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DIALKYL BIS[BIS(TRIMETHYLSILYL)AMIDO] GROUP IV A METAL COMPLEXES; PREPARATION OF BRIDGING CARBENE COMPLEXES BY γ-ELIMINATION OF ALKANE. CRYSTAL STRUCTURE OF $\{ZrCHSi(Me)_2NSiMe_3[N(SiMe_3)_2]\}_2$

Roy P. Planalp, Richard A. Andersen,
and Allan Zalkin

July 1982

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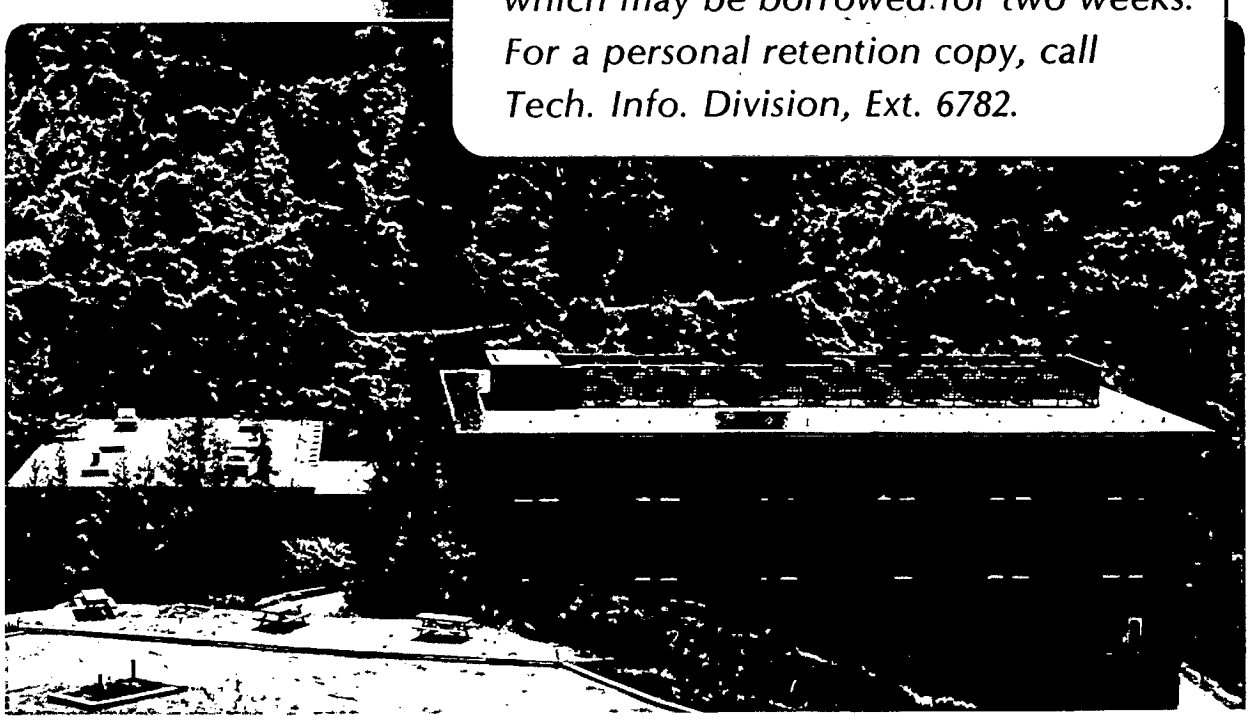

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LBL-14754

Dialkyl Bis[Bis(Trimethylsilyl)amido] Group IV A Metal Complexes; Preparation of Bridging Carbene Complexes by γ-Elimination of Alkane. Crystal Structure of $\{\overline{ZrCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]\}_2$

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Abstract

The dialkyls of zirconium of the type $R_2Zr[N(SiMe_3)_2]_2$, where R is Me, Et, or CH_2SiMe_3, thermally decompose (60°C, 10^{-2} mm) by elimination of alkane (MeH, EtH, or Me_4Si, respectively) to give the bridging-carbene compound $\{\overline{ZrCHSi(Me_2)N}SiMe_3[N(SiMe_3)_2]\}_2$. The 1:1 complex with pyridine is described. The related hafnium dialkyls decompose in a related manner though in this case the decomposition product could only be characterized as its pyridine complex, $\{\overline{HfCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]NC_5H_5\}_2$. The NMR spectra of the pyridine complexes of zirconium and hafnium are similar. In contrast, $Me_2Ti[N(SiMe_3)_2]_2$ is thermally stable to 190°C. The titanium-carbene, $\{\overline{TiCH-Si(Me)_2N}SiMe_3[N(SiMe_3)_2]\}_2$ may be prepared by sodium amalgam reduction of $Cl_2Ti[N(SiMe_3)_2]_2$. The crystal structure of $\{\overline{ZrCHSi(Me)_2N}SiMe_3[N(SiMe_3)]\}_2$ was determined by single crystal X-ray crystallography. The crystals are orthorhombic, Pbca, with cell dimensions $\underline{a}$ = 18.307(7) Å, $\underline{b}$ = 26.036(6) Å and $\underline{c}$ = 19.425(6) Å; for Z = 8, d_{calc} = 1.18 g cm^{-3}. The structure was refined to a conventional R factor of 0.061 using 3149 data where $F^2 > 3\sigma(F^2)$. The structure consists of three, fused, planar, four-membered rings giving the molecule a 'tub' conformation. The Zr-C distances are 2.16 and 2.21 Å and the Zr-N distances range from 2.04 to 2.09 Å.

The hafnium dialkyls $R_2Hf[N(SiMe_3)_2]_2$, where R = Me, Et or Me_3SiCH_2, have been described recently.[1] Isolation of the methyl or trimethylsilylmethyl derivatives is not surprising. However, isolation of the thermally stable diethyl derivative (the complex melts without decomposition at 68°C) is rather surprising since diethyl derivatives of transition metals are rather rare due to facile β-elimination of ethylene and ethane.[2] We suggested that the thermal stability was due to steric congestion about the metal atom due to the sterically large $(Me_3Si)_2N$ groups preventing the β-hydrogen atoms of the ethyl groups from getting close enough to the metal center to react. Thus, $Et_2Hf[N(SiMe_3)_2]_2$ is kinetically stable as a result of steric effects. In a related class of thermally stable amido-alkyls, $Et_2Mo_2(NMe_2)_4$, molybdenum to nitrogen π-bonding, $p\pi \rightarrow d\pi$, was suggested as the reason for the stability.[3] Though metal to nitrogen π-bonding may play a role in the stability of silylamido-alkyls we think it is a minor one since we have shown that this type of bonding is insignificant in $M-N(SiMe_3)_2$ complexes.[4a] Others, however, have shown that π-bonding is very important in $M-NR_2$ complexes where R is an alkyl group.[4b] In order to gain insight into the reasons for the thermal stability of $Et_2Hf[N(SiMe_3)_2]_2$ and related dialkyls, we began a study of the thermal decomposition reactions of $R_2M[N(SiMe_3)_2]_2$ where R is Me, Et, or Me_3SiCH_2 when M is Zr or Hf and R is Me when M is Ti.

<u>Synthetic Studies</u>. The three hafnium compounds and $Me_2Zr[N(SiMe_3)_2]_2$ have been described.[1] The diethyl and bis-trimethylsilylmethyl derivatives of zirconium were prepared in a similar fashion. If is of interest to note that $Et_2Hf[N(SiMe_3)_2]_2$ is rather more thermally stable than its zirconium analogue; the former melts without decomposition at 68°C, while the latter melts with decomposition at 25°C. This relative thermal stability trend is also observed

for the Me_3SiCH_2 derivatives; $(Me_3SiCH_2)_2Hf[N(SiMe_3)_2]_2$ melts without decomposition at 91-92°C whereas the zirconium analogue melts with decomposition at 53-55°C.

We wished to prepare the corresponding titanium derivatives so that the properties of all the group IVA derivatives could be compared. Though $Cl_3TiN(SiMe_3)_2$[5] and $ClTi[N(SiMe_3)_2]_3$[6] are known, $Cl_2Ti[N(SiMe_3)_2]_2$ is unknown. The latter compound was isolated as a dark red liquid that solidified to a red, waxy material after distillation (138°C at 10^{-2} mm). The $Me_2Ti[N(SiMe_3)_2]_2$ was isolated as a pale-yellow solid from reaction of $Cl_2Ti[N(SiMe_3)_2]_2$ and the methyl Grignard reagent. It is noteworthy that $Me_2Ti[N(SiMe_3)_2]_2$ is a solid at room temperature (20°C) with a melting point of 46-48°C whereas the zirconium and hafnium complexes are liquids at that temperature. We have been unable to prepare, in pure form, $Et_2Ti[N(SiMe_3)_2]_2$ or $(Me_3SiCH_2)_2Ti[N(SiMe_3)_2]_2$.

All three zirconium alkyls decompose at comparable rates at ca. 60°C under reduced pressure (10^{-2} mm) to give alkane and a yellow material whose empirical composition is derived from $R_2Zr[N(SiMe_3)_2]_2$ less two molar equivalents of alkane, viz. I. The ^1H NMR spectrum of (I), isolated in essentially

$$R_2\ Zr\ [N(SiMe_3)_2]_2 \xrightarrow{\Delta} 2RH + Zr[(SiMe_3)(SiMe_2CH)]_2 \qquad (I)$$

$$R = Me, Et, Me_3SiCH_2$$

quantitative yield after crystallization from pentane, consists of singlets at δ 7.08, 1.14, 0.44, 0.40, and 0.28 in area ratio of 1:3:9:18:3. The four upfield resonances are most reasonably ascribed to methyl groups on silicon and the downfield singlet of area one suggests that a methine group is present.[7] This inference is supported by the ^{13}C NMR spectrum which yields a downfield doublet centered at δ 201.4, J_{CH} = 122 Hz. The other resonances in the ^{13}C NMR spectrum are quartets clustered between δ 5-10 and are due to

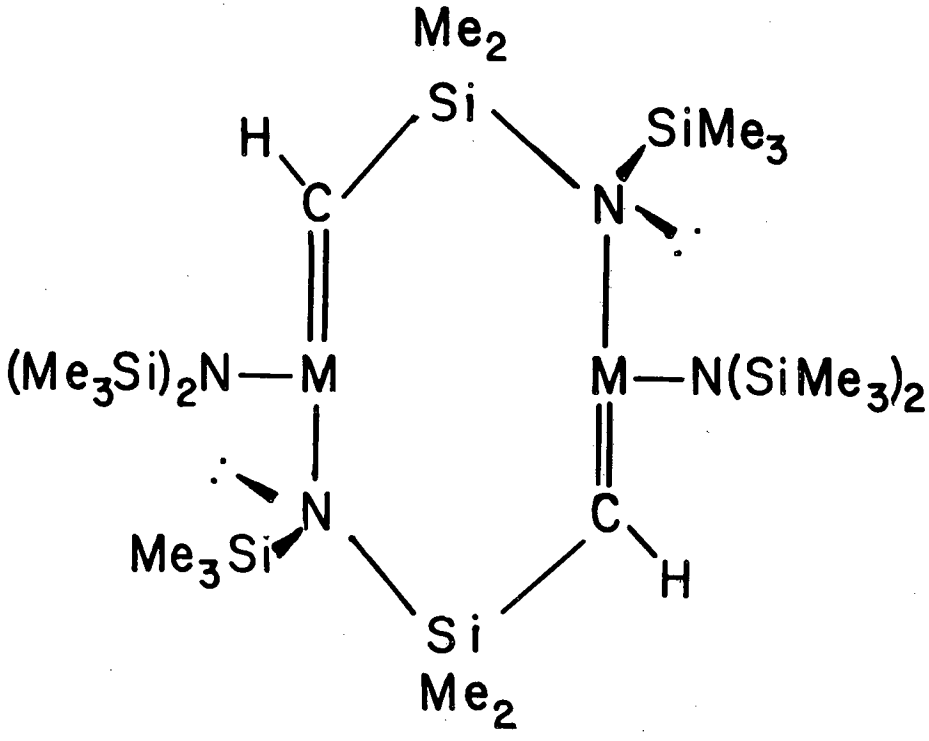
methyl groups bound to silicon (see experimental section for details). A structural unit that is consistent with these data is $\overline{Zr(CHSi(Me)_2N}SiMe_3)N-(SiMe_3)_2$, in which the methyl groups on the Me_2Si group are diastereotopic. In addition, the mass spectrum shows that (I) is dimeric. Two structural formulae that are consistent with all of the spectroscopic data are II and III, where M is zirconium. These data, however do not allow us to make a distinction between the two valence isomers but a crystal structure (see below) shows that III is the correct structural isomer.

(see illustration next page)

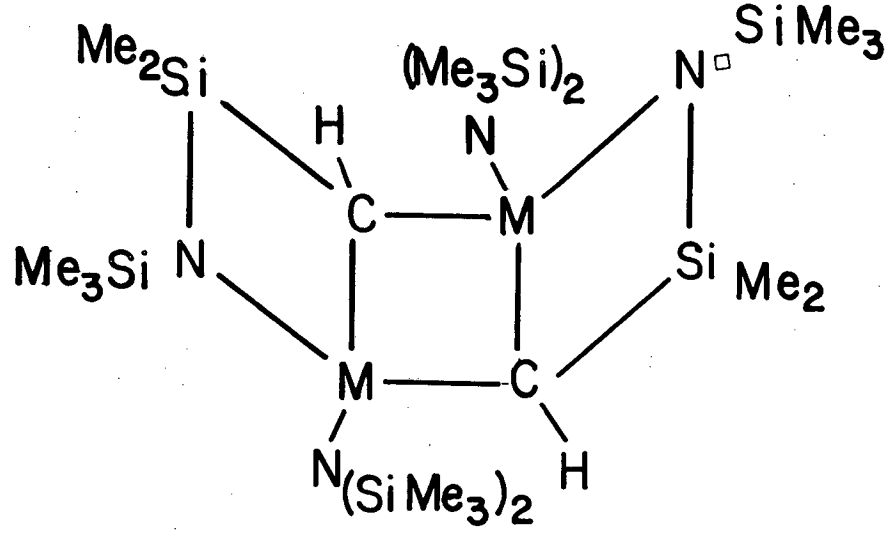
Thus, thermal decomposition of all three zirconium alkyls gives the same compound, III, derived by a formal elimination of alkane, the hydrogen atoms of the alkane coming from the methyl group of a $(Me_3Si)_2N$ ligand. It is important to note that we are describing the events in a phenomenological way; we intend to address the mechanistic question later. A single hydrogen γ-elimination from a coordinated $(Me_3Si)_2N$ group[8] or a β-elimination from a Me_2N or Et_2N group[9] is a well-known thermal decomposition pathway. Elimination of both hydrogen atoms from the same methyl group is without precedent in metal amide chemistry, though some examples of this are known in alkyl chemistry.[10]

The dimeric unit in III cannot be cleaved by pyridine, since a 1:2 coordination complex is isolated (see experimental section for details).

The three hafnium alkyls may be thermally decomposed at ca. 70°C under reduced pressure (10^{-2} mm), eliminating alkane and forming a yellow substance. We have not been able to crystallize this material though we have been able to isolate a pyridine complex. The similarity of the ^1H and ^{13}C NMR spectrum of the pyridine complex of hafnium to that of the zirconium pyridine



II



III

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complex suggests that they are isostructural (see experimental section for details). Thus, the zirconium and hafnium dialkyls decompose at similar rates to give the dimeric, bridging, carbene-like metallacycles III, where M is zirconium or hafnium.

In contrast, the titanium alkyl $Me_2Ti[N(SiMe_3)_2]_2$ is thermally stable. This dialkyl may be recovered unchanged after heating at 190°C for prolonged periods of time. This observation may be rationalized by noting that tetravalent titanium (IV) is smaller than either zirconium or hafnium. As a consequence, the steric congestion about the titanium atom in $Me_2Ti[N(SiMe_3)_2]_2$ is greater than that around the two heavier group IVB metal complexes and a γ-hydrogen atom of the $(Me_3Si)_2N$ group cannot get close enough to the titanium atom to become 'activated'. This explanation is a kinetic one and it implies that a titanium metallacycle, III M=Ti, should exist if a suitable preparative route could be found. Sodium amalgam reduction of $TiCl_2[N(SiMe_3)_2]_2$ yields orange-red III, M=Ti. The similarity of the NMR spectral properties of the titanium complex to that of its zirconium of hafnium congeners (see experimental section) shows that they are isostructural. The titanium complex does not react with pyridine, a result consistent with steric effects.

The inability to get $Me_2Ti[N(SiMe_3)_2]_2$ to thermally decompose whereas the related zirconium and hafnium dimethyls readily decompose to III has some mechanistic significance. Titanium-carbon bond strengths are less than the corresponding zirconium or hafnium-carbon bond strengths.[11] This suggests that radical processes are not involved.

<u>Structural Studies of III, M = Zr</u>. An ORTEP diagram showing the atom numbering scheme is shown in Figure I. Figure II shows a 'side-on' view that illustrates the overall stereochemistry. Tables I lists the positional parameters and Table II and Table III list some important bond angles and bond

distances.

The molecular structure consists of two planar four-membered ZrCSiN rings fused to the central planar, four-membered Zr_2C_2 ring along the Zr-C edges. The deviations of the atoms in each of the three planes is shown in Table IV. The angles formed by the intersection of the Zr(1)N(1)Si(1)C(1) and Zr(2)N(3)Si(5)C(13) planes with the Zr(1)C(1)Zr(2)C(13) plane are 124° and 111°, respectively. The overall conformation of the eight-membered ring is that of a 'tub' reminiscent of that found for cyclooctateraene in the gas phase.[12]

A line-drawing of III, M = Zr, looking towards the Zr_2C_2 ring is shown in Figure III. As can be seen no symmetry plane bisects the Me_2Si groups and the methyl groups are diastereotopic as described to earlier. This conformation is consistent with the solution ^1H NMR spectrum which is invarient from -90°C to +60°C. The molecule is either stereochemically rigid or highly fluxional on the NMR time scale in this temperature range.

