27	140	6	-5	5	384	14	9	11	137	6	-9	22	207	8	2	H, K=	5,	1	
29	91	5	5	7	363	13	8	13	110	8	-3	26	126	6	7	1	671	24	105
31	85	6	-2	9	369	14	-9	15	153	6	4	H, K=	4,	8	3	432	17	56	
	H, K=	3,	3	11	371	14	-8	H, K=	3,	19	0	628	23	32	5	375	14	-3	
1	584	21	57	13	235	9	-6	1	120	6	-8	2	95	4	17	7	366	14	-28
3	495	18	43	15	231	9	7	3	118	6	-6	4	603	22	32	9	182	7	-23
5	639	23	48	17	208	8	28	5	103	6	-3	6	135	6	-6	11	281	11	-17
7	635	23	23	19	135	6	7	7	109	6	4	8	454	17	21	13	278	11	8
9	543	20	-1	21	167	7	5	H, K=	4,	0	10	125	5	10	15	357	13	8	
11	467	17	2	23	108	5	-1	0	E22	22	46	12	389	14	14	17	382	14	-0
13	296	11	-2	25	134	6	1	4	E22	22	14	14	72	5	-2	19	230	9	23
15	297	11	-4	27	136	6	19	8	435	16	-36	16	421	18	19	21	209	8	13
17	207	8	12	H, K=	3,	11	12	361	14	-25	20	306	11	18	23	107	8	3	
19	232	9	-17	1	271	11	-27	16	405	15	5	24	192	7	12	25	99	5	-8
21	163	6	4	3	318	12	-0	20	390	15	-18	28	124	6	7	27	96	5	-0
23	158	6	13	5	306	11	-7	24	212	8	-8	H, K=	4,	18	29	99	6	1	
25	136	6	3	7	404	15	-19	28	136	6	4	2	460	18	4	H, K=	5,	3	
27	170	6	11	9	315	12	-11	H, K=	4,	2	4	132	5	0	1	612	22	86	
29	108	8	2	11	251	9	-16	2	763	27	115	6	363	14	-6	3	802	29	106
31	70	5	-5	13	175	7	-1	4	126	8	11	10	261	10	-8	5	430	16	43
	H, K=	3,	5	15	153	6	5	6	656	24	64	12	81	5	-8	7	559	21	36
1	469	17	32	17	141	10	-6	8	154	6	8	14	307	12	27	9	387	15	9
3	520	19	9	19	163	7	-3	10	557	20	32	16	64	6	7	11	309	12	27
5	489	18	9	21	125	5	-12	12	102	4	3	18	297	11	6	13	428	16	3
7	372	14	-5	23	161	7	2	14	479	18	10	20	72	5	-5	15	365	13	12
9	452	16	-18	25	130	6	10	16	64	6	3	22	197	8	-4	17	308	11	-0
11	383	14	-36	H, K=	3,	13	18	477	17	-5	26	136	6	9	19	314	12	18	
13	370	14	-26	1	181	7	10	20	118	5	2	H, K=	4,	12	21	210	8	15	
15	298	11	-27	3	197	7	12	22	293	11	10	0	361	13	14	23	151	6	11
17	328	12	-16	5	305	11	16	26	176	7	8	2	70	14	-1	25	145	6	-2
19	181	7	-15	7	282	11	34	30	125	6	7	4	350	13	4	27	89	5	5
21	164	6	-13	9	268	10	26	H, K=	4,	4	8	255	5	8	29	91	5	-6	
23	108	7	-0	11	195	7	16	0	867	31	63	12	214	8	20	H, K=	5,	5	
25	148	8	0	13	165	8	24	2	96	6	7	14	29	44	-0*	1	442	16	43
27	121	5	-1	15	138	6	-3	4	734	26	53	16	245	9	5	3	424	16	34
29	137	6	5	17	102	5	4	6	103	4	5	20	200	8	-8	5	486	18	24
31	99	5	2	19	139	6	3	8	542	20	27	24	143	6	4	7	268	10	7
	H, K=	3,	7	21	126	6	-1	10	139	6	-8	H, K=	4,	14	9	237	9	2	
