Title

BIS (PENTAMETHYLCYCLOPENTADIENYL) YTTERBIUM (II) AS A LEWIS ACID AND ELECTRON-TRANSFER LIGAND; PREPARATION AND CRYSTAL STRUCTURES OF [Yb(Me5C5)2(u-CO)x Mn(CO)5-x]y WHERE X AND Y ARE TWO AND X IS THREE AND Y IS INFINITE

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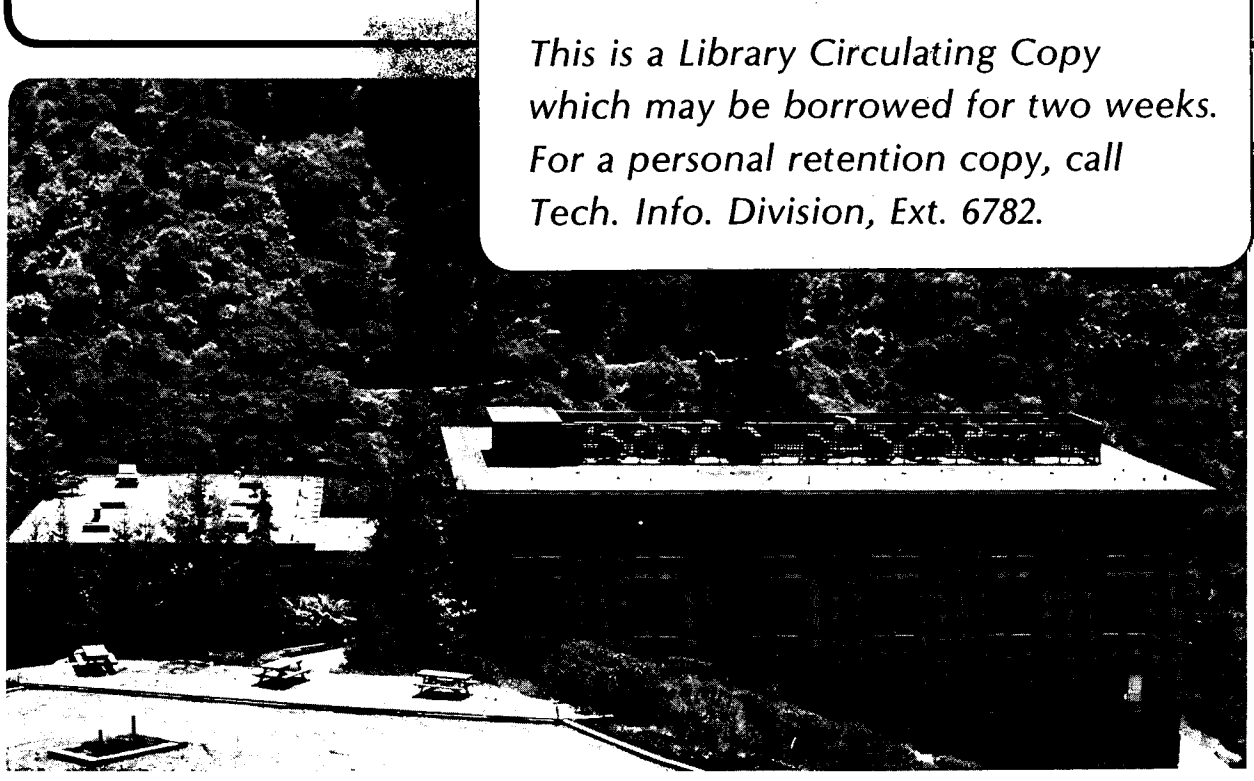

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Bis(Pentamethylcyclopentadienyl)Ytterbium (II) As A Lewis Acid and Electron-Transfer Ligand; Preparation and Crystal Structures of $[Yb(Me_5C_5)_2(\mu\text{-}CO)_x\ Mn(CO)_{5-x}]_y$ where X and Y Are Two and X is Three and Y is Infinite

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Abstract

The divalent ytterbium metallocene, $(Me_5C_5)_2Yb(OEt_2)$, reacts with $Mn_2(CO)_{10}$ to give a compound of composition $(Me_5C_5)_2YbMn(CO)_5 \cdot 1/4$ PhMe which was shown by an X-ray crystallographic study to be composed of a polymeric chain of $[(Me_5C_5)_2Yb(\mu\text{-}OC)_3Mn(CO)_2]$ units with dimeric units $[(Me_5C_5)_2Yb(\mu\text{-}OC)_2Mn(CO)_3]$ packed between the polymeric sheets. The toluene of solvation fills regular spaced voids in the network of dimer and polymer sheets. The space group is C2/m with a = 18.942(5)Å, b = 32.592(5)Å, c = 19.029(5)Å, β = 109.92(2)°, V = 11045(18)Å^3 and Z = 16. The contact ion-pair complex results from $(Me_5C_5)_2Yb$ acting as an electron-transfer reagent, $(Me_5C_5)_2Yb \rightarrow (Me_5C_5)_2Yb^+ + 1e^-$, and as a Lewis acid by way of Yb(μ-OC)Mn interactions. The solution and solid state infrared spectra are discussed relative to the alkali metal analogues. The rhenium carbonyl, $Re_2(CO)_{10}$, behaves similarily.