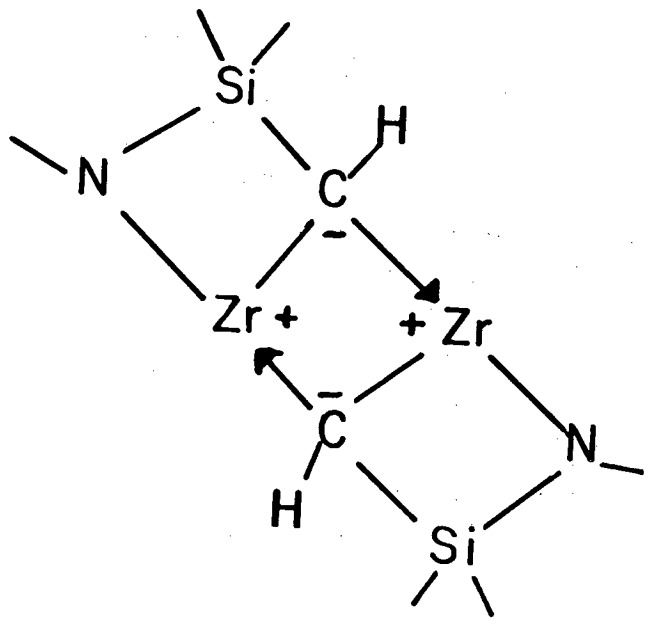
The averaged terminal Zr-N[N(2,4)] bond length of 2.09 ± .01 Å lies at the low end of zirconium-amido nitrogen bond lengths which range from 2.05 to 2,20 Å.[6b,13] The averaged Zr-N[N(1,3)] bond length of 2.06 ± .02 Å, which is part of the metallacyclic ring, is also within this range. Given the uncertainty in the individual bond lengths (Table II) this difference is probably not chemically significant.

The zirconium-carbon bond lengths in the Zr_2C_2 unit are unsymmetrical. The two Zr-C bonds that are part of the ZrCSiN framework, Zr(1)-C(1) and Zr(2)-C(13), are 2.16(2) Å and they are shorter than the two Zr-C bonds that are not part of the metallacyclic framework. The latter two distances, Zr(1)-C(13) and Zr(2)-C(1) are both 2.21(2) Å. These bond lengths are shorter than Zr-C(sp^3) bond lengths in compounds of the type Cp_2ZrR_2 which vary from 2.25

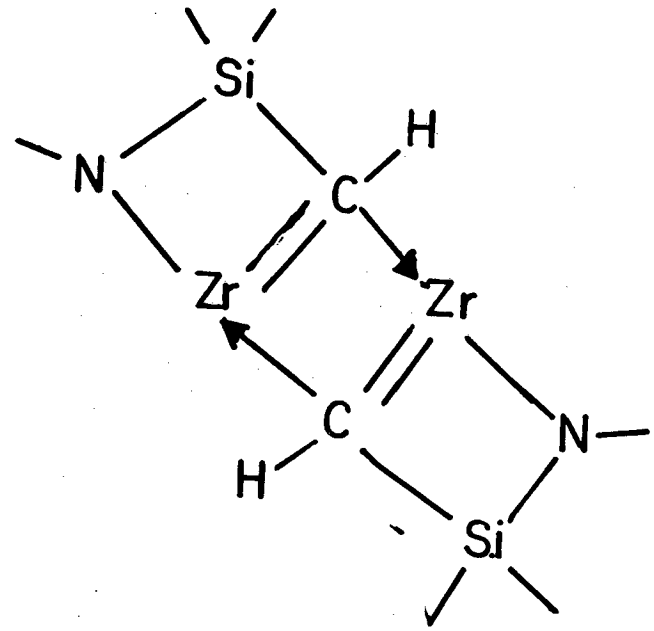
to 2.37 Å.[14] The zirconium-carbon bond lengths in III, M = Zr, are close to those found for Zr-C(sp^2) of 2.20 Å.[15] It is well known that the coordination number of a metal atom plays a significant role in determining bond lengths. In the Cp_2ZrR_2 compounds the coordination number of zirconium is eight, defining the coordination number of a Cp group as three,[16] whereas the coordination number of the zirconium atom in III, M = Zr, is only four. Since the ionic or covalent radius of Zr(IV) in eight coordination is estimated to be 0.78 or 0.92 Å, respectively, and 0.59 or 0.73 Å, respectively, in four coordination, the zirconium-carbon bond lengths in III, M = Zr, should be ca. 0.2 Å shorter than in the cyclopentadienyl derivatives.[17] Thus, adjusting the Zr-C bond lengths in the metallacycle for the coordination number change puts them within the region for Zr-C(sp^3) bond lengths.

It is probably best to view the bonding in the metallacyclic-Zr_2C_2 ring as IV, with an ylid-type structure rather than as V, with two discrete zirconium-carbon double bonds. This view is consistent with the NMR spectral data which imply that the carbon atoms carry a negative charge, as found in Cp_2Zr-$Cl(CHPPh_3)$.[18] This bonding scheme may also be used to rationalize the unsymmetrical nature of the Zr-C bond lengths, since the shorter lengths are associated with the 'clamped' ZrCSiN unit and the longer ones are 'unclamped.'

(see illustration next page)



IV



V

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Experimental Section

All operations were performed under argon. Elemental analyses were done by the microanalytical laboratory of this department. The ^{1}H and ^{13}C nuclear magnetic resonance spectra were recorded on a JEOL-FX90Q instrument operating at 89.56 and 22.50 MHz, respectively, in benzene-d_6 solutions at 26°C.

$TiCl_2[N(SiMe_3)_2]_2$. Titanium tetrachloride (6.5 g, 0.034 mol) in pentane (50 mL) at -30°C was added to a solution of lithium bis(trimethylsilyl)amide (11.4 g, 0.0683 mol) in pentane (150 mL) also at -30°C. The mixture was warmed to 0°C and stirred at that temperature for 40 min, then warmed to room temperature. The solution was filtered and the residue was extracted with pentane (50 mL). The red extracts were combined and the pentane was removed under reduced pressure giving a red, viscous liquid. The oil was fractionated and the fraction that distilled at 136-140°/10^{-3} mm was collected. The distillate solidified as a dark red, waxy solid in 61% yield (9.1 g), mp 60-62°C. Anal. Calcd for $C_{12}H_{36}Cl_2N_2Si_4Ti$: C, 32.8; H, 8.20; Cl, 16.2; N, 6.38. Found: C, 30.6; H, 8.10; Cl, 14.7; N, 5.91. IR: νM-N = 438 cm^{-1}; νM-Cl = 350 cm^{-1}. NMR: ^{1}H, 0.53 s; ^{13}C, 5.10 q, J = 119 Hz.

$TiMe_2[N(SiMe_3)_2]_2$. Methylmagnesium chloride (5.7 mL of a 0.62 M solution in diethyl ether, 0.0035 mol) was added to dichlorobis[bis(trimethylsilyl)amido]-titanium (0.70 g, 0.0032 mol) in pentane (50 mL) at -35°C. The mixture was stirred at that temperature for 50 min, then allowed to warm to 0°C. The volatile material was removed under reduced pressure at 0°C. The dark solid was extracted with pentane (20 mL), filtered, and the filtrate was concentrated to ca. 4 mL and cooled (-70°C). The yellow prisms (0.97 g, 77% yield) were collected and dried under reduced pressure, mp 46-48°C. Anal. Calcd for

$C_{14}H_{42}N_2Si_4Ti$: C, 42.2; H, 10.5; N, 7.03. Found: C, 42.0; H, 10.5; N, 6.63. NMR: ^1H, 1.63 s (6H); 0.47 s (36H). ^{13}C, 66.1 q, J = 114 Hz; 5.41 q, J = 121 Hz due to Me and Me_3Si, respectively.

$ZrEt_2[N(SiMe_3)_2]_2$. Diethylmagnesium (2.2 mL of a 1.0 M solution in diethyl ether, 0.0022 mol) was added to dichlorobis[bis(trimethylsilyl)amido]zirconium (1.0 g, 0.0021 mol) in pentane (20 mL) at -30°C. The suspension was stirred at that temperature for 40 min, then the volatile material was evaporated. The solid was extracted at -30°C with cold (-30°C) pentane (20 mL), filtered (-30°C), concentrated to ca. 3 mL (-30°C), then cooled (-70°C). The white prisms (0.41 g, 40% yield) were collected and dried under reduced pressure. The crystals were stored at 5°C since they decompose at ca. 25°C and reliable elemental analyses could not be obtained. NMR: ^1H (PhMe-d_8, -50°C), 1.64 t, J = 7 Hz, (6H); 1.12 q, J = 8 Hz, (4H); 0.43 s (36H). ^{13}C(PhMe-d_8, -40°C), 63.5 s, 13.9 s, 3.80 s due to CH_2, CH_3, and Me_3Si, respectively.

$Zr(CH_2SiMe_3)_2[N(SiMe_3)_2]_2$. Bis(trimethylsilylmethyl)magnesium (2.6 mL of a 1.3 M diethyl ether solution, 0.0034 mol) was added to dichlorobis[bis(trimethylsilyl)amido]zirconium (1.5 g, 0.0035 mol) in pentane (60 mL) at -30°C. The mixture was slowly allowed to warm to 0°C (3 h) with stirring. The volatile material was removed under reduced pressure (0°C) and the solid was extracted with cold (0°C) pentane (50 mL). The extract was filtered (0°C) and the filtrate was concentrated to ca. 6 mL (0°C) and cooled (-70°C). The white prisms (1.7 g, 83% yield) were collected and dried under reduced pressure, mp 53-55°C (dec.). NMR: ^1H, 1.04 s (4H); 0.34 s (36H); 0.27 s (18H). $^{13}C\{^1H\}$, 69.4 s, 5.70 s, and 3.30 s, due to CH_2, $SiMe_3$, and $(Me_3Si)_2N$, respectively. The compound did not give satisfactory elemental analyses, possibly due to

thermal decomposition.

$\{\overline{TiCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]\}_2$. Sodium amalgam (0.78 mL of a 1% amalgam, 0.0046 mol) was added to dichlorobis[bis(trimethylsilyl)amido]titanium (1. g, 0.0023 mol) in toluene (30 mL) under argon. The red solution turned green then back to red over 5 h. After stirring for 72 h, the red solution was filtered and the filtrate was evaporated to dryness giving a red oil. The oil was extracted with pentane (50 mL), filtered, concentrated to ca. 5 mL and cooled (-70°C). The red material that crystallized was recrystallized twice from pentane (-70°C) giving 0.44 g (58%) of bright orange-red prisms, mp 168-169°C. Anal. Calcd. for $C_{12}H_{34}N_2Si_4Ti$: C, 39.3; H, 9.28; N, 7.64. Found: C, 40.4; H, 9.45; N, 7.35. The mass spectrum consisted of a molecular ion at 732. NMR: ^1H; 10.5 s (1H), 1.43 s (3H); 0.12 s (3H), 0.42 s (18H), 0.43 s (9H). ^{13}C; 271.4 d (J = 128 Hz), 8.10 q (J = 117 Hz), 3.40 q (J = 118 Hz), 4.90 q (J = 117 Hz), 4.60 q (J = 120 Hz) due to CH, $SiMe_2$ (diastereotopic), $(Me_3Si)_2N$, and Me_3SiN, respectively. The complex does not form an adduct with pyridine.

$\{\overline{ZrCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]\}_2$. Dimethylbis[bis(trimethylsilyl)-amido]zirconium (1.2 g, 0.0027 mol) was heated to 60°C under dynamic vacuum (10^{-2} mm). Within 5 min the clear, colorless liquid turned yellow and began to froth. After heating for 6 h the frothing ceased and a light yellow, clear glassy solid remained. The gases that were evolved were collected (liquid nitrogen) and shown to be methane by gas phase infrared spectroscopy. The solid was dissolved in pentane (30 mL), filtered, and the yellow filtrate was concentrated to ca. 7 mL and cooled (-20°C). The yellow needles were collected and dried under reduced pressure. The yellow mother liquor yielded an

additional crop of yellow needles and the combined yield was 1.0 g, 94%, mp 150-151°C. Elemental analyses were not satisfactory. NMR: ^1H; 7.08 s (1H), 1.14 s (3H), 0.28 s (3H), 0.44 s (9H), 0.40 s (18H). ^{13}C; 201.4 d (J = 122 Hz), 9.50 q (J = 119 Hz), 4.50 q (J = 117 Hz), 4.90 q (J = 117 Hz), 4.30 q (J = 117 Hz) due to CH, Me_2Si (diastereotopic), Me_3SiN, and $(Me_3Si)_2N$, respectively. Pyrolysis of diethyl- and bis(trimethylsilylmethyl)-bis[bis(trimethylsilyl)amido]zirconium were performed similarly, yielding the metallacycle in essentially quantitative yield, as shown by mp and ^1H NMR spectroscopy. The gaseous materials were identified as ethane and tetramethylsilane, respectively, by gas phase infrared spectroscopy.

$\{\overline{ZrCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]_2[NC_5H_5]\}_2$. Pyridine (0.4 mL, 0.0052 mol) was added to a solution of the metallacycle (1.0 g) in pentane (15 mL). The yellow precipitate was collected and dried under reduced pressure. Toluene (10 mL) was added and the solution was heated, filtered, and the filtrate was cooled to -20°C then to -70°C giving 1.2 g (95%) of bright yellow prisms, mp 133-134°C (dec.). Anal. Calcd for $C_{17}H_{39}S_3Si_4Zr$: C, 41.8; H, 7.98; N, 8.60. Found: C, 40.4; H, 7.91; N, 7.59. The mass spectrum contained a molecular ion at 897 due to $M-NC_5H_5$. NMR: ^1H; 8.80 m (2H), 7.02 m (2H), 6.77 m (1H), 7.11 s (1H), 1.24 s (3H), 0.53 s (3H), 0.55 s (18H), 0.25 s (9H). $^{13}C\{^1H\}$; 195.7 s, 11.0 s, 5.60 s, 6.30 s, 5.00 s, 151.4 s, 137.5 s, 124 s due to CH, Me_2Si (diastereotopic), $(Me_3Si)_2N$, Me_3SiN, and the o-, p- and m- resonances of pyridine, respectively.

$\{\overline{HfCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]NC_5H_5\}_2$. Dimethylbis[bis(trimethylsilyl)amido]-hafnium (1.1 g, 0.0021 mol) was heated to 70°C under dynamic vacuum (10^{-2} mm) for 6 h. The pale yellow material was dissolved in pentane (10 mL) and the

solution was filtered. Pyridine (0.2 mL, 0.0025 mol) was added and the small, bright yellow prisms were isolated by filtration. The prisms, 0.94 g (78%), were crystallized from toluene (10 mL) at -70°C, mp 137-139°C (dec.). The mass spectrum contained a molecular ion at 1073 amu due to M-py$^+$. NMR: ^{1}H; 8.96 m (2H), 7.18 m (2H), 6.79 m (1H), 4.95 s (1H), 2.32 s (3H), 1.36 s(3H), 0.63 s (18H), 0.34 s (9H). ^{13}C; 180.3 d (J = 166 Hz), 10.8 q (J = 118 Hz), 3.20 q (J = 119 Hz), 6.60 q (J = 118 Hz), 5.40 q (J = 117 Hz), 151.8 d (J = 182 Hz), 138.0 d (J = 116 Hz), 124.1 d (J = 168 Hz), due to CH, Me_2Si (diastereotopic), $(Me_3Si)_2N$, Me_3SiN, and o-, p- and m-CH of pyridine, respectively. The pyridine complex was also prepared by a similar pyrolysis of diethylhafniumbis[bis(trimethylsilyl)amide], as shown by mp and ^{1}H NMR spectroscopy.

X-Ray Study. Yellow crystals of the zirconium complex were grown from heptane (-20°C) and loaded into quartz capillaries at room temperature under an atmosphere of argon and sealed. A crystal was examined with a Picker FACS-I automated diffractometer equipped with a graphite monochromator and a Mo X-ray tube ($\lambda(K\alpha_1)$ 0.70930 Å). The space group is Pbca. The setting angles of twelve manually centered reflections (41° < 2θ < 45°) were used to determine the cell parameters by least-squares. The cell dimension are a = 18.307(7) Å, b = 26.036(6) Å and c = 19.425(6) Å. For Z = 8 the calculated density is 1.18 g/cm^3.

Intensity data were collected using a θ-2-θ scan technique with a scan speed of 2°/min on 2θ. Each peak was scanned 0.7° before the $K\alpha_1$ peak to 0.7° after the $K\alpha_2$ peak, and backgrounds were counted for 10 s at each end of the scan range. The temperature during the data collection was 23 ± 1°C. Three standard reflections were measured every 250th scan, and no significant varia-

tions of their intensities were observed. A total of 10,589 scans ($4° < 2\theta < 45°$) yielded 5966 unique data of which 3149 had $F^2 > 3\sigma(F^2)$. An absorption correction ($\mu = 6.6\ cm^{-1}$) was applied[19] which ranged from 1.35 to 1.43.

A three dimensional Patterson calculation showed the two zirconium positions, and subsequent least-squares refinements and electron density calculation revealed all of the non-hydrogen atoms in the structure. The least-squares function used minimizes the function $\Sigma \underline{w}(|F_o| - |F_c|)^2/\Sigma \underline{w} F_o^2$. The expressions used in processing the data and estimating weights are given in the supplementary material; the "ignorance factor" $\underline{p}$ was set to 0.065. An extinction correction was made; $F_{corr} = F_{obs}(1 + 0.167 \times 10^{-6} I)$, where I is the raw intensity, and F is the structure factor. The scattering factors were from International Tables.[20] In the final refinements the zirconium, silicon, nitrogen, C(1) - C(3), and C(13) - C(15) atoms were assigned anisotropic thermal parameters, and hydrogen atoms (1) and (23) were included. Only the carbons atoms C(1) - C(3), C(13) - C(15) were given anisotropic thermal parameter as they are in the region of the fused rings, and confirmation of the hydrogen atoms on the bridging atoms C(1) and C(13) was sought. In the difference electron density maps these hydrogen atoms H(1) and H(23) were found and were included in the least-squares refinements. Because of the large computer costs no more parameters were added and the refinement was terminated at this point.

The discrepancy indices for the data were $F^2 > 3\sigma$ are: $R = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0.061$ and $R_w = [\Sigma \underline{w}(|F_o| - |F_c|)^2/\Sigma \underline{w}|F_o|^2]^{1/2} = 0.082$. R for all the data is 0.12. The error in the observation of unit weight is 1.71.