1	475	17	10	23	139	6	12	12	355	13	1	2	406	15	71	11	294	12	-3
3	405	15	-0	H, K=	3,	15	14	103	5	-4	4	70	13	15	13	119	5	-10	
5	445	16	7	1	182	7	18	16	453	17	-2	6	346	13	34	15	203	8	-10
7	356	13	-15	3	204	8	9	18	26	13	0	10	256	10	11	17	222	9	10
9	357	13	4	5	219	11	15	20	327	12	-7	14	240	9	7	19	187	7	14
11	241	9	-17	7	203	10	4	22	60	6	8	16	33	12	14	21	172	8	14
13	406	15	-20	9	187	9	-1	24	183	7	5	18	207	8	5	23	138	8	3

STRUCTURE FACTORS CONTINUED FOR  
 YB ((CH<sub>3</sub>)<sub>3</sub>Si)2N<sub>12</sub> ((CH<sub>3</sub>)<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>F(CH<sub>3</sub>)<sub>2</sub>)

L	F <sub>OB</sub>	SG	DEL	L	F <sub>CB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	L	F <sub>CB</sub>	SG	DEL	L	F <sub>OB</sub>	SG	DEL	
25	92	5	1	21	119	6	2	4	381	14	24	17	156	6	-5	17	111	5	-11	
27	85	5	-4	H, K=	5,	15		6	42	8	-3	19	96	6	-8	19	168	8	-1	
29	49	7	-4	1	223	8	14	8	572	21	4	21	143	6	5	21	108	5	-3	
	H, K=	5,	7	3	278	10	15	12	321	12	11	23	149	6	8	H, K=	7,	11		
1	40	5	15	29	5	166	7	8	16	158	6	45	25	132	6	6	1	117	9	8
3	342	13	24	7	177	7	-3	20	156	7	7	27	130	6	1	3	87	12	10	
5	393	15	24	9	155	6	-9	24	167	7	-0	H, K=	7,	3	5	203	11	14		
7	382	14	6	11	129	6	8	H, K=	6,	8	1	340	13	14	7	184	7	16		
9	250	9	14	13	156	6	-3	2	493	18	37	3	511	19	35	9	200	8	4	
11	318	12	2	15	140	7	13	4	86	5	7	5	338	13	32	11	197	7	7	
13	181	7	7	17	124	6	-8	6	564	21	12	7	451	17	24	13	136	6	-9	
15	246	9	0	H, K=	5,	17		8	35	18	7	9	493	18	22	19	112	6	-13	
17	219	8	15	1	125	6	3	10	538	20	35	11	263	10	15	17	101	7	-5	
19	223	9	14	3	95	6	-0	12	129	6	-0	13	417	16	36	19	51	8	-14	
21	182	8	3	5	140	6	-7	14	330	12	46	15	205	8	20	H, K=	7,	13		
23	160	6	2	7	104	6	-3	16	28	37	17*	17	141	7	8	1	214	8	-7	
25	91	5	6	9	104	6	-5	18	262	10	12	19	212	8	3	3	174	7	4	
27	94	5	-0	11	100	6	-7	20	54	18	8	21	147	6	4	5	242	9	4	
	H, K=	5,	9	H, K=	6,	0		22	229	8	8	23	172	7	5	7	216	8	17	
1	412	15	39	2	466	17	51	H, K=	6,	10	25	175	7	0	9	208	8	6		
3	455	18	15	6	290	11	12	0	331	12	47	H, K=	7,	5	11	213	8	10		
5	288	11	10	10	323	12	8	2	103	5	8	1	214	8	33	13	132	6	-11	
7	295	11	4	14	411	16	-0	4	310	11	29	3	202	9	26	15	140	6	3	
9	282	11	1	18	270	10	25	6	124	6	3	5	320	12	20	H, K=	7,	15		
11	188	7	22	22	112	12	7	8	295	11	30	7	257	10	7	1	122	6	-5	
13	271	10	16	26	149	7	-9	12	293	11	14	9	281	11	7	3	185	7	-3	