The concept of transition metal carbonyl basicity, the ability of the lone pair of electrons on the oxygen atom to act as a Lewis base, is well known.[1] In particular, Group IIIb compounds form acid-base complexes with the bridging carbonyl groups in, for example, $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ or $Cp_4Fe_4(\mu_3\text{-}CO)_4$.[2] The acid-base interaction leads to a reduction in the C-O stretching frequency, e.g., the bridging CO stretching frequency in $Cp_2Fe_2(\mu CO\text{-}A\ell Et_3)_2(CO)_2$ is lowered 113 cm^{-1} relative to that found in the acid-free complex.[2a,b] Carbonyl complexes whose solid-state structures do not contain bridging carbonyl groups and whose solution behavior is stereochemically rigid, e.g., $Mn_2(CO)_{10}$,[3] do not form complexes with aluminum compounds.[2b,d]

Early transition metal complexes also can act as Lewis acids towards metal carbonyls giving complexes with M-CO-M' interactions.[4] In these complexes the C-O stretching frequency also is lowered relative to that in the uncoordinated complex. In addition, it is generally observed that the M-C-O angle is essentially linear and the C-O-M' angle is less than 180°. In particular, the Mo-C-O bond angle is 178.8(4)° and the O-C-Ti angle is 144.3(3)° in $CpMo(CO)_2[\mu\text{-}CO\text{-}Ti(Me_5C_5)_2Me]$.[4d] The bond angles in the titanium complex are remarkably similar to that found in $Cp_2W_2(CO)_4[\mu\text{-}CO)_2\text{-}A\ell Me_2]$ in which the W-C-O and C-O-Aℓ angles are 172(2)° and 149(2)°, respectively.[5] Thus, the $Me_2A\ell^+$ and $(Me_5C_5)_2TiMe^+$ groups have similar effects when these groups are bonded to the oxygen atom.

In the above examples, the oxidation state of the main group or early transition metal does not change in the synthesis reaction, i.e., no formal electron-transfer is observed. In a recent example, reaction of a divalent zirconium species with $Cp_2Fe_2(\mu\text{-}CO)_2(CO)_2$ gives the tetravalent zirconium complex, $Cp_2Fe_2(\mu\text{-}CO)_2C_2O_2Zr(Me_5C_5)_2$.[6a] The two-electron transfer process results in the formation of a carbon-carbon bond. The related reaction of

$Cp_2Ti(CO)_2$ with $Cp_2Mo_2(CO)_4$ gives $Cp_2Ti(thf)(\mu\text{-}OC)Mo(CO)_2Cp$, the results of a one electron transfer process. We have shown that the divalent f- block metal complex, $Yb((Me_5C_5)_2(OEt_2)$, acts as a Lewis acid and a one electron-transfer agent towards the metal-metal bonded transition metal carbonyl $Co_2(CO)_8$, giving $(CO)_3Co[\mu\text{-}CO\text{-}Yb(Me_5C_5)_2(thf)]$.[7] The paramagnetism and bond lengths of this complex show that the ytterbium fragment is trivalent, the result of a one electron-transfer process. Several bridging carbonyl, f-element complexes have been postulated on the basis of infrared data.[8] A plausible mechanism for the formation of the ytterbium-cobalt complex is to postulate an interaction between two Yb(II) atoms and the bridging carbonyl groups in $Co_2(CO)_8$, similar to that observed in $Co_2(CO)_6(\mu\text{-}CO)(\mu\text{-}COA\ell Br_3)$[2d], followed by an electron-transfer into the lowest unoccupied molecular orbital of $Co_2(CO)_8$. Population of this orbital, which is metal-metal σ-antibonding, causes cleavage of the metal-metal bond giving $Co(CO)_4$-fragments.[9] This coordination, electron-transfer mechanism may be used to rationalize the formation of $(CO)_7Fe[(\mu_3\text{-}CO)_4\text{-}Yb_2(Me_5C_5)_4]$[10] and the cleavage of binuclear transition metal carbonyls by main group metals.[11]

It was of interest to extend the reaction of $Yb(Me_5C_5)_2(OEt_2)$ with other metal-metal bonded carbonyls to test the scope of the electron-transfer reaction. We were particularily interested in the reaction of $Mn_2(CO)_{10}$ since its h.o.m.o.'s are metal-metal anti-bonding[12] (similar to that found in $Co_2(CO)_8$) but it does not contain bridging carbonyl groups[3] (dissimilar to that found in $Co_2(CO)_8$). In addition, considerable effort has been spent on trying to reduce the bond order of coordinated carbon monoxide so that the C-O bond can be reduced by, for example, hydrogen to give synthetically useful oxygenated and other hydrocarbons.[13] The $Yb(Me_5C_5)_2$ group acts as a Lewis acid, polarizing the coordinated carbon monoxide molecule, and as a one

electron-transfer reagent, putting electron density into the lowest unoccupied molecular orbitals of carbon monoxide which are C-O antibonding and metal-carbon bonding. These two processes will activate carbon monoxide and reduce its bond order. In this regard, this strategy might be a useful model for the "oxide mechanism" of Fischer-Tropsch chemistry.[14]