Tables of the thermal parameters, and a list of observed structure factors is given in the supplementary materials.

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Table I. Positional Parameters[a]

Atom	X	Y	Z
ZR(1)	.12720(6)	.06047(4)	.21461(5)
ZR(2)	.15127(6)	.17194(4)	.14944(6)
SI(1)	.1641(2)	.12331(14)	.3251(2)
SI(2)	.0540(2)	.0430(2)	.3786(2)
SI(3)	.2325(2)	-.0406(2)	.1943(2)
SI(4)	.0827(2)	-.04306(13)	.1282(2)
SI(5)	.0003(2)	.16088(13)	.1522(2)
SI(6)	.0301(2)	.2768(2)	.1740(2)
SI(7)	.2815(2)	.23425(14)	.0872(2)
SI(8)	.2216(3)	.1514(2)	-.0089(2)
N(1)	.1603(5)	.0719(3)	.3155(5)
N(2)	.1501(5)	-.0126(3)	.1759(5)
N(3)	.0574(5)	.2140(3)	.1684(4)
N(4)	.2226(6)	.1859(3)	.0679(4)
C(1)	.1974(8)	.1256(5)	.2344(7)
C(2)	.1153(9)	.1832(5)	.3558(8)
C(3)	.2400(8)	.1077(6)	.3870(6)
C(4)	.029(2)	-.023(1)	.348(1)
C(5)	.107(2)	.032(1)	.461(2)
C(6)	-.029(2)	.074(1)	.400(2)
C(7)	.292(1)	.0079(7)	.241(1)
C(8)	.223(1)	-.0953(7)	.257(1)
C(9)	.279(1)	-.0631(7)	.1147(9)
C(10)	-.0084(9)	-.0157(6)	.1524(8)
C(11)	.080(1)	-.1160(7)	.1388(9)
C(12)	.0952(9)	-.0325(6)	.0298(9)
C(13)	.0724(7)	.1106(5)	.1386(6)
C(14)	-.0626(7)	.1451(6)	.2271(7)
C(15)	-.0563(8)	.1706(5)	.0725(7)
C(16)	-.0708(9)	.2829(6)	.2011(8)
C(17)	.048(1)	.3116(7)	.091(1)
C(18)	.083(1)	.3127(7)	.2452(9)
C(19)	.2586(8)	.2555(6)	.1779(8)
C(20)	.379(1)	.2154(7)	.087(1)
C(21)	.2683(9)	.2921(6)	.0303(8)
C(22)	.275(1)	.182(1)	-.078(1)
C(23)	.124(1)	.1496(9)	-.046(1)
C(24)	.247(1)	.0816(9)	.011(1)
H(1)	.237(5)	.128(4)	.234(5)
H(23)	.048(7)	.085(5)	.104(6)

[a] Here and in the following tables the number in parentheses is the estimated deviation in the least significant digit.

Table II. Selected Interatomic Distances (Å)

Zr(1)	- N(1)	2.04(1)	Zr(2)	- N(3)	2.07(1)
	- N(2)	2.09(1)		- N(4)	2.08(1)
	- C(1)	2.16(2)		- C(13)	2.16(2)
	- C(13)	2.21(2)		- C(1)	2.21(2)
N(1)	- Si(1)	1.79(1)	N(3)	- Si(5)	1.76(1)
	- Si(2)	1.70(1)		- Si(6)	1.71(1)
N(2)	- Si(3)	1.71(1)	N(4)	- Si(7)	1.70(1)
	- Si(4)	1.74(1)		- Si(8)	1.74(1)
Si(1)	- C(1)	1.87(2)	Si(5)	- C(13)	1.88(2)
	- C(2)	1.89(2)		- C(14)	1.90(2)
	- C(3)	1.88(2)		- C(15)	1.88(1)
Si(2)	- C(4)	1.80(3)	Si(6)	- C(16)	1.93(2)
	- C(5)	1.89(4)		- C(17)	1.87(2)
	- C(6)	1.80(4)		- C(18)	1.93(2)
Si(3)	- C(7)	1.90(2)	Si(7)	- C(19)	1.89(2)
	- C(8)	1.89(2)		- C(20)	1.85(2)
	- C(9)	1.86(2)		- C(21)	1.88(2)
Si(4)	- C(10)	1.87(2)	Si(8)	- C(22)	1.85(3)
	- C(11)	1.91(2)		- C(23)	1.92(3)
	- C(12)	1.95(2)		- C(24)	1.92(3)

Table III. Selected angles (deg.)

N(1) - Zr(1) - N(2)	121.7(4)	N(3) - Zr(2) - N(4)	124.3(4)
N(1) - Zr(1) - C(1)	81.9(5)	N(3) - Zr(2) - C(13)	81.6(4)
N(1) - Zr(1) - C(13)	116.5(4)	N(3) - Zr(2) - C(1)	118.2(5)
N(2) - Zr(1) - C(1)	131.2(5)	N(4) - Zr(2) - C(13)	118.2(4)
N(2) - Zr(1) - C(13)	112.8(4)	N(4) - Zr(2) - C(1)	115.0(5)
C(1) - Zr(1) - C(13)	85.8(5)	C(1) - Zr(2) - C(13)	85.7(5)
N(1) - Si(1) - C(1)	98.1(6)	N(3) - Si(5) - C(13)	99.0(6)
N(1) - Si(1) - C(2)	110.0(6)	N(3) - Si(5) - C(14)	113.2(6)
N(1) - Si(1) - C(3)	112.8(6)	N(3) - Si(5) - C(15)	111.6(6)
C(1) - Si(1) - C(2)	115.2(7)	C(13) - Si(5) - C(14)	112.5(6)
C(1) - Si(1) - C(3)	111.6(7)	C(13) - Si(5) - C(15)	111.4(6)
C(2) - Si(1) - C(3)	108.9(7)	C(14) - Si(5) - C(15)	109.0(7)
Zr(1) - N(1) - Si(1)	92.9(4)	Zr(2) - N(3) - Si(5)	92.6(4)
Zr(1) - N(1) - Si(2)	127.6(6)	Zr(2) - N(3) - Si(6)	139.3(6)
Si(1) - N(1) - Si(2)	128.0(6)	Si(5) - N(3) - Si(6)	126.0(6)
Zr(1) - C(1) - Zr(2)	93.9(6)	Zr(1) - C(13) - Zr(2)	93.9(5)
Zr(1) - C(1) - Si(1)	87.0(6)	Zr(2) - C(13) - Si(5)	86.6(5)
Zr(2) - C(1) - Si(1)	126.7(8)	Zr(1) - C(13) - Si(5)	129.5(6)

Table IV. Deviations (Å) of Atoms from Selected Least Squares Planes.

Plane	Zr(1) C(1) C(13) Zr(2)	Zr(1) C(1) N(1) Si(1)	Zr(2) C(13) N(3) Si(5)
	Zr(1) -.06	Zr(1) -.02	Zr(2) -.03
	C(1) .06	C(1) .02	C(13) .03
	Zr(2) -.06	Si(1) -.02	Si(5) -.04
	C(13) .06	N(1) .02	N(3) .03

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SUPPLEMENTARY MATERIAL AVAILABLE

Data processing formulas, a table of thermal parameters and the listing of structure factor amplitudes (17 pages). Ordering information is given on any current masthead page.

Figure Captions

Figure I An ORTEP diagram of $\{\overline{ZrCHSi(Me)_2N}SiMe_3[N(SiMe_3)_2]\}_2$ showing the atom numbering scheme.

Figure II An ORTEP diagram showing a side-on view.

Figure III A line drawing showing the diastereotopic Me_2Si groups.

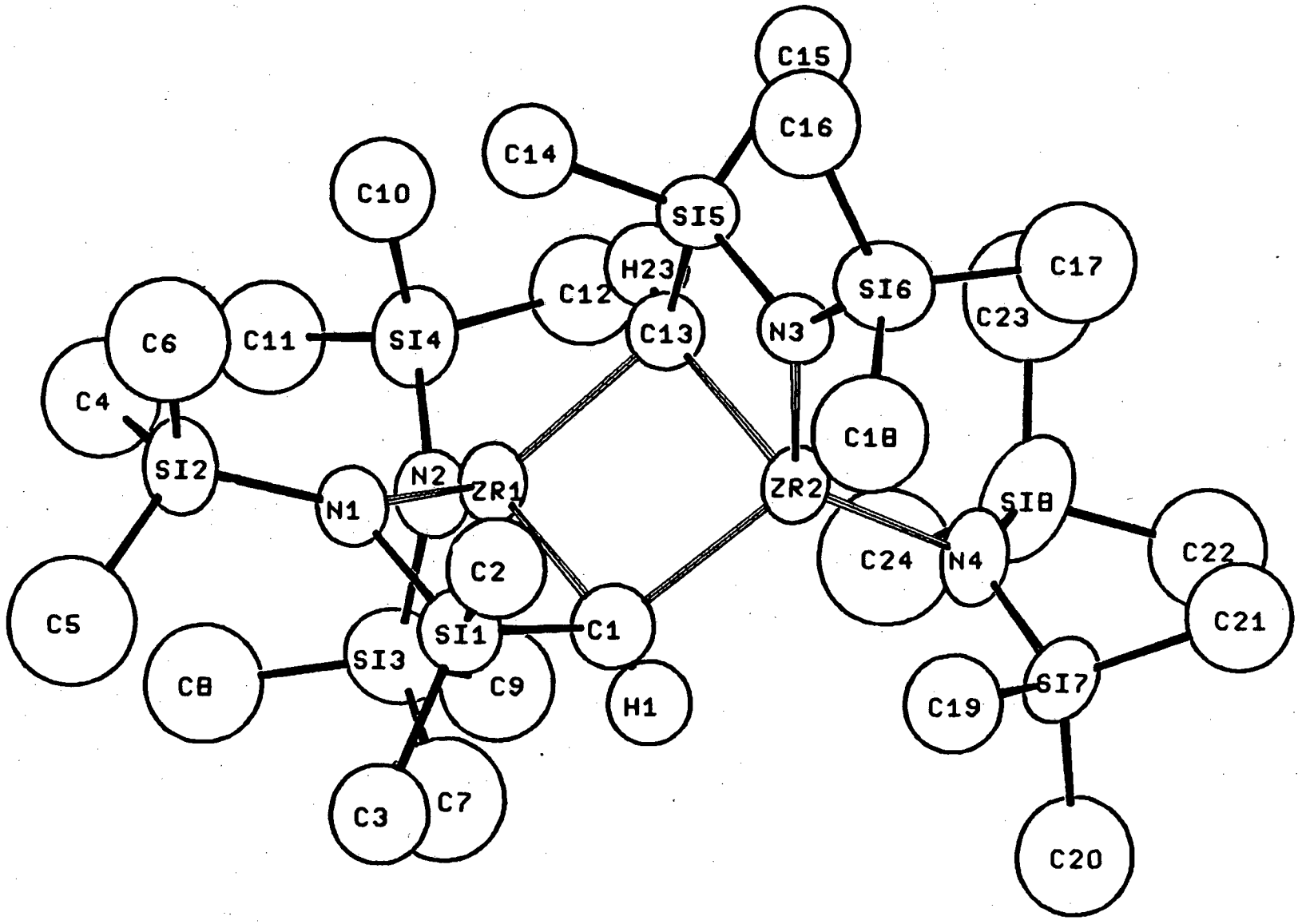


Figure I

XBL 816-10254

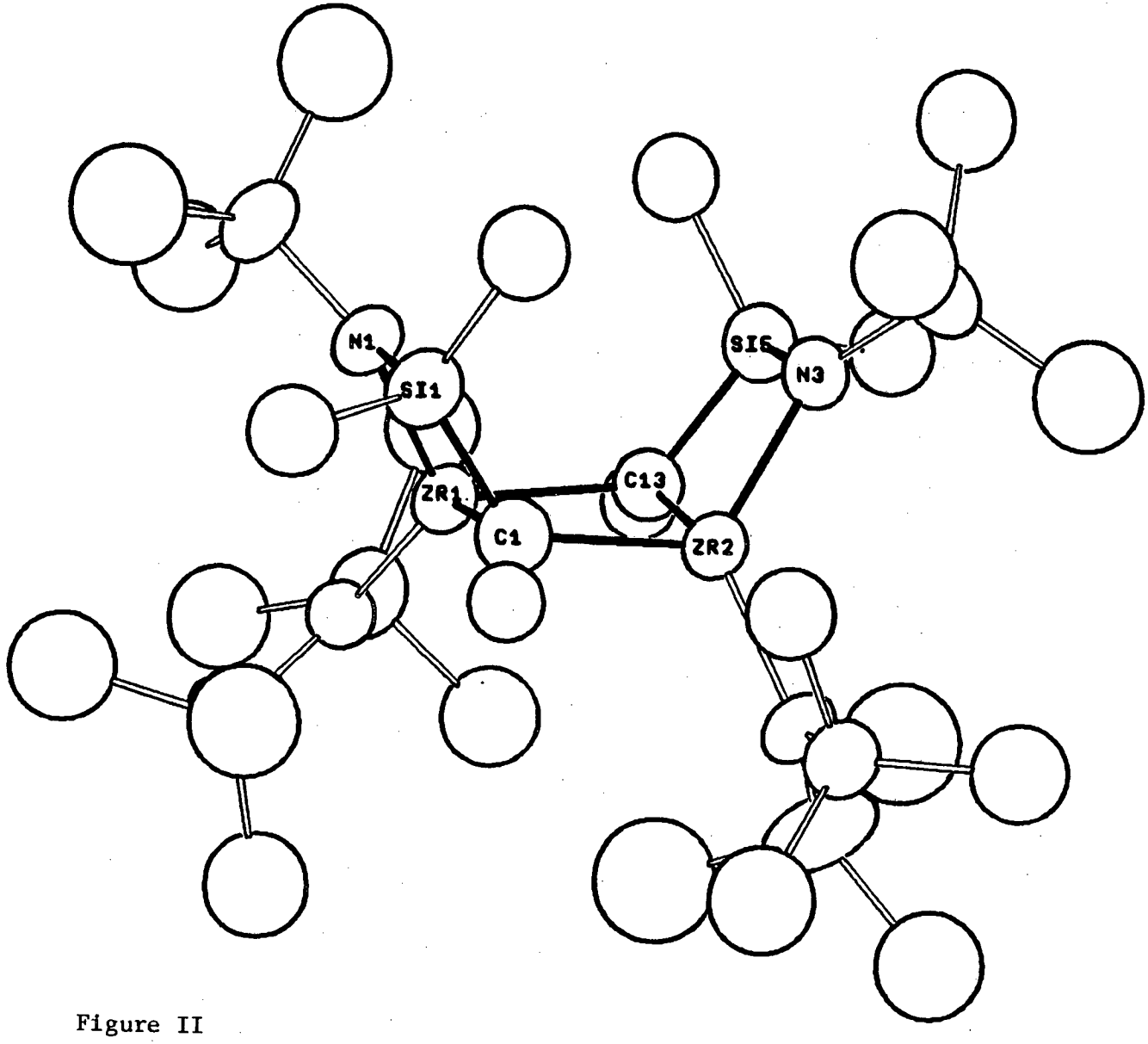
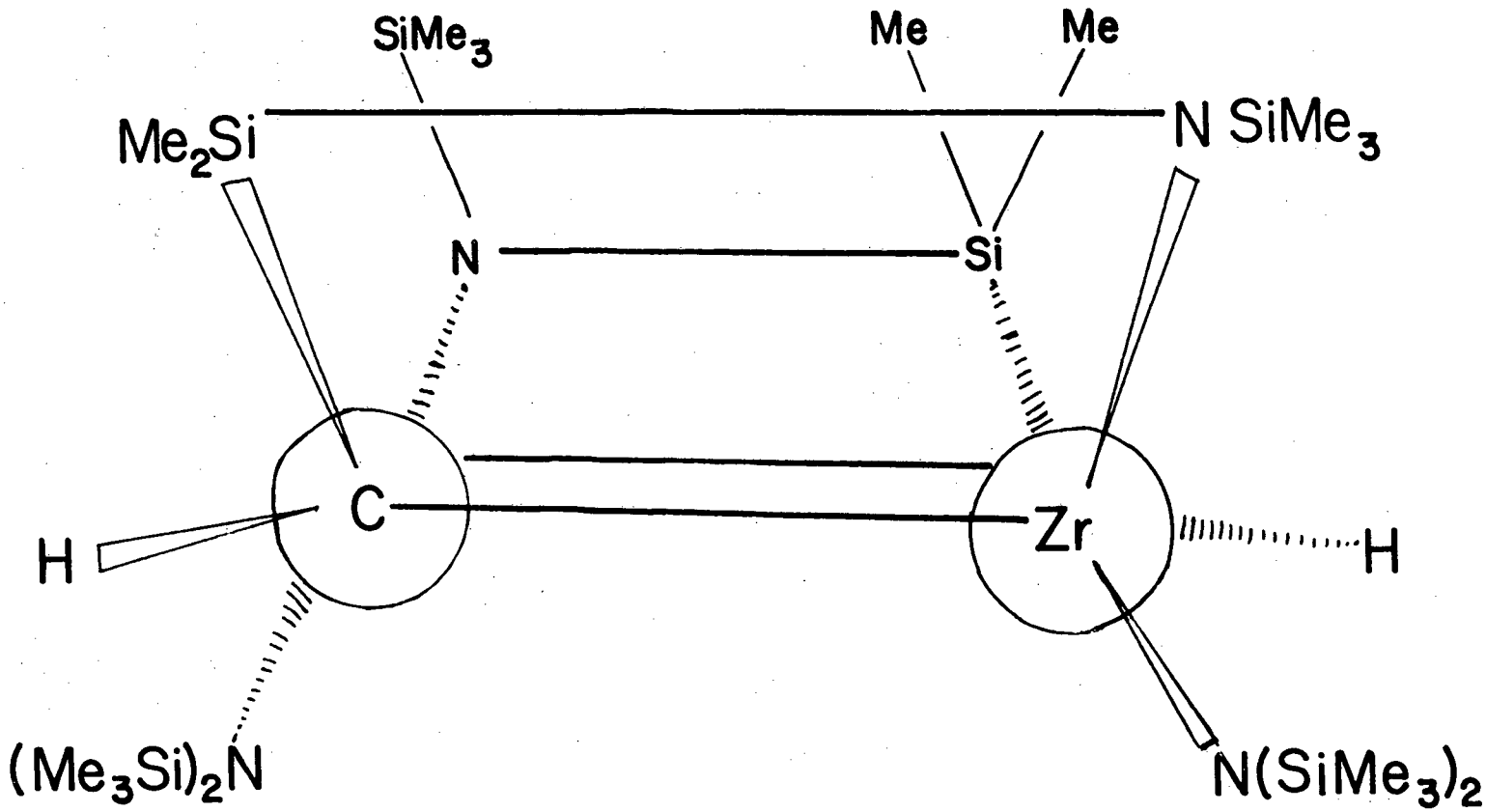


Figure II

XBL 816-10257



XBL 828-10910

Figure III

Supplementary Materials For

Dialkyl Bis[Bis(Trimethylsilyl)amido] Group IVA Metal Complexes; Preparation of Bridging Carbene Complexes by γ-Elimination of Alkane. Crystal Structure of $\{\overline{ZrCHSi(Me_2)N}SiMe_3[N(SiMe_3)_2]\}_2$.