15	272	11	25	H, K=	6,	2	16	227	8	-4	11	336	12	24	5	136	7	7		
17	243	9	29	0	807	29	95	18	55	12	-2	13	204	8	34	7	165	7	1	
19	246	9	-2	2	172	6	16	20	162	7	-4	15	171	7	31	9	196	8	11	
21	180	7	9	4	748	27	85	H, K=	6,	12	17	151	6	13	11	120	6	-9		
23	137	6	1	6	55	14	5	2	282	11	23	19	87	5	5	H, K=	8,	0		
25	125	5	7	8	585	22	46	4	60	19	16	21	108	5	-4	0	269	10	-5	
	H, K=	5,	11	10	94	10	3	6	205	8	8	23	126	6	6	4	386	14	43	
1	283	11	20	12	533	20	24	10	230	9	-7	25	100	5	1	9	491	18	63	
3	223	8	21	14	85	5	9	14	239	9	-5	H, K=	7,	7	12	314	12	43		
5	177	7	3	16	401	15	11	18	169	7	3	1	285	11	30	16	159	10	-11	
7	157	6	-11	18	35	11	-15	H, K=	6,	14	3	3	242	10	26	20	220	8	3	
9	136	6	-18	20	226	9	25	0	373	14	-8	5	384	11	21	24	185	7	3	
11	160	7	2	24	197	7	2	4	323	12	8	7	328	12	17	H, K=	8,	2		
13	167	7	12	28	175	7	-6	8	283	11	0	9	269	10	13	2	549	20	13	
15	198	8	8	H, K=	6,	4	10	49	12	5	11	338	13	39	4	87	5	6		
17	205	8	2	2	575	21	69	12	260	10	2	13	188	8	31	6	498	18	53	
19	130	6	4	4	113	5	6	16	204	8	-3	15	210	8	22	8	62	7	-3	
21	119	8	-6	6	674	24	38	H, K=	6,	16	17	150	7	-1	10	430	16	50		
23	87	6	2	8	96	8	-1	2	146	6	-4	19	111	5	-6	12	70	6	-2	
	H, K=	5,	13	10	552	20	21	6	192	7	-3	21	145	6	2	14	263	10	16	
1	351	13	55	12	162	7	6	10	174	7	-9	23	128	6	1	18	252	9	-8	
3	281	11	36	14	377	14	22	H, K=	7,	1	H, K=	7,	9	20	45	9	-4			
5	247	10	19	16	50	7	9	1	223	8	-9	1	226	8	32	22	240	9	1	
7	169	8	8	18	229	9	36	3	153	6	7	3	331	12	46	H, K=	8,	4		
9	149	10	-2	22	212	8	5	5	367	14	38	5	234	9	20	0	547	20	29	
11	183	8	-12	26	170	7	-7	7	379	14	57	7	319	12	35	2	104	5	3	
13	196	8	14	28	36	20	-5	9	385	15	35	9	349	13	28	4	407	15	29	
15	193	7	7	H, K=	6,	6	11	396	15	30	11	206	8	22	6	107	5	9		
17	203	8	15	0	368	14	56	13	230	9	10	13	266	10	9	8	348	13	50	
19	124	6	-2	2	34	9	16	15	214	8	15	15	178	7	-4	10	96	5	9	

STRUCTURE FACTORS CONTINUED FCF  
 $\text{YB} (((\text{CH}_3)_3\text{Si})_2\text{N})_2 ((\text{CH}_3)_2\text{P}\text{C}\text{H}_2\text{C}\text{H}_2\text{F}(\text{CH}_3)_2)$

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
12	341	13	34	1	360	13	39	2	402	15	29	11	190	7	-5
14	29	31	2*	3	356	13	36	6	305	11	-15	H, K =	11,	7	
16	289	11	-5	5	205	8	16	10	265	10	-13	1	111	6	-3
18	47	8	1	7	242	9	24	14	295	11	7	3	133	8	-4
20	217	9	-6	9	194	9	13	18	227	9	-3	5	193	7	-8