Roy P. Planalp, Richard A. Andersen* and Allan Zalkin

Thermal Parameters[a]

ATOM	B11	B22	B33	B12	B13	B23
ZR(1)	4.46(6)	3.61(5)	3.36(5)	-.25(5)	.30(5)	.11(4)
ZR(2)	3.80(6)	3.74(5)	3.94(5)	-.16(5)	.44(5)	.46(5)
SI(1)	5.4(2)	5.4(2)	3.7(2)	-.5(2)	-.3(1)	-.4(1)
SI(2)	6.3(2)	6.9(2)	4.0(2)	-.4(2)	.8(2)	1.1(2)
SI(3)	6.3(3)	5.4(2)	7.7(3)	1.8(2)	-.1(2)	-.5(2)
SI(4)	7.2(3)	4.3(2)	5.5(2)	-1.1(2)	-.1(2)	-.4(2)
SI(5)	4.0(2)	4.9(2)	4.5(2)	-.1(1)	-.5(1)	.2(1)
SI(6)	5.5(2)	5.0(2)	7.5(2)	1.2(2)	-.2(2)	-.4(2)
SI(7)	4.4(2)	5.1(2)	6.4(2)	-.9(2)	.6(2)	1.2(2)
SI(8)	9.9(3)	9.3(3)	5.6(2)	-3.1(3)	3.1(2)	-1.7(2)
N(1)	4.3(5)	4.9(5)	3.2(4)	-.2(4)	.3(4)	.4(4)
N(2)	5.1(6)	4.3(5)	4.0(5)	.7(4)	.7(4)	.2(4)
N(3)	3.8(5)	4.1(5)	4.0(5)	.1(4)	-.4(4)	.4(4)
N(4)	6.1(6)	4.2(5)	3.6(5)	-.4(4)	1.2(4)	.1(4)
C(1)	4.0(8)	4.3(6)	4.4(7)	-1.1(6)	-.5(6)	-.1(5)
C(2)	8.1(9)	6.0(8)	7.1(8)	.8(7)	.4(7)	-2.2(7)
C(3)	7.8(10)	9.7(10)	4.0(6)	-.2(8)	-2.3(6)	-.5(7)
C(13)	5.1(7)	4.6(6)	2.9(5)	-.6(5)	-.0(5)	-.0(5)
C(14)	4.0(7)	8.2(9)	6.5(8)	-.4(6)	.8(6)	.4(7)
C(15)	6.3(8)	7.2(8)	5.6(7)	-.3(7)	-2.7(6)	.3(6)
C(4)	15.8(9)					
C(5)	20.0(11)					
C(6)	21.2(12)					
C(7)	10.8(5)					
C(8)	10.0(5)					
C(9)	9.5(5)					
C(10)	7.4(4)					
C(11)	9.0(4)					
C(12)	8.5(4)					
C(16)	8.1(4)					
C(17)	10.3(5)					
C(18)	9.7(5)					
C(19)	6.9(3)					
C(20)	10.1(5)					
C(21)	8.3(4)					
C(22)	15.4(8)					
C(23)	12.4(6)					
C(24)	13.0(7)					
H(1)	2.5(30)					
H(23)	6.9(34)					

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

DATA PROCESSING FORMULAE

$$I = C - (t_c/2t_b)(B_1+B_2)$$

$$\sigma(B) = \mathrm{Max}[(t_c/2t_b)(B_1+B_2)^{\frac{1}{2}},\ (t_c/2t_b)|B_1-B_2|]$$

$$\sigma(I) = [C + \sigma^2(B)]^{\frac{1}{2}}$$

$$F^2 = (D\cdot A/Lp)I$$

$$\sigma(F^2) = (D\cdot A/Lp)\sigma(I)$$

$$F_a^2 = \Sigma F^2/n$$

$$\sigma(F_a^2) = [\Sigma\sigma^2(F^2)]^{\frac{1}{2}}/n$$

When $S(F_a^2) > 4\sigma(F_a^2)$, $\sigma(F_a^2)$ is replaced by $S(F_a^2)$.

$$S(F_a^2) = [\Sigma|F^2-F_a^2|^2/n(n-1)]^{\frac{1}{2}}$$

$$\sigma(F_o^2) = [\sigma^2(F_a^2) + (pF_a^2)^2 + q^2]^{\frac{1}{2}}$$

$$F_o = (F_a^2)^{\frac{1}{2}}$$

$$\sigma(F) = F_o - [F_a^2 - \sigma(F_o^2)]^{\frac{1}{2}} \text{ when } \sigma(F_o^2) \leq F_a^2 \text{ or } [\sigma(F_a^2]^{\frac{1}{2}} \text{ when } \sigma(F_a^2) > F_a^2$$

$$Lp = [\cos^2 2\theta_m + \cos^2 2\theta]/[\sin 2\theta\ (1 + \cos^2 2\theta_m)]$$

$$wtg = 1/\sigma^2(F)$$

C = counts recorded during a scan

I = individual raw intensity, background removed.

t_c = scan count time

t_b = background count time

B_1 = individual background count

$\sigma(B)$ = estimated standard deviation of the total background count

F = structure factor

D = decay correction; an empirically applied correction obtained from the fluctuations of the standard reflections.

A = absorption correction

Lp = Lorentz and polarization corrections

θ_m = monochromater angle

θ = crystal diffraction angle

S = scatter

a = average

q = additional uncertainty that affects the weak intensities

p = estimate of non-statistical errors

wtg = weighting factors in least squares

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 2.0)
ZR(2)SI(8)N(4)C(24)H(68) F(0,0,0) = 5643

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
H,L=		0,	0	22	86	9	-14	12	282	10	-10	8	202	10	13	11	363	12	5
4	49	4	3	24	200	8	-5	14	247	9	-23	10	85	8	11	12	193	7	-4
6	469	16	63	H,L=		0,	5	16	91	9	-15	12	172	7	-1	13	116	5	-5
8	797	27	17	4	892	30	39	18	100	7	10	16	113	8	13	14	206	7	19
10	585	20	-83	6	280	9	-45	20	156	9	-12	H,L=		0,	17	15	108	5	20
14	245	9	9	8	296	10	22	24	141	7	5	2	181	11	6	17	126	6	-9
16	97	6	6	10	464	16	-26	H,L=		0,	11	4	95	8	3	18	213	8	-8
18	516	19	-12	14	195	8	-22	2	223	8	-10	6	112	7	12	19	291	10	-8
20	199	8	4	16	200	8	-10	4	594	20	-31	8	91	12	2	20	74	10	-4
24	49	13	5	20	69	11	-5	6	117	6	20	10	89	12	7	21	55	11	-2
26	87	8	-9	22	240	9	-12	8	236	9	3	12	115	10	0	26	80	12	-6
H,L=		0,	1	26	57	13	6	10	80	8	-8	14	66	12	-8	H,L=		1,	3
4	123	5	-4	H,L=		0,	6	12	196	8	16	16	82	14	22	1	349	12	3
6	216	7	5	0	646	21	-28	14	206	8	14	H,L=		0,	18	2	193	7	9
8	278	9	14	4	115	5	-36	16	155	7	5	0	57	12	-1	3	157	7	23
10	692	23	20	6	399	13	-61	22	204	9	11	2	96	15	9	6	314	11	71
14	143	8	-16	10	101	5	-4	H,L=		0,	12	6	74	10	-13	7	186	7	5
16	239	10	-10	14	90	6	-2	2	590	20	19	12	64	12	-5	9	423	14	-53
18	356	13	4	16	215	8	19	4	96	6	4	14	110	8	8	10	435	14	-20
20	316	11	-2	18	177	9	3	6	235	9	-14	H,L=		0,	19	11	184	7	-6
28	212	9	11	20	186	8	16	8	355	12	18	4	205	8	8	14	52	12	-13
H,L=		0,	2	26	60	12	13	10	269	10	16	H,L=		0,	20	15	74	5	-4
0	925	31	-46	H,L=		0,	7	12	208	8	-10	6	146	8	8	16	156	6	-4
2	471	16	6	6	235	8	-10	16	83	17	-5	8	80	12	26	17	172	7	-16
4	92	8	27	10	393	14	-20	H,L=		0,	13	H,L=		1,	1	18	149	6	-4
6	252	9	-7	12	140	6	9	2	213	8	-7	2	338	11	8	19	183	7	9
8	154	9	-63	14	166	7	0	4	64	9	26	3	281	9	-3	20	184	7	-7
10	208	7	19	18	84	8	5	6	226	8	-9	4	630	21	-13	21	69	12	-1
14	74	6	-16	22	59	12	-23	8	141	9	-6	6	71	4	-2	24	108	6	2
16	283	10	-4	H,L=		0,	8	10	231	9	-33	7	381	13	52	H,L=		1,	4
18	300	12	-3	4	306	10	3	12	89	9	-19	8	62	16	14	0	566	19	90
20	85	9	7	6	230	8	-23	22	93	9	12	9	321	11	-18	1	573	19	9
22	61	12	18	8	39	10	-17	H,L=		0,	14	10	350	12	3	2	354	12	-17
26	123	8	-2	10	132	6	24	4	132	7	-8	11	115	5	-17	3	57	5	-20
H,L=		0,	3	12	74	8	-4	6	164	8	-8	12	165	6	1	5	249	9	1
4	622	21	26	14	199	8	-0	8	376	13	-6	14	265	9	25	6	254	9	17
8	233	8	43	16	133	14	12	10	214	8	-16	15	109	5	-2	7	172	7	-33
10	54	7	-28	20	78	20	-7	12	200	8	8	16	105	5	0	8	277	9	-74
14	419	15	-6	H,L=		0,	9	16	73	10	-13	17	81	8	6	10	321	11	-7
16	226	9	-10	4	391	13	-0	18	189	10	3	18	128	6	0	11	273	10	27
20	186	8	-3	8	285	10	1	H,L=		0,	15	19	109	6	1	12	114	5	3
22	142	7	8	10	170	7	14	2	280	10	3	21	73	9	10	13	146	6	-20
H,L=		0,	4	12	254	9	1	4	90	10	12	H,L=		1,	2	14	92	5	-3
0	758	25	-2	14	182	9	-18	6	249	10	-5	0	959	33	-12	17	219	8	-3
2	324	12	-3	16	146	7	-6	8	119	11	6	1	540	18	15	18	208	7	10
4	171	8	31	22	196	8	16	10	257	10	-9	2	183	6	-5	19	186	8	10
6	408	14	47	H,L=		0,	10	12	124	9	-7	3	509	17	17	23	61	12	14
8	91	5	-4	0	130	6	7	14	60	11	6	5	577	19	30	26	112	8	-7
14	571	20	13	2	337	12	1	16	186	8	-1	7	173	9	29	H,L=		1,	5
16	195	7	-1	4	242	8	-0	H,L=		0,	16	8	394	13	8	1	381	13	48
18	165	7	-2	6	599	20	-25	2	106	14	3	9	347	12	-1	2	258	9	19
20	204	8	15	10	200	8	-14	6	61	11	28	10	276	9	6	3	205	8	16

TRUCTURE FACTCRS CONTINUED FCR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
5	60	11	32	0	147	7	-2	17	175	7	-7	19	52	14	17	7	53	10	1
6	70	5	15	1	138	5	-8	18	100	7	7	21	73	8	-7	9	113	11	10
7	134	6	-17	2	256	9	-23	19	127	6	1	H,L=	1,	14		10	73	15	-2
8	111	5	-8	3	433	14	39	21	129	7	-12	0	87	6	-12	H,L=	1,	20	
9	303	10	-23	4	72	4	-23	22	71	10	2	1	143	6	-7	3	65	16	13
10	341	12	7	5	333	11	11	H,L=	1,	11		2	124	6	-9	5	80	8	-6
11	86	5	2	6	419	14	12	1	295	10	-24	3	59	8	-13	6	48	12	-0
12	201	8	-9	10	254	9	10	2	240	9	-2	7	200	8	-1	8	100	10	-10
14	158	6	-2	12	214	8	-5	3	201	7	3	10	46	13	9	H,L=	2,	0	
15	140	5	6	13	271	10	-16	4	110	5	-10	11	65	7	12	0	264	9	21
17	72	6	-7	14	202	7	-25	7	110	5	4	12	98	8	7	1	890	29	-7
19	74	16	-3	15	110	6	4	8	107	6	10	15	52	10	13	2	175	6	13
20	165	6	-7	16	184	7	-16	9	139	6	-5	20	90	7	11	3	610	21	18
22	106	10	10	17	206	8	-11	10	143	6	1	H,L=	1,	15		4	285	10	28
23	105	7	11	20	104	6	2	11	95	6	-6	1	59	8	0	5	309	10	31
25	59	13	-12	21	139	7	3	13	65	11	5	2	76	7	-3	6	212	8	76
27	56	15	-0	23	91	8	1	14	103	6	4	6	49	14	-15	7	529	18	-2
H,L=	1,	6		24	134	8	-2	16	64	12	-3	17	67	8	7	8	166	11	15
0	160	8	7	H,L=	1,	9		17	162	9	-5	H,L=	1,	16		9	504	17	125
1	78	8	6	1	115	4	16	18	121	7	-5	0	197	7	5	11	534	18	6
2	375	12	-15	2	150	5	-7	19	56	9	6	1	77	9	10	12	192	9	30
3	221	8	-53	3	169	6	-9	20	134	6	-0	3	123	7	5	13	116	5	8
5	567	19	-50	4	331	11	11	21	70	8	10	4	61	8	-5	14	115	6	-23
6	297	10	-17	5	266	9	-11	22	70	9	12	7	82	12	4	15	340	12	-6
7	135	5	13	7	257	9	15	H,L=	1,	12		8	65	11	-11	16	226	8	-14
8	175	6	5	8	89	4	12	0	322	11	-15	10	51	12	4	17	46	9	14
9	51	5	9	9	50	6	24	1	265	9	-3	11	64	7	-8	19	440	15	-7
10	70	4	-1	10	133	6	18	2	58	7	-5	14	63	8	-10	21	48	12	4
12	263	9	19	12	260	10	-16	3	196	7	3	15	71	9	2	22	46	13	11
13	365	12	1	13	44	9	17	4	275	9	4	16	52	11	10	25	86	6	18
14	115	5	-2	14	122	6	-5	5	124	6	-8	H,L=	1,	17		27	172	9	-1
15	149	6	4	15	232	8	14	6	147	6	-21	1	175	7	-7	H,L=	2,	1	
16	148	7	-2	16	135	8	22	7	201	7	-10	2	174	8	-6	11	201	49	-41
20	91	7	-12	17	81	15	-14	8	171	6	10	3	69	16	-5	2	48	3	6
21	55	16	4	18	93	13	6	10	66	7	8	6	72	7	-3	3	42	8	20
23	95	8	-9	20	92	6	-8	11	197	7	-6	8	51	13	4	4	347	12	9
24	126	7	9	22	120	6	-1	12	95	7	-8	9	138	7	-9	5	137	6	40
H,L=	1,	7		23	87	13	9	13	59	8	-8	10	63	9	2	7	292	10	10
3	418	14	-3	H,L=	1,	10		15	68	13	-5	15	64	8	21	8	229	8	-15
5	246	8	-1	0	123	5	-8	16	104	8	9	16	120	6	3	9	584	19	-38
6	326	11	24	1	60	5	7	18	155	7	4	H,L=	1,	18		10	226	8	16
7	278	10	19	2	261	9	-16	19	109	6	-2	0	218	9	9	11	103	5	7
8	337	11	16	3	211	7	-5	20	94	7	-4	1	120	6	-8	12	55	5	1
9	81	5	7	4	200	7	-2	H,L=	1,	13		3	147	7	-2	13	161	6	0
10	179	7	-10	5	73	6	23	1	210	7	-11	4	79	7	-7	15	58	6	0
11	234	9	18	6	121	5	-18	2	371	13	-6	5	46	10	11	16	64	15	7
12	264	9	31	7	160	6	-3	3	188	7	-7	7	155	6	-11	17	433	15	-7
14	283	10	-12	8	153	6	-7	5	74	8	3	8	105	10	-0	18	241	9	-1
15	306	10	-4	9	96	5	-1	6	165	6	14	10	97	8	-1	19	111	6	7
16	62	10	8	10	76	7	-13	8	165	7	9	11	103	8	3	21	166	7	12
18	100	10	-0	11	158	6	2	9	212	8	5	12	76	10	19	23	60	9	4
20	46	13	23	12	119	7	-5	10	69	7	-2	H,L=	1,	19		24	73	6	2
21	65	13	-10	13	74	6	-22	13	65	10	4	1	104	14	4	25	91	7	-4
22	198	8	-1	14	86	6	-1	15	77	7	-0	2	133	13	10	27	98	9	-8
23	115	7	-4	15	53	9	10	16	140	7	-10	3	47	12	16	H,L=	2,	2	
H,L=	1,	8		16	182	8	-7	17	84	8	1	6	68	14	-17	0	384	10	13

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
1	462	15	31
2	600	20	20
3	307	11	-8
5	362	12	10
6	73	14	21
7	225	8	49
8	93	5	14
9	250	8	1
11	274	9	12
12	67	4	-14
13	272	9	9
14	216	7	-7
15	238	8	-16
16	132	6	6
19	274	9	-11
21	74	10	10
23	46	10	6
24	83	7	-2
25	41	12	22
27	111	9	16
H,L=		2,	3
1	73	9	-34
4	40	8	30
5	307	10	29
7	458	15	46
8	86	5	-4
9	48	5	2
10	70	4	-2
11	231	8	5
12	39	7	2
13	233	8	-11
14	65	9	-15
15	299	10	-8
16	93	5	-8
17	171	6	5
18	44	11	8
19	55	11	-16
20	105	6	-8
22	48	10	3
23	159	7	3
25	105	6	5
27	73	8	7
H,L=		2,	4
0	667	22	-6
1	224	8	25
2	378	13	23
3	306	11	32
5	576	19	52
6	138	6	3
7	152	5	3
9	105	4	9
10	90	4	-5
11	89	4	-7
12	167	6	13
13	431	15	-1
16	187	7	8

K	FOB	SG	DEL
17	105	5	10
19	71	7	-6
20	91	6	2
21	183	7	-6
23	93	6	-8
25	75	10	-0
27	59	14	19
H,L=		2,	5
1	406	14	-32
2	111	10	61
3	761	25	97
4	53	11	-3
5	390	13	23
6	90	6	44
7	326	11	-20
8	42	11	10
9	162	6	-21
11	239	8	-4
12	59	6	9
13	131	5	28
15	320	11	-4
16	45	9	13
17	129	6	-3
19	56	8	4
21	99	8	3
22	68	7	12
23	191	8	-5
24	64	8	-14
25	58	9	-2
H,L=		2,	6
0	227	8	37
1	570	19	30
2	90	6	-41
3	166	6	7
4	279	9	-7
5	383	13	8
6	169	6	-12
7	44	5	-8
8	122	5	-10
9	59	5	-2
10	128	5	-2
11	116	5	12
13	184	7	-0
14	82	5	-12
16	70	7	-7
17	113	5	4
18	99	7	11
19	175	7	2
20	46	11	7
21	154	8	5
23	63	9	-5
24	53	15	-12
25	65	8	4
H,L=		2,	7
1	251	9	41
2	57	5	35

K	FOB	SG	DEL
3	145	7	0
4	88	6	-12
5	143	5	-14
8	85	4	1
9	60	5	-12
11	119	5	-4
13	40	9	19
15	67	6	5
16	45	9	34
17	98	6	-6
18	45	13	-2
19	64	13	-10
21	69	7	-5
24	57	13	0
26	57	12	15
H,L=		2,	8
0	90	4	4
1	67	9	11
2	221	8	9
3	180	6	-4
4	210	7	27
5	196	7	12
6	47	5	17
7	166	6	2
8	63	5	7
10	145	5	24
12	172	6	-10
13	220	8	-14
14	244	8	3
17	54	10	2
18	61	8	-2
21	43	11	22
22	43	12	-1
H,L=		2,	9
1	77	5	2
2	58	5	19
3	288	10	1
4	188	7	-20
5	261	9	10
6	60	6	-2
7	108	5	-4
8	157	6	-16
9	101	6	9
10	77	7	4
11	116	5	-10
12	130	6	-3
13	91	5	-4
14	91	8	1
15	333	11	-2
17	63	8	9
21	52	9	9
23	126	6	-11
24	58	12	8
H,L=		2,	10
0	252	9	4
1	279	10	-1

K	FOB	SG	DEL
2	44	7	5
3	301	10	-15
5	399	14	-4
7	136	6	-16
8	115	5	10
9	50	10	5
10	160	7	-9
13	339	12	-2
16	106	6	9
17	75	15	-12
19	81	7	4
20	76	6	4
21	164	7	-0
23	53	15	-10
H,L=		2,	11
1	174	6	-3
2	89	5	-6
3	446	15	26
5	137	5	17
6	154	6	-3
7	311	11	1
8	59	7	-19
9	99	7	5
10	48	13	-6
11	300	10	5
15	157	6	2
19	97	6	-2
23	108	11	6
H,L=		2,	12
0	166	7	5
2	49	9	-4
3	172	6	-9
5	293	10	1
7	59	10	-4
8	71	6	-11
10	92	8	1
11	189	7	3
13	120	7	3
14	98	9	14
19	75	7	8
H,L=		2,	13
1	253	9	-18
5	55	8	-2
7	231	8	-9
8	59	8	-9
9	328	11	-4
10	115	6	-0
11	81	6	-5
17	163	6	6
19	95	8	-5
H,L=		2,	14
1	153	7	6
2	90	6	-0
3	126	6	-6
4	48	10	-5
5	71	7	-1

K	FOB	SG	DEL
7	269	11	-6
8	107	6	2
9	108	6	4
11	240	9	-1
15	91	8	-6
16	42	11	20
19	150	8	3
H,L=		2,	15
1	133	6	-10
3	113	6	5
4	74	7	-4
6	143	6	-0
7	130	9	4
9	295	10	7
11	99	11	1
13	66	9	12
17	202	8	8
19	75	10	16
H,L=		2,	16
1	137	7	10
3	119	8	-1
4	95	8	12
5	69	9	3
6	65	12	2
7	200	7	3
9	88	13	3
11	165	6	8
15	114	8	6
H,L=		2,	17
1	99	12	15
7	88	7	9
9	112	6	7
12	42	11	27
15	63	10	-8
H,L=		2,	18
3	98	6	6
4	87	6	2
5	144	7	-4
13	130	7	-5
H,L=		2,	19
5	72	8	5
7	81	9	9
11	115	8	9
H,L=		2,	20
0	43	13	8
1	58	11	13
5	96	6	9
7	98	12	-4
H,L=		3,	1
1	244	8	-2
2	286	10	3
3	126	9	23
5	191	7	-23
6	132	10	-57
7	49	13	36
8	267	9	-1

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
9	338	11	-7	5	52	9	-1	16	128	6	-20	9	145	5	1	14	66	13	18
10	47	13	-37	6	54	7	-39	17	111	5	7	10	138	7	-24	15	119	7	5
11	101	5	-1	7	286	10	-3	18	46	10	-7	11	250	9	6	18	61	8	-5
14	74	5	5	8	210	7	30	21	189	7	-3	12	112	5	12	19	168	7	-0
15	68	6	-10	9	189	6	19	22	77	12	2	14	120	7	11	H,L=		3,	13
16	60	8	-6	11	356	12	3	23	72	10	-11	15	212	8	-4	1	61	8	4
17	67	6	-7	12	67	7	10	24	129	6	-5	18	136	7	-2	3	160	7	-6
18	41	11	27	13	63	6	1	25	67	12	-3	19	99	6	-6	4	144	6	15
19	49	13	24	14	98	6	-5	26	79	9	9	20	147	6	9	6	118	7	13
20	162	7	-8	15	172	6	16	H,L=		3,	7	22	80	11	-5	8	51	9	-5
23	83	9	3	16	128	5	13	1	147	5	-6	23	111	11	7	9	143	6	-5
25	83	8	12	18	204	7	-4	2	99	5	-46	H,L=		3,	10	10	53	15	-15
H,L=		3,	2	19	109	6	3	3	315	11	-34	0	295	10	10	11	129	6	1
0	112	9	-0	21	51	11	-5	4	579	19	-8	1	281	10	2	17	120	6	-11
1	194	8	-1	23	64	12	7	5	338	11	23	2	159	6	8	19	51	10	8
3	363	12	70	24	100	8	-2	6	278	10	-17	3	203	7	-4	H,L=		3,	14
4	351	12	43	25	54	13	17	7	264	9	30	5	267	9	-1	0	93	7	9
7	502	17	-7	26	78	7	-1	8	182	6	-2	6	127	6	-15	3	51	12	32
8	73	6	-36	27	116	6	3	11	228	8	-1	8	147	6	-1	5	61	8	6
9	263	9	-12	H,L=		3,	5	12	244	9	-24	9	74	5	-4	6	99	6	23
10	147	5	-4	1	299	10	23	14	230	10	1	10	190	8	-3	7	65	11	10
11	315	11	20	3	114	7	33	15	341	12	-1	12	51	14	2	8	98	6	-9
12	81	4	9	4	121	5	-70	18	127	6	3	13	197	7	7	9	82	7	-2
13	206	7	8	5	118	5	4	19	131	6	10	14	60	11	-4	13	50	11	-9
14	35	9	0	6	665	22	6	21	45	11	-8	15	74	18	8	16	51	9	6
15	248	9	1	7	289	10	-18	22	75	7	7	16	132	6	9	19	56	10	9
18	220	8	13	8	125	5	-14	23	185	7	8	18	74	16	4	H,L=		3,	15
19	95	9	-2	9	128	5	-13	H,L=		3,	8	19	143	7	-13	1	63	11	-18
21	48	10	12	10	43	8	13	0	82	4	3	24	49	12	0	4	67	8	29
25	93	10	-6	11	185	6	-4	1	35	7	1	H,L=		3,	11	14	47	14	43
26	73	11	-1	12	123	5	9	2	245	8	-12	1	216	8	9	H,L=		3,	16
27	137	6	-2	13	205	8	6	3	386	13	-2	2	152	6	13	0	96	7	13
H,L=		3,	3	14	228	9	9	4	49	5	19	3	121	6	-7	1	120	7	6
1	210	8	-32	16	236	9	-11	5	285	10	-8	4	89	5	17	2	73	12	-6
2	370	12	36	17	157	6	1	6	204	7	7	5	73	5	0	3	45	13	3
3	140	7	-35	19	86	6	4	7	93	4	-7	7	74	12	-10	4	83	10	-1
4	157	10	76	22	58	10	7	8	269	9	24	8	97	7	3	8	49	12	5
5	380	13	10	23	81	9	-3	9	65	6	-8	9	161	8	-10	10	82	15	-14
6	151	6	42	25	94	9	-4	10	43	10	38	10	146	7	-16	15	47	11	5
7	275	9	-62	H,L=		3,	6	13	405	14	-11	12	157	6	-7	H,L=		3,	17
8	125	5	-3	0	282	9	69	14	150	7	7	13	60	8	9	1	93	7	-3
9	368	12	2	1	159	6	0	15	43	11	6	17	201	7	10	2	149	6	-4
10	169	6	-1	2	247	8	48	16	194	8	10	18	128	7	-10	3	89	8	-9
11	93	4	3	3	154	5	-5	20	51	11	-17	20	89	9	-20	4	76	7	7
12	98	4	14	4	183	6	34	21	196	7	-1	21	68	8	-9	6	86	8	-1
15	144	7	-15	5	229	8	-28	22	64	10	-16	H,L=		3,	12	8	97	6	1
16	62	6	3	6	139	5	-14	24	98	6	9	0	184	7	0	9	122	6	-13
17	275	9	-3	7	159	6	11	25	55	14	-15	1	309	10	2	11	71	7	13
20	110	7	-8	8	171	6	-15	H,L=		3,	9	2	129	6	7	12	52	11	9
23	111	7	-8	9	142	5	11	1	267	9	4	3	79	15	6	13	45	11	12
25	151	9	3	10	143	6	-11	3	104	8	-13	6	136	6	-3	H,L=		3,	18
H,L=		3,	4	11	155	6	23	4	232	8	25	7	149	7	-5	0	96	9	-13
0	295	10	29	12	56	8	-4	5	291	10	3	8	149	6	3	1	118	8	-6
1	83	14	29	13	266	9	-8	6	112	6	1	10	123	7	9	2	65	8	6
2	77	20	-79	14	182	7	-3	7	68	8	-12	11	91	6	14	3	63	9	-3
3	82	11	-6	15	55	8	2	8	189	7	-8	13	58	9	2	7	72	12	-10

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
11	91	8	19
H,L=		3,	19
1	82	10	0
2	98	6	2
4	95	10	4
6	113	8	3
H,L=		3,	20
0	97	7	7
2	48	11	21
3	54	15	-8
4	55	13	45
5	124	7	8
6	81	12	24
H,L=		4,	0
0	89	15	38
1	228	9	42
2	371	12	-36
3	452	15	22
4	264	9	7
5	700	23	-36
6	148	7	56
7	238	8	14
8	636	21	12
9	118	10	23
10	164	6	5
11	217	8	-5
12	42	7	13
13	84	5	-4
15	196	9	6
16	468	16	30
18	279	10	11
19	113	7	4
20	119	7	3
23	85	6	5
25	96	11	-10
26	229	9	5
H,L=		4,	1
1	94	8	17
2	653	23	38
3	665	22	39
4	334	12	-3
5	75	11	30
6	576	19	18
7	306	10	56
9	154	5	24
10	339	12	17
11	194	7	-2
12	233	8	-6
14	209	8	-2
16	178	8	-13
17	162	6	-3
18	201	7	-20
20	173	7	7
21	88	7	-7
23	75	8	-3
24	123	12	6

K	FOB	SG	DEL
26	78	12	-4
27	60	10	2
H,L=		4,	2
0	556	18	12
1	63	5	39
4	284	10	33
5	167	6	8
6	180	6	32
7	170	6	26
8	539	18	38
9	61	7	-13
10	170	6	0
12	105	5	2
13	41	9	-13
14	168	6	-9
15	113	5	-1
16	331	11	-12
18	158	6	-6
19	68	7	8
22	87	8	12
24	122	7	-8
26	121	8	5
H,L=		4,	3
1	341	12	12
2	367	12	27
3	228	8	13
4	699	23	70
5	256	9	55
6	206	7	-27
7	44	6	11
9	55	7	-3
11	388	13	-7
12	338	11	-9
13	100	5	5
14	162	6	4
15	79	6	2
16	124	5	6
20	53	13	18
21	96	6	5
22	136	7	-15
25	62	10	6
26	48	14	25
H,L=		4,	4
2	317	11	26
3	115	7	16
4	264	9	-16
5	53	7	-51
6	395	13	0
7	219	7	20
8	64	8	-5
9	181	6	-1
10	181	6	-3
11	49	6	-17
12	100	5	6
13	150	6	-15
14	205	8	-6

K	FOB	SG	DEL
15	142	7	4
16	117	5	10
19	84	8	7
20	104	9	6
22	107	9	1
24	162	6	11
25	78	10	-4
H,L=		4,	5
1	127	6	-13
2	194	7	30
4	487	16	8
5	157	6	-9
7	175	6	-3
8	38	10	-14
9	32	8	17
10	60	5	15
11	149	6	6
12	221	8	-11
13	215	8	5
14	160	6	3
15	108	6	-5
16	141	7	-3
17	155	8	6
18	207	8	10
20	109	7	10
21	101	12	-8
22	168	7	1
23	70	7	19
24	69	10	1
H,L=		4,	6
0	122	5	12
1	174	6	-13
2	78	5	5
4	187	7	32
5	238	8	6
6	110	5	-28
7	105	4	-8
8	50	5	14
9	46	6	-12
10	190	7	-6
11	114	5	2
12	134	6	-8
13	170	6	-9
14	229	9	-16
15	146	7	7
16	172	6	3
19	44	12	-5
20	139	10	-7
22	66	9	-0
24	52	10	2
H,L=		4,	7
1	206	7	-6
2	205	7	-21
3	134	5	2
5	117	5	25
6	140	5	0

K	FOB	SG	DEL
10	157	6	11
11	162	6	2
13	87	8	-1
14	46	9	9
15	113	10	-10
16	138	8	0
17	106	7	-6
22	58	11	2
23	73	7	3
H,L=		4,	8
0	31	8	-3
1	127	5	17
2	252	9	-0
4	229	8	7
5	108	4	28
6	72	7	-15
7	86	4	20
8	124	5	14
11	130	6	6
14	203	7	-12
15	97	7	17
16	67	9	-8
17	79	7	-4
20	62	10	15
22	64	12	-28
24	54	10	8
H,L=		4,	9
1	212	7	6
2	75	5	12
3	225	8	3
4	426	14	-3
5	67	8	15
6	127	6	16
10	117	5	3
11	141	7	-6
12	192	8	-5
13	171	6	-18
14	211	8	8
16	57	9	7
17	82	7	3
18	102	7	-4
24	48	12	4
H,L=		4,	10
0	140	6	9
1	145	5	-4
2	242	8	6
4	68	6	-11
6	236	8	6
7	191	7	11
11	95	5	-13
12	79	8	-10
13	131	7	5
14	252	9	-2
15	125	7	-2
16	73	8	-1
19	62	8	-3

K	FOB	SG	DEL
20	85	8	-4
21	93	8	12
22	105	8	4
24	103	6	13
H,L=		4,	11
1	245	9	9
2	58	10	-13
3	149	8	-24
4	265	9	24
5	125	5	8
6	137	5	-9
7	67	11	9
9	174	7	-10
10	66	10	3
12	246	9	-7
13	58	13	1
14	110	7	-10
15	110	9	-5
20	102	8	12
22	142	8	6
23	72	7	4
H,L=		4,	12
0	330	11	10
2	61	8	-2
3	133	9	-15
4	55	11	-4
5	173	7	-8
6	152	7	-5
7	60	11	8
8	146	6	-4
10	230	8	-5
14	129	6	-1
15	77	9	-3
18	104	6	-3
20	67	11	9
H,L=		4,	13
1	62	11	-37
2	94	6	-6
3	81	8	19
4	185	7	-5
5	82	8	13
6	165	7	-5
8	64	8	1
9	102	6	-9
10	179	8	-9
11	94	11	16
12	111	6	4
13	128	11	-8
14	57	16	-5
16	50	9	-3
20	109	8	-6
H,L=		4,	14
0	230	8	-23
1	139	7	-8
2	70	7	15
6	110	7	-14