24	153	8	4	11	158	7	-10	H, K =	10,	2		7	200	8	-13
	H, K =	8,	6	13	195	7	-4	0	326	12	15	H, K =	12,	0	
2	425	16	54	15	200	8	-7	4	299	11	-12	0	297	11	-15
4	42	14	16	17	179	7	-3	8	274	10	-21	4	258	10	-14
6	271	10	64	19	213	8	5	12	250	9	-15	H, K =	12,	2	
8	52	7	10	21	129	6	-13	16	222	8	-7	2	206	8	-23
10	272	10	47	H, K =	9,	5		H, K =	10,	4		4	66	7	4
14	308	11	11	1	333	13	29	2	273	10	-6				
18	218	8	3	3	259	10	21	4	73	6	-0				
22	133	6	1	5	233	9	28	6	255	10	-11				
	H, K =	8,	8	7	152	10	22	10	247	9	-9				
0	503	19	36	9	148	8	20	14	229	9	-10				
2	56	13	33	11	179	7	6	18	209	8	6				
4	393	15	12	13	179	7	-1	H, K =	10,	6					
6	63	9	21	15	185	7	-12	0	286	11	0				
8	302	11	21	17	208	8	-3	4	291	11	7				
10	71	10	14	19	140	6	-2	8	269	10	4				
12	305	11	5	21	135	9	11	12	242	9	-7				
16	270	10	-4	H, K =	9,	7		16	213	8	-3				
20	197	8	-6	1	319	12	3	H, K =	10,	8					
	H, K =	8,	10	3	223	9	-6	2	249	9	-15				
2	274	11	5	5	244	10	9	6	219	8	-16				
4	59	16	14	7	114	5	-4	10	213	8	-18				
6	294	11	7	9	150	6	6	H, K =	10,	10					
10	256	9	2	11	164	6	7	0	279	10	2				
12	61	7	4	13	201	8	-12	2	37	16	15				
14	173	7	-13	15	182	7	-3	4	229	9	-3				
18	142	6	-13	17	193	8	-3	6	33	13	20				
	H, K =	8,	12	19	112	6	-6	8	191	7	-11				
0	199	8	-5	H, K =	9,	9		H, K =	11,	1					
2	29	17	22	1	254	9	-7	1	213	8	4				
4	245	9	3	3	263	10	-4	3	225	8	-8				
8	270	10	6	5	164	7	-10	5	192	7	-0				
12	185	7	1	7	164	6	-5	7	196	8	-11				
	H, K =	8,	14	9	164	6	5	9	192	7	-12				
2	248	9	-9	11	144	6	-10	11	187	7	-7				
4	34	15	-12	13	153	6	-5	13	190	7	-9				
6	239	9	-11	15	127	6	-18	H, K =	11,	3					
	H, K =	9,	1	H, K =	9,	11		1	139	6	-13				
1	347	13	57	1	198	8	3	3	138	6	-6				
3	308	11	53	3	159	6	-3	5	189	7	-19				
5	300	11	44	5	177	7	-3	7	177	7	-19				
7	255	9	32	7	147	6	-2	9	171	7	-5				
9	188	9	18	9	123	6	-11	11	173	7	-13				
11	195	8	9	11	140	7	2	13	126	6	-6				
13	135	7	-5	13	93	9	-4	H, K =	11,	5					
15	160	6	3	H, K =	9,	13		1	124	6	11				
17	181	7	5	1	162	7	-2	3	169	7	-13				
19	171	7	8	3	140	8	-9	5	203	8	3				
21	155	6	-1	5	160	6	-9	7	250	9	-6				
	H, K =	9,	3	H, K =	10,	8		9	231	9	-5				

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TECHNICAL INFORMATION DEPARTMENT  
LAWRENCE BERKELEY LABORATORY  
UNIVERSITY OF CALIFORNIA  
BERKELEY, CALIFORNIA 94720