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
7	188	8	-2	20	60	12	16	15	186	7	19	4	487	16	1	7	89	7	16
8	280	10	3	21	58	13	15	16	179	7	-1	8	77	5	-22	8	75	9	10
9	56	13	14	22	116	7	-7	17	63	8	-14	9	271	9	4	9	157	7	-14
10	117	7	-2	24	60	12	-9	18	109	6	-7	10	97	6	11	10	183	7	-6
11	114	10	12	H,L=	5,		2	21	57	11	-23	12	268	10	-13	11	158	7	-12
H,L=	4,		15	0	152	10	6	22	49	10	14	13	276	9	-7	12	119	7	-19
1	86	11	10	1	192	10	29	23	46	12	8	14	258	9	3	14	50	10	-7
2	204	8	12	2	180	8	-3	24	91	10	2	16	216	8	-6	16	74	17	8
4	64	12	-12	4	143	6	11	26	130	6	9	17	99	8	-11	18	92	7	2
5	88	10	7	5	171	6	4	H,L=	5,		5	18	52	10	14	19	88	7	0
6	168	7	10	6	534	18	-8	2	67	7	20	19	67	11	-0	H,L=	5,		11
8	121	8	2	7	326	11	4	3	139	5	22	20	90	8	-8	1	177	7	-1
9	202	8	4	8	430	14	18	4	210	7	21	22	209	8	2	2	370	13	12
10	221	9	16	9	51	9	18	6	286	10	3	23	115	17	-4	3	160	6	-12
14	89	7	-3	10	139	6	12	7	97	4	-10	25	57	13	0	5	95	5	-7
H,L=	4,		16	11	47	6	15	8	80	6	1	H,L=	5,		8	6	58	7	-3
0	232	8	10	12	380	13	-10	10	130	6	-19	0	132	5	12	7	99	5	7
2	72	18	-2	13	55	6	-19	12	239	8	-4	1	270	9	27	8	190	7	-14
7	95	8	-5	14	150	6	-4	14	72	6	6	2	223	8	-2	9	203	7	3
8	199	8	-2	17	110	6	1	15	189	8	7	3	142	5	16	10	103	7	3
10	89	9	-6	18	172	11	-9	16	89	6	2	5	234	8	-10	11	44	11	6
13	68	7	9	19	61	8	11	17	83	7	-9	6	457	16	-23	12	85	8	-8
H,L=	4,		17	20	79	9	-4	18	87	6	-5	7	179	6	9	15	90	8	1
1	85	8	-4	23	61	8	8	19	55	9	8	10	57	9	-5	16	85	8	2
2	69	9	0	26	157	7	-4	20	58	12	12	11	262	9	-7	18	84	7	-4
4	107	6	4	H,L=	5,		3	21	56	13	-7	12	353	12	-5	19	79	7	-2
6	126	7	3	1	163	7	-18	22	113	6	-0	13	60	8	-10	20	77	10	3
9	50	10	17	2	491	16	-51	23	52	10	5	14	301	10	1	H,L=	5,		12
10	54	10	-5	3	52	11	20	25	123	8	11	15	59	11	12	0	355	12	-23
12	69	8	8	5	166	6	13	26	50	12	-3	16	113	6	8	1	125	5	-5
14	101	8	4	6	368	12	-65	H,L=	5,		6	18	46	11	12	2	69	16	-24
H,L=	4,		18	7	203	7	7	0	101	6	5	19	106	9	7	3	63	7	11
2	91	7	-2	8	425	14	4	1	202	7	9	20	115	7	-12	4	78	6	19
6	95	11	3	9	103	4	17	2	246	8	21	21	77	7	11	5	199	7	-4
7	64	11	1	10	424	15	8	3	291	10	22	24	120	8	9	6	110	5	-9
10	63	11	14	11	228	8	11	5	219	7	-2	H,L=	5,		9	8	180	7	-4
H,L=	4,		19	12	148	5	-17	6	372	13	21	1	224	8	-20	9	72	7	-8
4	77	18	-1	14	97	7	15	7	269	9	-27	2	111	9	-16	10	132	7	-8
8	69	11	21	15	113	13	3	8	96	5	11	3	139	5	0	12	121	7	3
9	122	9	13	16	370	12	6	10	65	7	-12	4	506	17	14	13	78	10	4
H,L=	5,		1	17	125	6	12	11	213	7	11	5	36	9	21	17	62	8	12
1	108	15	15	19	50	11	4	12	54	7	-2	6	160	6	-3	18	114	8	-4
2	335	12	81	22	87	6	4	13	191	7	-13	7	185	7	18	20	123	13	9
3	208	8	-5	24	80	10	-13	14	277	9	-5	9	287	10	-0	H,L=	5,		13
4	94	10	19	H,L=	5,		4	15	121	7	3	10	128	5	-0	2	70	8	-13
5	201	7	44	0	281	9	18	16	186	7	-11	12	100	6	1	3	131	7	1
6	301	10	-36	2	143	5	16	17	97	7	-4	14	282	10	-15	4	199	7	-16
7	181	6	-17	3	255	9	-40	18	48	10	6	15	64	14	11	7	145	6	3
8	259	9	-12	5	201	7	-4	20	121	8	-8	17	89	11	-19	9	56	12	-2
9	169	6	23	6	228	8	51	21	93	6	4	20	75	11	10	10	241	9	-8
10	206	7	8	7	253	9	43	22	75	11	-8	23	69	11	3	14	62	11	5
11	198	7	3	8	403	14	8	24	164	8	8	H,L=	5,		10	16	60	8	-5
12	54	5	20	10	102	5	-5	H,L=	5,		7	0	452	15	22	18	135	7	10
13	60	8	4	11	62	6	-6	1	213	7	30	1	71	5	-4	20	105	6	10
16	234	9	-7	12	331	11	-4	2	49	8	34	3	44	8	11	H,L=	5,		14
17	115	6	-6	13	165	6	-7	3	145	5	25	6	173	7	-9	0	73	7	15

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
4	64	8	-16	16	62	7	-18	11	106	5	-1	7	194	7	-0	15	92	8	4
5	74	9	-1	18	243	9	-4	14	60	11	8	8	43	7	2	16	132	8	-4
6	147	7	3	19	212	8	6	15	245	9	-9	9	128	5	-6	20	51	9	4
8	106	7	10	20	226	8	3	17	55	9	15	11	52	11	6	23	101	8	12
12	93	12	-4	21	93	8	5	19	130	6	1	12	218	8	-5	H,L=	6,	10	
14	75	9	16	22	79	12	13	22	64	8	14	13	126	6	-7	0	431	14	18
H,L=	5,	15		24	44	12	-9	23	90	6	6	14	160	7	-3	1	79	8	11
1	52	10	29	25	52	15	18	25	86	12	-10	15	183	7	-5	2	144	6	23
4	105	6	-8	26	136	8	7	H,L=	6,	4		18	152	7	-9	3	120	5	15
9	57	9	5	H,L=	6,	1		0	293	10	-15	20	149	7	0	4	107	5	14
H,L=	5,	16		1	501	17	98	1	58	6	-0	21	74	8	-1	5	378	13	1
0	152	7	-0	2	477	16	-19	2	288	10	10	23	69	8	3	6	287	10	11
2	89	9	-10	4	224	8	4	3	313	10	-19	25	76	7	15	7	115	5	6
4	77	12	13	5	139	5	27	4	183	6	-12	H,L=	6,	7		8	123	6	-9
5	83	10	9	7	259	9	-20	5	547	18	-3	1	111	5	-10	10	157	6	-4
6	71	11	13	8	371	13	7	6	481	16	15	2	177	6	-4	12	202	8	-3
8	65	8	3	9	387	13	-0	7	35	8	-7	4	122	5	2	13	227	8	5
12	58	10	14	10	207	7	0	8	98	4	-3	6	132	5	0	14	111	6	1
H,L=	5,	17		12	67	9	16	9	46	7	-17	7	45	8	4	16	65	17	-7
2	171	7	2	13	339	12	23	11	63	6	7	8	127	6	-1	18	104	9	3
4	80	7	-8	15	135	6	4	12	339	12	3	10	43	8	-4	20	88	13	2
7	66	8	-7	16	276	10	-1	13	326	11	-8	12	56	7	9	21	93	8	8
8	85	8	-9	17	371	12	2	16	66	7	1	15	56	9	12	23	72	11	27
10	135	7	-1	19	48	10	6	18	81	9	-2	16	114	7	1	H,L=	6,	11	
H,L=	5,	18		21	77	12	-1	20	121	7	-7	22	67	8	4	1	73	6	-2
0	180	8	-0	22	155	10	-5	21	120	6	-15	H,L=	6,	8		2	194	7	-2
3	75	9	11	23	86	8	-1	23	74	9	6	0	140	5	9	3	68	7	-17
4	61	12	6	25	167	8	1	26	69	8	-1	1	44	7	11	4	176	6	-13
5	170	8	1	H,L=	6,	2		H,L=	6,	5		2	169	6	-3	5	169	6	-6
8	112	7	-3	0	291	10	-34	1	60	9	-45	3	268	9	-6	6	137	6	-12
10	52	10	10	1	216	8	28	2	409	14	20	4	102	5	-4	7	141	6	7
H,L=	5,	19		3	567	19	27	3	430	14	1	5	129	6	-14	8	102	6	-11
2	91	7	-1	4	96	5	-18	4	371	12	43	6	62	6	-5	9	108	6	12
3	72	10	18	5	248	8	24	5	143	5	0	7	84	5	20	10	177	7	-14
6	46	12	17	6	214	7	6	6	90	6	-5	8	162	7	5	11	65	8	-4
7	63	16	-16	7	370	12	10	7	91	4	-9	9	139	6	-5	12	51	10	-7
9	51	12	13	8	48	6	7	8	389	13	17	11	97	5	7	14	74	12	-0
H,L=	5,	20		9	108	5	7	10	266	9	-13	12	174	7	-17	15	187	7	-16
0	118	8	1	11	332	11	-6	11	243	9	-13	13	118	6	-5	16	96	12	-5
2	81	7	11	12	84	7	1	14	81	8	-12	15	71	7	-2	18	72	13	8
3	83	10	-6	13	170	7	9	15	110	5	8	20	77	9	35	19	63	14	-1
H,L=	6,	0		15	157	7	-6	16	281	10	4	23	48	11	35	20	59	14	-1
0	399	13	97	18	79	7	-2	17	52	10	4	H,L=	6,	9		22	73	11	1
1	321	11	20	19	64	8	3	18	49	10	5	1	63	6	-10	H,L=	6,	12	
2	198	7	-42	20	63	15	-11	19	89	11	6	2	214	7	-19	0	229	8	5
3	379	13	27	21	153	7	2	21	66	8	1	3	193	7	16	1	84	6	-9
4	305	10	10	H,L=	6,	3		22	153	7	9	4	279	9	21	2	115	5	2
5	233	8	-19	1	282	9	9	23	124	8	8	5	144	6	-1	3	130	6	-2
6	603	20	58	2	61	4	57	H,L=	6,	6		6	99	6	-2	4	44	10	14
7	298	10	1	3	231	8	-32	0	475	16	22	7	187	7	-16	5	114	6	-0
8	82	4	22	4	57	6	-19	1	87	4	-4	8	154	6	-3	6	84	6	10
9	123	5	-9	5	79	5	12	2	231	8	-17	9	133	6	17	7	87	8	11
10	41	9	-3	7	196	7	12	3	90	4	9	10	222	8	-14	9	71	7	-5
11	521	18	-2	8	144	5	-8	4	125	5	-23	11	184	7	-8	10	48	11	18
12	405	14	-18	9	218	8	3	5	192	7	-21	13	57	12	2	11	94	7	-6
15	267	11	-6	10	121	5	-9	6	404	14	4	14	150	7	5	12	84	9	-7

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
13	211	8	2
14	109	9	3
18	63	10	7
19	92	7	4
20	62	12	21
21	107	8	-6
H,L=	6,	13	
1	113	6	-4
3	74	7	25
5	92	8	-8
6	159	7	5
7	147	6	-1
8	59	12	11
9	210	8	-4
10	74	13	7
14	65	7	-5
15	134	6	7
16	52	14	3
17	123	8	2
19	81	7	-5
H,L=	6,	14	
0	90	8	9
1	169	7	-2
3	125	6	4
5	173	7	12
6	109	6	9
7	172	8	10
8	186	8	9
9	63	16	-4
10	69	7	6
11	138	6	-7
12	147	6	-0
13	78	7	-9
14	64	10	-1
15	99	11	16
18	65	9	10
19	153	7	-1
H,L=	6,	15	
1	254	9	2
2	131	8	4
3	52	13	14
4	139	7	13
7	99	8	-0
8	112	6	-5
9	251	9	1
10	182	7	7
14	103	8	3
16	79	11	3
17	141	7	1
H,L=	6,	16	
0	221	8	-14
1	152	8	4
3	109	8	2
4	59	8	14
5	109	7	-1
6	120	6	-3

K	FOB	SG	DEL
7	121	6	-1
8	126	6	-7
10	94	14	-0
11	128	6	3
12	66	9	1
13	62	10	5
H,L=	6,	17	
1	122	7	-0
3	81	8	3
4	69	7	15
6	44	12	20
9	102	8	7
10	78	19	8
H,L=	6,	18	
1	61	8	12
2	50	10	15
3	90	10	2
5	67	11	19
6	46	12	-9
H,L=	6,	19	
2	62	13	8
4	99	8	15
6	55	15	-1
8	74	11	8
H,L=	7,	1	
1	97	7	16
4	60	7	-3
5	142	5	-19
8	95	5	15
9	212	7	20
10	59	9	-6
11	108	5	-16
12	124	5	-0
13	145	6	-26
15	141	6	6
17	187	7	7
21	63	10	-1
22	56	13	10
H,L=	7,	2	
0	92	6	-16
1	393	13	-15
2	336	11	-37
3	103	8	-12
4	82	5	-26
5	133	5	16
6	146	6	1
7	443	15	-9
8	45	9	-4
9	129	5	-15
10	229	8	5
11	407	14	-8
12	224	8	-13
13	179	8	1
14	69	6	-3
15	192	7	6
16	83	6	-6

K	FOB	SG	DEL
17	278	10	-1
18	63	12	9
19	95	6	3
20	96	9	-9
21	54	16	-31
H,L=	7,	3	
1	395	13	24
2	108	6	22
3	291	10	-12
4	139	6	-2
5	366	12	27
7	90	4	-1
8	181	7	12
9	563	19	3
10	194	7	-7
11	272	9	-15
12	170	6	22
13	275	10	7
14	114	5	-7
15	116	7	1
17	180	7	3
19	69	9	-3
20	89	7	11
21	139	6	4
25	82	10	-0
H,L=	7,	4	
1	221	8	5
2	353	12	-11
3	245	8	7
4	103	4	-6
6	113	5	2
7	484	16	-12
9	178	7	-15
10	158	6	-21
11	347	12	-24
12	154	6	11
15	181	7	-14
16	165	7	7
17	84	9	-8
19	97	10	-8
20	90	9	3
22	53	10	-3
25	52	13	12
H,L=	7,	5	
1	89	4	11
2	173	6	-6
3	217	8	-4
4	152	6	-3
5	52	6	-16
6	111	5	10
7	202	7	15
8	90	5	4
9	185	7	3
10	44	10	1
11	143	6	11
12	205	7	9

K	FOB	SG	DEL
14	94	6	5
15	190	8	-1
17	105	8	4
18	84	9	-2
19	90	8	-5
20	125	9	-5
22	63	11	-9
23	54	10	5
25	106	9	3
H,L=	7,	6	
0	296	10	35
1	194	7	-11
3	193	7	7
4	112	5	17
5	390	13	-1
7	139	5	2
8	203	7	12
9	111	5	-6
10	84	5	3
11	62	8	-13
12	61	7	6
13	297	10	2
16	128	6	4
17	108	8	-6
21	188	8	15
23	95	7	-1
24	58	11	13
25	71	8	2
H,L=	7,	7	
1	69	5	-18
2	208	7	-30
3	351	12	-2
5	290	10	4
6	188	7	3
7	353	12	-15
9	182	7	-13
10	228	8	-7
11	345	12	-4
12	89	6	13
14	67	7	11
15	256	9	-6
16	99	7	-1
18	112	11	0
19	67	7	-1
20	118	7	3
21	105	8	-8
23	162	7	-2
H,L=	7,	8	
0	297	10	8
1	211	7	-15
3	174	7	-11
4	69	6	-1
5	591	20	-1
7	260	10	-12
8	286	10	18
9	58	11	1

K	FOB	SG	DEL
10	165	7	7
11	104	7	15
13	343	12	10
14	49	11	-8
15	54	10	1
17	130	9	-1
18	143	7	4
21	133	6	-2
23	97	9	-11
H,L=	7,	9	
1	92	5	7
2	100	6	-3
3	261	9	13
4	136	5	-9
5	140	6	-5
6	187	9	0
7	339	11	-18
8	138	7	16
9	62	7	-3
10	196	8	-9
11	186	7	-3
12	91	6	-6
13	70	10	1
14	48	11	2
15	191	7	5
17	86	11	-2
22	75	10	21
23	89	12	5
H,L=	7,	10	
0	192	7	-12
1	119	6	0
2	125	6	-12
3	256	9	9
4	158	6	3
5	133	6	3
6	94	6	-9
7	246	8	-10
8	228	9	-14
10	85	8	-20
13	112	8	-3
14	113	6	12
15	87	16	6
18	68	10	-11
21	78	14	15
H,L=	7,	11	
1	197	7	16
2	62	7	-6
3	149	6	1
4	223	8	-1
6	102	6	0
7	45	11	29
9	282	10	1
10	116	7	19
12	73	10	13
13	52	10	-3
16	51	9	14

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
17	72	8	-5
19	76	10	12
21	96	9	6
H,L=	7,	12	
0	42	12	14
1	133	6	0
2	60	8	0
5	95	6	-17
6	125	7	6
7	188	8	-9
9	76	8	-1
11	149	7	-18
13	70	11	-5
14	102	6	-6
19	167	7	6
H,L=	7,	13	
1	83	6	-25
3	129	6	7
4	96	6	2
5	125	6	-8
9	191	7	10
11	69	13	-6
13	59	13	5
15	133	7	4
17	125	6	5
H,L=	7,	14	
0	107	9	6
1	130	6	4
3	117	6	2
5	155	7	7
9	62	12	6
11	144	7	-1
12	50	10	7
13	103	6	-2
14	53	10	-1
H,L=	7,	16	
1	141	6	-11
3	43	12	-12
4	70	9	5
5	58	9	-3
6	67	8	0
7	80	8	-13
11	96	8	9
H,L=	7,	17	
1	116	6	2
2	54	10	5
3	190	7	0
5	61	12	1
8	51	11	-6
9	123	8	-6
10	60	10	22
H,L=	7,	18	
5	66	12	-8
6	80	11	-13
7	76	8	-5
10	47	12	39

K	FOB	SG	DEL
H,L=	7,	19	
1	107	13	-16
4	97	15	4
H,L=	8,	0	
0	446	15	-14
1	608	21	16
2	158	6	-3
3	171	6	26
4	44	7	32
5	186	6	19
6	64	9	-9
7	201	7	-22
8	368	13	-12
9	155	6	14
10	264	9	-26
12	276	9	18
13	76	6	-12
14	120	8	16
15	207	7	-3
16	165	7	4
17	267	9	1
18	150	6	-4
19	155	10	2
21	193	7	-4
22	88	10	-8
24	111	6	-5
25	121	7	4
H,L=	8,	1	
1	63	5	-3
2	252	9	6
3	268	9	32
4	82	4	-22
5	167	6	-2
6	233	8	-1
7	246	9	-13
9	168	7	-0
10	442	15	2
11	218	8	9
12	256	9	16
13	65	6	1
14	106	7	-0
16	99	10	15
17	187	7	1
18	88	9	-3
20	193	8	4
21	86	11	-11
22	92	6	-10
H,L=	8,	2	
0	219	8	-1
1	253	9	23
2	331	11	38
3	111	5	1
4	112	5	3
5	117	5	-1
6	148	6	3
7	137	6	19

K	FOB	SG	DEL
8	361	13	-2
10	289	10	22
11	57	8	-12
12	85	6	13
16	131	6	-9
17	102	8	-3
18	148	7	-1
22	65	8	8
24	89	8	7
H,L=	8,	3	
1	37	9	17
2	72	11	7
3	103	6	21
4	299	10	-5
6	248	9	7
7	44	11	0
10	134	6	-3
11	87	6	3
12	196	7	3
13	153	6	-2
14	157	7	11
15	150	7	5
17	45	12	-13
19	55	14	15
20	115	7	-2
22	105	6	6
H,L=	8,	4	
0	146	7	-24
1	445	15	11
2	380	13	27
3	81	6	-4
4	125	5	9
5	211	7	-7
6	324	11	-2
7	263	9	18
8	195	7	13
9	105	7	-0
10	153	7	6
11	159	6	8
12	246	9	-5
13	129	6	-6
15	95	8	-5
16	77	8	-3
17	132	6	3
19	76	16	-12
20	66	8	0
21	111	6	-2
23	63	11	27
25	69	11	3
H,L=	8,	5	
1	154	6	-11
2	86	6	-3
3	357	12	31
4	318	11	-17
5	135	8	-1
6	178	7	-13

K	FOB	SG	DEL
7	211	8	1
8	154	6	-5
9	238	8	1
10	135	6	9
11	269	9	-11
12	59	10	-7
13	83	6	5
14	124	7	-17
15	106	6	10
16	55	13	9
17	122	6	2
21	135	6	4
22	86	9	7
23	97	7	-3
H,L=	8,	6	
0	158	6	-29
1	243	9	-9
3	38	8	33
4	39	9	5
5	198	8	-1
6	260	10	10
7	175	6	-13
9	79	5	7
10	104	7	14
12	153	7	-2
14	62	8	-16
15	147	7	-4
16	58	14	-4
17	86	8	-2
19	142	7	5
20	49	10	27
21	136	7	7
H,L=	8,	7	
1	43	12	6
3	151	6	5
5	127	6	7
7	246	8	-17
8	56	11	-23
9	50	11	12
10	96	9	1
11	128	6	-6
13	90	9	-14
21	67	11	20
H,L=	8,	8	
0	162	7	12
1	90	7	6
2	239	8	21
3	72	6	-8
4	162	6	19
6	94	5	14
7	207	7	1
8	65	9	15
9	88	7	-2
10	123	6	-13
11	62	9	-0
12	111	6	-4

K	FOB	SG	DEL
13	136	7	3
14	76	7	8
20	56	13	16
H,L=	8,	9	
1	103	6	12
3	214	8	8
4	193	7	4
5	167	7	-0
6	55	8	-6
8	140	6	7
9	283	10	-5
11	176	7	6
12	83	7	4
14	115	8	-1
15	96	17	4
16	70	10	-7
21	88	9	8
22	77	10	-1
H,L=	8,	10	
0	79	6	9
1	171	7	8
2	183	9	-8
3	50	11	-7
5	253	9	8
6	234	9	3
7	184	7	6
8	52	10	7
9	87	6	18
10	68	10	16
11	130	6	8
12	141	7	3
13	143	14	-0
14	75	21	1
16	106	7	0
19	116	6	-1
H,L=	8,	11	
1	106	6	1
2	54	13	-10
3	87	6	-1
4	183	7	-5
5	86	6	-5
8	106	6	-1
9	91	9	8
11	71	12	7
12	129	10	10
14	109	8	-3
15	101	8	6
17	90	7	6
18	71	8	-1
20	105	8	11
21	60	13	6
H,L=	8,	12	
0	76	12	-18
1	111	7	4
2	72	14	-0
3	144	6	8

TRUCTURE FACTCRS CONTINUED FC#
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
5	62	8	5	4	88	16	-13	15	89	6	7	18	69	7	7	3	49	10	17
6	127	7	-2	6	64	10	6	16	152	7	7	19	171	7	-2	4	80	7	-9
7	131	6	-12	9	65	12	14	18	74	12	1	20	97	9	-4	5	313	11	-1
8	134	6	-6	10	63	10	8	19	62	12	4	23	70	8	15	7	90	7	-0
14	101	11	-6	H,L=	8,		18	20	95	6	0	H,L=	9,		7	8	121	6	-14
16	143	7	6	1	65	11	25	H,L=	9,		4	1	105	8	-10	10	72	11	-13
18	96	7	-2	2	50	12	-9	0	462	15	-10	4	296	10	-2	11	108	11	15
19	102	7	4	6	63	14	3	1	68	8	6	6	45	12	-1	13	73	13	4
H,L=	8,		13	7	52	13	2	3	117	5	-2	7	187	7	-7	14	94	6	2
2	158	7	2	H,L=	8,		19	4	135	5	8	8	170	7	1	16	87	9	-1
4	134	6	6	3	89	7	13	6	47	11	-5	9	204	8	-6	17	53	9	9
5	53	13	19	H,L=	9,		1	7	180	7	4	10	51	14	49	18	55	9	5
6	147	8	10	1	131	6	-2	8	202	7	-16	11	111	6	2	H,L=	9,		11
7	67	12	-3	2	164	6	-22	9	117	7	-1	12	202	8	3	2	166	7	-4
9	73	9	4	3	83	6	11	10	161	8	-12	13	109	8	-3	3	161	6	-0
10	75	10	4	4	46	7	-9	11	81	13	3	14	160	7	-0	6	188	7	-5
11	51	14	6	5	82	6	16	12	63	8	11	15	74	13	-8	7	178	7	1
12	141	8	-1	6	72	7	3	13	111	6	-7	16	94	16	-13	8	94	10	-5
13	53	14	4	7	97	5	-4	17	51	11	-0	17	174	9	2	10	61	16	7
14	87	9	-9	8	202	7	-6	18	155	9	2	20	94	6	-1	12	83	8	-1
18	77	8	8	9	112	6	14	19	76	9	3	22	146	7	-14	13	76	11	-7
H,L=	8,		14	10	189	7	-4	20	61	16	-6	H,L=	9,		8	16	109	8	-2
0	250	9	-4	11	139	6	7	21	105	6	4	1	76	6	-5	20	57	10	5
7	147	10	0	13	84	6	-1	H,L=	9,		5	2	308	11	-8	H,L=	9,		12
8	182	7	-3	15	100	8	3	1	246	9	5	3	139	6	4	0	86	6	13
9	57	9	-3	16	83	9	9	2	86	8	-2	5	68	8	-6	2	45	12	5
10	138	8	-5	17	113	6	-5	3	100	5	7	6	252	9	10	4	64	9	-6
11	114	8	6	19	78	14	7	4	197	7	-16	7	252	9	9	5	128	6	0
13	94	9	-8	22	55	9	17	5	55	7	-15	8	84	6	-3	6	84	7	1
14	62	12	4	H,L=	9,		2	7	97	6	-4	9	163	6	-6	8	151	7	2
16	101	7	6	0	335	12	9	9	46	9	-14	10	109	7	-2	12	101	10	-10
H,L=	8,		15	1	246	9	-3	10	206	9	3	11	91	6	-9	13	83	6	1
1	92	7	8	2	217	7	4	11	191	7	-6	12	174	7	-2	18	77	11	-5
2	198	8	3	3	325	11	13	12	130	6	2	14	126	8	2	19	67	14	10
3	152	8	2	5	56	8	22	13	60	8	-8	15	69	11	-6	H,L=	9,		13
4	91	7	2	6	141	6	10	14	124	6	0	16	118	9	2	1	59	9	9
5	106	6	3	8	244	8	-7	17	125	8	-7	19	101	6	-6	2	121	11	-7
6	125	8	-16	9	98	6	6	18	89	10	4	20	119	6	-3	3	55	9	21
8	103	6	3	10	74	19	1	20	105	13	16	22	58	10	-1	4	82	7	-8
9	141	6	-5	12	222	8	-3	22	113	8	1	H,L=	9,		9	5	99	13	-0
10	100	7	-1	13	172	6	-2	H,L=	9,		6	1	172	7	18	10	118	7	6
12	134	7	16	18	126	6	-18	0	315	11	-3	2	64	11	-9	13	57	14	-10
13	69	12	-7	20	128	9	1	1	64	6	-3	3	70	7	9	14	59	13	21
14	68	11	9	21	82	9	-7	2	290	10	-8	4	219	8	-10	15	91	9	-5
15	117	10	-5	H,L=	9,		3	4	121	7	-7	5	67	9	-12	16	80	10	9
H,L=	8,		16	1	134	6	22	5	39	11	1	6	177	7	-0	H,L=	9,		14
0	213	8	10	2	229	8	-1	6	304	10	-0	7	140	6	-10	0	98	9	-5
1	123	6	-5	3	292	10	2	8	135	6	17	8	43	13	7	1	80	11	-19
2	93	13	-13	5	174	7	4	9	154	6	-15	9	204	8	-19	3	53	13	-5
3	48	13	2	6	110	5	1	10	169	7	5	10	62	11	11	6	54	9	1
5	80	8	-7	7	59	6	-1	11	102	6	-3	12	198	8	4	8	75	8	3
10	123	6	12	8	252	9	-1	12	198	7	-3	14	113	7	9	H,L=	9,		15
11	83	12	-9	10	415	14	12	14	91	6	0	17	66	9	-2	2	49	11	-9
13	91	9	7	11	264	9	2	15	112	6	-4	H,L=	9,		10	5	56	9	11
H,L=	8,		17	13	115	8	13	16	98	10	24	1	56	8	11	7	54	11	8
2	66	9	-11	14	72	10	6	17	101	7	5	2	67	10	24	H,L=	9,		16

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
0	94	7	1	24	72	12	-14	4	118	7	-14	2	154	6	6	13	106	9	-2
1	67	8	1	H,L=	10,		2	6	77	6	16	3	126	6	-4	15	82	11	-0
5	61	8	-4	0	181	6	12	7	124	7	-10	4	45	12	8	H,L=	10,		15
6	65	8	2	1	61	9	-2	8	80	12	3	6	88	9	-2	1	140	6	9
8	63	13	-12	2	54	7	13	11	68	11	-2	8	97	8	-3	2	70	11	1
9	59	14	9	3	44	8	17	12	131	6	1	9	67	13	-1	3	67	8	3
H,L=		9,	17	4	71	7	4	13	49	12	-10	11	84	10	-1	4	89	6	9
1	44	13	33	5	362	12	23	16	158	6	-7	12	127	7	-3	5	65	11	20
2	108	12	-1	6	62	9	5	17	84	9	-5	13	73	12	-5	7	88	9	-10
3	96	7	1	9	107	5	1	18	78	7	-13	14	65	10	-14	8	65	12	12
4	58	12	22	10	57	11	-2	22	122	8	1	18	72	8	-3	9	116	6	13
7	75	10	19	11	171	7	8	23	54	15	50	19	81	7	6	10	127	6	2
8	60	13	15	13	198	9	2	H,L=		10,	6	20	104	19	-0	11	50	11	-11
10	64	13	-5	14	59	9	8	0	257	9	10	H,L=		10,	11	H,L=		10,	16
H,L=		9,	18	18	50	14	1	1	79	8	7	1	121	6	-7	3	118	6	-10
0	127	7	3	19	151	6	9	2	154	7	2	3	47	12	8	4	45	13	15
H,L=		10,	0	21	88	11	-6	3	195	7	-7	4	155	6	4	5	87	11	-4
0	394	13	-10	23	71	12	-9	5	62	8	9	7	132	7	7	8	95	11	0
1	87	6	-4	H,L=		10,	3	6	92	7	8	10	80	12	-15	11	51	12	7
2	96	7	-19	1	328	11	-4	7	78	8	1	11	86	7	-5	H,L=		10,	17
3	263	9	1	2	124	6	7	10	64	11	-4	12	88	6	11	1	76	11	-10
4	57	8	19	3	139	6	-5	14	102	8	16	15	58	17	-2	5	72	11	16
5	168	7	14	4	61	14	0	15	130	16	16	16	52	13	4	7	70	16	17
6	183	7	-5	5	54	7	-29	17	52	14	13	17	115	10	6	H,L=		11,	1
7	240	9	5	6	63	10	20	18	72	7	8	18	88	7	4	3	123	7	-4
8	168	7	16	7	251	9	23	20	135	6	5	19	55	10	1	4	158	8	4
9	102	5	3	8	147	7	10	22	56	15	1	H,L=		10,	12	9	111	6	5
11	248	9	1	9	196	7	11	H,L=		10,	7	1	105	7	0	10	148	6	-6
13	233	9	-7	11	214	8	-16	4	174	8	6	2	71	16	4	11	111	8	2
14	171	7	-5	12	80	6	-5	6	116	6	-2	3	132	6	-4	15	86	12	9
18	83	8	-12	16	66	13	-4	9	102	8	7	5	163	7	-2	20	57	12	21
19	103	8	6	17	111	16	-12	13	54	10	-2	11	100	6	5	H,L=		11,	2
20	116	6	-4	19	48	11	-10	18	93	6	14	12	45	11	31	0	53	8	-31
21	110	8	-7	22	80	20	1	21	71	20	5	13	86	8	-12	1	82	14	-19
23	105	7	-7	23	98	8	32	H,L=		10,	8	15	93	9	-4	3	85	9	-10
24	77	8	2	H,L=		10,	4	3	75	7	-6	H,L=		10,	13	4	78	9	8
H,L=		10,	1	0	241	8	-5	8	112	6	6	1	177	7	23	6	304	10	-11
1	156	6	-29	1	128	6	6	9	119	8	-13	6	92	6	1	7	133	7	-8
2	213	7	-5	2	79	7	10	12	61	10	-5	7	123	7	7	8	133	7	-7
3	182	7	0	3	97	6	-4	19	54	10	-2	9	83	10	-4	9	177	7	-5
4	99	6	3	4	62	9	16	H,L=		10,	9	10	44	12	10	12	213	10	13
5	133	6	23	6	194	7	-8	1	175	7	0	11	86	7	-13	13	52	12	4
6	46	12	11	7	46	13	29	2	161	6	-6	13	82	9	10	14	189	8	9
7	162	6	1	8	86	8	-0	3	124	7	6	15	88	10	5	15	67	19	-16
8	149	7	4	11	173	9	1	5	45	12	-14	16	50	12	-2	19	124	6	-3
9	424	14	18	12	77	9	13	6	155	7	-4	H,L=		10,	14	20	55	14	13
10	148	9	5	13	90	8	-8	8	102	6	-11	0	66	8	10	H,L=		11,	3
12	62	11	-10	14	181	7	12	9	205	8	-1	1	92	8	-5	1	70	9	-17
14	83	9	23	18	60	9	-3	10	69	16	-4	3	180	7	10	2	59	7	-4
15	193	8	13	19	80	9	-3	13	83	16	-5	4	56	8	13	3	61	11	-11
16	177	7	13	20	125	6	5	14	71	21	-3	5	84	9	8	4	432	15	-16
17	74	10	-3	21	92	9	-6	16	107	8	-6	6	73	7	3	6	63	15	7
18	53	11	8	22	53	15	32	18	49	11	12	7	91	6	-9	7	127	9	-7
19	77	8	-2	H,L=		10,	5	19	82	7	11	8	103	7	-10	9	103	6	-13
22	76	10	4	1	237	9	-10	H,L=		10,	10	11	94	9	1	10	214	8	-1
23	94	9	-0	2	190	10	9	0	73	9	-4	12	88	9	-11	11	78	7	23

TRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
14	184	8	-8
16	129	7	8
17	152	7	1
22	99	9	3
H,L=	11,		4
0	51	13	16
1	153	7	-3
2	99	6	8
3	52	12	3
4	63	13	-16
5	152	7	-0
6	176	7	-13
8	68	7	13
9	78	7	6
10	56	13	-2
11	97	7	-1
12	145	7	-15
13	140	7	5
14	174	8	6
16	75	18	-0
19	142	7	5
H,L=	11,		5
1	375	13	8
2	92	6	7
3	116	8	11
4	147	7	10
6	69	7	-18
7	180	7	-3
8	127	6	15
9	177	7	6
10	70	11	-16
11	219	8	-2
14	117	7	3
17	102	6	4
20	74	11	-9
H,L=	11,		6
0	262	10	-5
3	145	7	-5
4	84	8	1
5	152	7	4
8	146	6	-4
10	58	13	-8
11	100	10	-6
13	140	6	12
16	89	6	-9
18	132	6	2
20	50	13	-3
21	110	12	7
H,L=	11,		7
1	254	11	3
2	283	12	7
3	213	8	-5
4	87	9	-24
5	74	11	-8
6	117	11	1
7	149	6	3

K	FOB	SG	DEL
8	66	12	0
9	198	7	9
10	200	8	-2
11	138	8	-8
12	65	8	5
15	88	12	-10
16	120	6	-4
18	111	8	-8
19	105	7	-2
20	85	8	2
H,L=	11,		8
0	420	15	-1
3	191	7	8
5	57	13	3
6	96	8	-5
7	81	9	16
8	203	8	-4
9	52	12	13
10	109	8	-7
11	131	8	-0
12	135	7	-0
13	140	6	-2
16	66	9	8
18	126	8	-5
H,L=	11,		9
2	173	8	-2
5	67	10	6
6	181	8	-7
7	59	15	5
9	91	11	-4
10	120	10	8
11	74	7	-3
12	87	11	-7
13	116	7	-2
15	88	8	-3
16	90	13	-11
19	73	14	-7
H,L=	11,		10
2	138	9	-2
3	94	8	-1
5	149	8	-4
8	117	10	11
10	53	14	10
11	126	7	-2
14	46	13	8
19	69	16	32
H,L=	11,		11
2	53	11	15
4	141	8	-3
6	83	10	6
7	116	8	5
11	55	10	21
12	94	6	-2
13	68	11	2
14	68	8	3
16	68	12	0

K	FOB	SG	DEL
17	122	9	12
H,L=	11,		12
0	111	8	3
1	85	9	-3
2	100	9	-8
6	97	7	8
7	108	9	-5
11	48	12	-7
14	113	7	1
15	57	16	-27
H,L=	11,		13
1	69	10	13
2	82	9	-6
4	77	10	-2
8	102	6	3
9	89	9	-4
10	57	14	-9
12	83	7	6
H,L=	11,		14
2	47	11	18
3	47	11	20
6	88	9	3
7	55	9	11
8	77	13	-5
12	64	9	3
H,L=	11,		15
3	52	11	-1
6	84	8	-4
H,L=	11,		16
0	77	11	-12
2	58	9	22
4	65	13	-15
6	61	10	-3
7	67	10	4
H,L=	11,		17
1	76	11	30
2	84	8	8
4	87	13	10
H,L=	12,		0
0	69	10	4
1	121	7	20
3	102	7	2
4	215	12	11
5	268	10	15
6	297	11	7
7	254	9	2
8	189	7	4
9	102	8	-11
10	79	10	-8
11	95	10	2
12	84	7	9
13	106	7	6
14	218	8	4
15	104	16	-7
16	115	9	-4
18	61	12	-0

K	FOB	SG	DEL
19	102	8	16
H,L=	12,		1
1	229	10	2
3	88	10	-10
4	372	14	6
5	203	9	5
6	325	11	18
7	62	10	23
9	110	8	3
12	151	7	10
13	54	11	-4
14	159	10	-14
15	144	17	-4
17	88	16	0
18	61	13	28
19	52	13	17
21	56	12	2
22	135	6	13
H,L=	12,		2
0	66	10	25
2	206	7	-9
3	80	9	4
4	56	13	-11
5	44	12	9
6	200	8	-9
8	154	12	-12
9	87	9	3
10	77	20	8
11	56	10	12
12	76	8	4
13	58	10	15
14	140	9	14
16	110	8	-6
18	62	13	-9
19	63	10	-0
H,L=	12,		3
2	125	6	-8
3	103	6	3
4	116	7	16
7	75	11	-14
9	54	14	2
10	159	7	-10
11	88	9	3
12	92	7	12
14	87	19	5
18	62	12	13
20	121	11	-7
21	60	9	14
H,L=	12,		4
0	289	10	1
1	135	7	-13
2	113	8	-6
3	46	11	-10
4	152	8	-9
5	117	6	-5
6	71	7	1

K	FOB	SG	DEL
7	159	7	-0
8	122	7	11
10	139	7	-3
12	60	16	5
13	107	12	12
15	77	10	-1
16	63	8	3
17	80	11	13
18	146	7	13
19	55	11	-8
21	51	12	-11
H,L=	12,		5
1	171	7	5
2	243	10	6
3	199	7	-8
4	118	8	1
5	182	7	5
7	98	18	10
10	111	8	2
12	69	13	-3
15	163	8	-5
16	61	14	-19
17	92	7	-1
18	99	9	10
20	106	7	-7
21	72	10	-2
H,L=	12,		6
0	329	11	4
1	165	7	-5
3	50	11	7
4	90	9	7
5	229	9	4
6	76	8	26
7	61	13	-0
10	76	8	-8
11	94	9	-4
13	120	11	14
16	61	9	1
17	68	12	35
18	81	9	14
19	62	16	7
H,L=	12,		7
2	168	8	6
3	93	7	-14
5	118	7	-11
15	47	13	7
16	72	10	2
H,L=	12,		8
1	138	10	3
5	58	16	-15
7	96	8	-1
8	116	11	17
H,L=	12,		9
2	98	7	-4
3	135	6	-5
4	72	11	7

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL
5	61	15	6
9	84	25	2
10	93	9	-12
11	88	10	-20
12	78	10	-6
14	80	7	-3
15	100	8	6
16	59	14	8
17	69	13	-12
H,L= 12, 10			
0	232	9	-1
1	142	13	4
4	54	15	17
5	73	11	26
7	128	6	7
8	123	8	-2
10	135	8	6
11	72	11	9
12	74	10	-2
13	126	7	7
15	69	11	3
H,L= 12, 11			
2	166	7	6
3	155	7	8
4	93	13	10
5	63	15	-8
6	107	9	-3
8	101	8	9
10	78	16	2
11	118	8	8
12	76	8	-6
16	86	7	3
H,L= 12, 12			
0	141	6	11
2	106	6	2
4	79	10	5
5	99	9	-11
8	121	9	6
10	93	6	0
H,L= 12, 13			
2	144	7	-4
4	148	8	9
6	84	7	-5
8	49	11	5
9	83	10	-5
12	84	7	-3
H,L= 12, 14			
0	84	8	4
1	102	6	-2
2	117	6	8
5	60	9	10
6	105	10	-1
7	75	11	-6
8	63	9	2
11	74	8	10
12	54	12	-1

K	FOB	SG	DEL
H,L= 12, 15			
3	84	7	1
4	157	8	6
8	101	7	2
9	104	7	3
H,L= 12, 16			
2	85	7	-2
6	143	8	9
H,L= 13, 1			
1	161	6	5
2	117	6	3
3	157	10	-4
4	69	12	13
5	157	6	-9
6	63	9	18
7	62	14	-5
9	147	6	-1
11	65	15	2
12	76	8	2
15	111	11	-4
H,L= 13, 2			
0	145	7	4
1	143	6	11
5	343	12	-8
6	60	13	8
7	212	8	-1
9	133	6	-2
11	154	6	-8
13	219	9	1
16	107	8	5
17	65	9	-2
19	96	7	8
H,L= 13, 3			
1	160	6	-1
2	157	7	-0
3	162	7	-19
4	55	15	11
5	241	8	-16
6	90	9	17
7	56	16	-28
8	88	10	-10
9	176	8	4
11	103	10	-10
12	95	17	3
14	48	12	-16
15	259	9	3
18	59	15	-22
20	53	11	-5
H,L= 13, 4			
0	144	8	-11
1	47	13	-9
2	174	7	-1
3	124	6	-11
4	110	7	-1
5	225	8	-3
8	130	8	-9

K	FOB	SG	DEL
9	55	15	2
11	83	18	-11
13	193	7	3
16	114	10	8
18	64	14	-5
H,L= 13, 5			
2	156	7	-5
4	149	8	-6
5	66	14	-10
6	120	6	-0
7	64	10	8
9	87	20	4
12	97	11	5
14	91	9	-6
15	87	7	2
17	60	15	-3
20	71	16	-7
H,L= 13, 6			
0	129	9	7
1	187	8	1
2	187	8	-7
3	100	9	7
4	55	15	26
6	108	10	-13
7	147	6	-11
8	142	8	-10
10	108	8	0
11	134	10	1
12	81	9	-11
15	78	7	18
16	91	7	-11
18	65	13	5
19	93	10	-19
H,L= 13, 7			
1	245	9	-8
2	60	15	16
3	207	8	2
4	180	10	-16
5	93	7	-1
6	151	8	6
9	237	9	8
12	103	6	-9
13	75	7	-4
14	76	10	5
15	94	9	-2
17	146	7	3
18	64	13	14
H,L= 13, 8			
0	114	7	-9
1	191	8	-8
2	73	12	17
3	78	11	3
4	68	13	1
5	75	14	3
6	147	7	2
7	189	8	-7

K	FOB	SG	DEL
8	75	17	-3
10	125	8	7
11	208	8	-4
13	97	7	-5
14	48	13	-18
15	86	19	-10
16	60	10	-4
17	77	10	22
H,L= 13, 9			
1	103	16	-11
4	114	12	-5
5	76	15	-9
9	119	6	5
10	93	10	2
12	76	17	5
13	67	8	5
14	55	14	15
17	92	10	-9
H,L= 13, 10			
3	78	17	2
6	66	8	8
7	67	12	-2
8	89	9	5
9	71	8	13
11	60	14	5
12	59	14	12
16	72	12	6
H,L= 13, 11			
3	88	10	-25
4	71	8	-1
5	49	11	15
7	75	7	1
8	69	8	20
10	114	8	-3
14	64	13	-5
15	103	10	2
H,L= 13, 12			
0	82	7	7
1	156	9	-15
5	138	6	-1
7	116	6	-6
8	64	11	-6
13	126	8	-0
H,L= 13, 13			
3	189	8	-4
5	84	7	8
6	63	9	7
7	84	10	-2
9	104	9	-2
11	108	9	-3
H,L= 13, 14			
7	119	7	3
H,L= 14, 0			
0	339	12	-0
1	59	10	8
2	92	9	4

K	FOB	SG	DEL
3	182	8	-6
5	436	15	-2
6	209	8	-1
7	59	16	-18
8	102	9	-3
9	66	11	19
10	119	9	-1
12	140	8	-10
13	202	9	-6
14	98	24	-6
15	71	12	-5
18	121	7	11
19	66	13	1
H,L= 14, 1			
2	143	6	-6
3	158	8	-5
4	182	8	-10
5	63	12	1
6	53	14	-8
7	208	9	-9
8	89	8	20
10	97	12	21
11	117	9	-5
13	59	10	-11
14	96	9	-3
15	145	8	3
16	127	8	11
H,L= 14, 2			
3	161	8	-8
5	171	7	-8
7	62	14	-11
11	82	16	3
13	138	8	3
H,L= 14, 3			
1	115	8	-3
2	49	13	6
4	119	7	2
7	88	12	-5
9	124	7	-9
14	55	15	-15
15	70	9	3
17	108	10	7
H,L= 14, 4			
0	152	7	-5
1	107	7	5
2	69	11	-1
3	64	10	-4
5	57	12	20
6	129	8	9
9	90	19	1
11	117	7	14
12	94	9	-2
14	105	16	-1
15	54	10	6
19	146	8	7
H,L= 14, 5			

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
1	143	7	10	1	92	10	-9	H,L=	15,		6	9	59	13	36	1	67	9	3
2	132	7	2	2	72	12	9	0	233	11	-10	10	76	13	8	5	65	13	-6
3	77	14	-2	5	56	11	-9	2	69	13	26	11	72	8	-5	8	109	19	-12
4	220	9	7	8	58	15	2	3	138	8	-0	12	92	8	8	H,L=	16,		11
8	81	12	-3	H,L=	14,		14	5	151	8	-9	13	48	13	-17	2	115	8	12
9	148	7	12	0	149	8	-2	7	65	9	-8	14	118	8	7	3	50	13	23
10	120	6	-4	2	69	13	16	8	129	8	0	15	67	15	24	6	67	14	-3
14	114	8	8	3	85	13	-14	10	107	6	-3	H,L=	16,		1	H,L=	16,		12
16	78	11	-7	5	129	8	4	13	108	8	2	2	67	17	-2	0	156	8	11
17	133	8	2	H,L=	15,		1	14	71	12	16	4	185	7	2	H,L=	17,		1
H,L=	14,		6	2	79	14	-23	H,L=	15,		7	6	110	6	-3	4	80	8	-6
1	121	8	-7	4	149	9	-12	1	68	18	-3	9	58	14	-6	14	65	14	2
4	126	9	6	8	78	15	12	2	157	10	0	10	56	14	33	H,L=	17,		2
5	71	12	5	10	69	11	-3	5	72	8	12	12	156	7	4	1	69	12	1
6	202	10	-10	14	96	9	7	7	78	8	-5	14	81	10	-10	2	98	7	-17
8	78	9	2	16	84	9	-4	8	126	13	3	16	57	10	23	6	60	10	-5
11	78	11	-6	H,L=	15,		2	9	73	13	-16	H,L=	16,		2	12	86	11	6
12	108	9	6	0	262	10	-6	10	169	8	-4	0	104	18	-1	13	84	8	-5
14	55	10	-5	1	89	23	2	15	95	10	8	2	63	16	2	H,L=	17,		3
H,L=	14,		7	2	95	15	10	H,L=	15,		8	8	77	7	11	3	59	15	-5
1	96	16	-8	3	123	8	3	0	143	7	-7	10	101	9	-4	4	112	8	-3
13	66	15	11	6	144	19	5	3	73	9	4	14	72	9	6	7	84	7	7
H,L=	14,		8	8	78	11	0	5	132	6	8	16	64	17	12	9	55	11	3
0	117	11	-4	11	65	12	5	6	83	10	-14	H,L=	16,		3	11	101	8	-7
11	69	8	7	12	96	7	-1	8	156	8	-6	2	78	22	-14	13	54	13	-6
H,L=	14,		9	13	60	15	19	11	68	9	-3	7	45	12	21	H,L=	17,		4
2	84	7	1	14	165	10	-4	12	76	12	-3	12	85	17	-10	0	98	9	-5
3	68	12	11	15	52	12	1	13	71	13	2	H,L=	16,		4	6	115	8	1
4	72	11	-2	18	78	16	-0	H,L=	15,		9	0	135	8	-20	13	80	8	7
8	86	7	6	H,L=	15,		3	2	65	13	-6	5	96	9	-5	H,L=	17,		5
9	84	13	-7	1	126	16	-19	3	77	12	9	8	115	8	22	1	104	15	4
10	116	6	-2	3	97	15	3	6	57	10	4	13	73	12	0	2	79	8	-0
11	51	13	34	4	169	13	-2	7	89	21	26	H,L=	16,		5	4	106	8	14
12	60	10	15	8	78	11	-11	9	100	12	-3	2	94	17	-9	6	66	14	-7
H,L=	14,		10	10	104	14	-10	10	124	6	-4	8	67	19	-13	7	71	12	0
0	130	13	9	11	70	8	1	H,L=	15,		10	9	65	10	14	9	64	14	0
1	91	7	-4	12	114	7	-7	6	58	10	26	10	115	9	-14	11	79	14	8
4	96	9	7	13	80	12	21	8	52	11	38	11	78	13	8	12	77	9	-1
6	145	8	7	14	95	10	6	11	63	9	16	15	61	14	13	H,L=	17,		6
7	140	8	-3	16	86	8	-3	H,L=	15,		11	H,L=	16,		6	0	91	9	-1
11	98	7	-3	H,L=	15,		4	1	82	10	18	0	113	8	-10	7	63	14	-12
12	89	7	1	1	89	22	4	4	104	9	18	7	62	13	6	8	57	12	-11
14	75	11	11	3	175	9	-8	8	60	10	10	8	81	10	13	10	75	12	17
H,L=	14,		11	4	60	15	0	9	80	8	-8	13	61	13	-2	11	59	11	-7
1	115	6	-4	6	144	8	-4	H,L=	15,		12	H,L=	16,		7	H,L=	17,		7
2	106	6	-3	7	69	14	4	0	99	9	-3	2	64	13	12	1	106	7	-7
4	125	8	-0	11	50	12	-13	2	93	8	7	8	66	12	14	2	91	7	4
9	146	8	-3	12	81	10	11	4	64	14	-7	H,L=	16,		8	5	52	12	9
10	61	12	-3	13	102	9	10	6	130	7	-2	1	47	13	22	6	66	15	11
H,L=	14,		12	14	76	11	2	H,L=	15,		13	5	79	11	-5	8	54	12	-8
1	103	9	7	H,L=	15,		5	1	61	13	11	9	75	12	24	9	141	7	7
3	144	9	-4	1	91	23	-9	2	88	7	8	H,L=	16,		9	10	86	13	-9
5	90	10	13	7	100	8	3	4	111	12	4	3	58	12	7	H,L=	17,		8
7	117	8	1	11	61	11	1	H,L=	16,		0	10	93	8	-5	0	65	10	-2
11	59	11	-2	12	72	11	-0	2	180	8	-7	H,L=	16,		10	1	68	19	-17
H,L=	14,		13	15	92	10	3	6	93	7	-8	0	89	10	2	2	58	11	-3

STRUCTURE FACTORS CONTINUED FOR
ZR(2)SI(8)N(4)C(24)H(68)

K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL	K	FOB	SG	DEL
7	80	11	17	5	89	11	14												
8	117	9	-7																
9	69	10	16																
H,L=	17,	9																	
2	56	11	12																
6	93	11	12																
H,L=	17,	10																	
0	94	8	1																
2	49	13	21																
H,L=	18,	0																	
0	71	12	-2																
1	75	15	-8																
3	79	8	2																
5	151	15	-8																
7	86	11	2																
8	63	14	34																
H,L=	18,	1																	
1	74	11	31																
3	128	10	2																
4	60	11	3																
7	136	8	10																
10	59	17	-1																
11	122	9	8																
H,L=	18,	2																	
0	51	12	12																
3	75	11	13																
5	82	11	-5																
H,L=	18,	3																	
1	83	11	5																
4	59	10	28																
9	113	10	8																
H,L=	18,	4																	
1	82	11	3																
7	117	7	6																
H,L=	18,	5																	
1	85	11	-4																
2	62	11	2																
3	71	11	-2																
9	106	10	-18																
H,L=	18,	6																	
1	82	12	-17																
4	75	9	-1																
6	60	15	21																
H,L=	19,	1																	
3	74	14	-6																
H,L=	19,	2																	
5	111	10	-5																
6	110	8	7																
7	104	10	13																
H,L=	19,	3																	
1	68	14	32																
3	135	9	4																
4	74	13	-9																
5	95	11	2																
H,L=	19,	4																	
2	71	14	-9																

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