The diethyl ether complex of bis(pentamethylcyclopentadienyl)ytterbium reacts with decacarbonyldimanganese in toluene to give a blue complex of empirical composition $Mn(CO)_5Yb(Me_5C_5)_2 \cdot {}^1/_4\,PhMe$. Decacarbonyldirhenium behaves similarily, giving red $Re(CO)_5Yb(Me_5C_5)_2 \cdot {}^1/_4\,PhMe$. Both complexes react with methyl iodide to give $MeM(CO)_5$, where M is Mn or Re as shown by the infrared spectrum of a pentane extract of the reaction residue. Both complexes are paramagnetic based upon the width and shift of the Me_5C_5 resonances in the ^1H NMR spectra, (see experimental section). The manganese complex follows Curie-Weiss behaviour [$\chi_M = C_M(T - \theta)^{-1}$] from 5-20 K with C_M = 1.58 ± 0.02 and θ = -0.69 ± 0.18 K and μ_{eff} = 3.57 ± 0.02 B.M. and from 80-300 K with C_M = 2.225 ± 0.005 and θ = -13.46 ± 0.51 K and μ_{eff} = 4.237 ± 0.005 B.M. The susceptibility values are indicative of trivalent ytterbium.[15] Thus, a one electron-transfer from $Yb(Me_5C_5)_2$ to the transition metal fragment has occurred similar to earlier observations.[7,10]

The infrared spectrum of the ytterbium-manganese complex in tetrahydrofuran is similar (five absorption bands) to that of $NaMn(CO)_5$ in thf (Table I). The infrared spectrum of $NaMn(CO)_5$ in thf has been interpreted as arising from either an equilibrium between solvent separated and contact ion-pairs, or a single contact-ion-pair with local C_{2v} symmetry.[16] The five line pattern observed for the ytterbium complex suggests a similar explanation. We cannot distinguish between these two explanations, though some support for the existance of a contact-ion pair of C_s symmetry is found by examining the

infrared spectrum of the related complex $(Me_5C_5)_2Yb(\mu\text{-}OC)Co(CO)_3(thf)$ in tetrahydrofuran (Table I). In the solid state this molecule is a contact-ion pair in which the ytterbium atom is bonded to a carbonyl-oxygen atom and a tetrahydrofuran molecule.[7] The infrared spectrum of this complex in tetrahydrofuran has four absorptions expected for a structure of local C_s symmetry. The infrared spectrum of the ytterbium-manganese complex in tetrahydrofuran is consistent with a solution structure analogous to that of the ytterbium-cobalt complex, i.e., a contact-ion pair in which the ytterbium atom is coordinated to a carbonyl-oxygen atom and a tetrahydrofuran molecule.

The infrared spectra of the ytterbium-manganese complex in solid state or in cyclohexane solution are much more complex than in tetrahydrofuran suggesting that other species are present in a non-coordinating solvent or in the solid. This is confirmed by the crystal and molecular stucture of the complex.

Figure I shows a stereopair view of a portion of the unit cell oblique to the a-c plane. Only half of the b axis is shown. A full layer of the structure at 0 and 0.25 in y is shown. A portion of the y = 0.5 layer shows how these layers pack in the unit cell.

Inspection of Figure I shows that the structure consists of layers of infinite, planar, polymeric sheets of the stoichiometry $\{[(Me_5C_5)_2Yb]\text{-}[Mn(CO)_5]\}^{\infty}$. Dimeric molecules of the formula $\{[(Me_5C_5)_2Yb][Mn(CO)_5]_2\}$ are packed between polymeric sheets. The solvating toluene molecules fill regularly spaced voids in the network of dimers and polymer sheets.

Close insepction of the polymeric sheet reveals that it consists of essentially trigonal bipyramidal $Mn(CO)_5$groups which are each coordinated to 3 different $(Me_5C_5)_2Yb$ groups through their equitorial carbonyls. Each $(Me_5C_5)_2Yb$ cation is in turn coordinated only to the equitorial carbonyls of

the $Mn(CO)_5$ units and all the Mn and Yb atoms in the polymer are essentially coplanar. The largest deviation of a metal atom from the least squares plane through them is 0.065Å by Yb(1).

The dimeric $Mn(CO)_5Yb(Me_5C_5)_2$ units, which are non-planar, lie on the mirror plane at y = 0 such that two ytterbium atoms lie in the mirror plane and the manganese atoms lie above and below the mirror plane. In addition all four Me_5C_5 rings in the dimer are normal to the mirror plane. The dimers pack in the a-c plane at y = 0 with the disordered toluene molecule filling the voids such that the overall composition of the crystal is $[Mn(CO)_5Yb(Me_5C_5)_2]_4[PhMe]$. The crystal structure, then, consists of alternate planar, polymeric sheets normal to b with dimers at 0, $1/2$ 1, etc. and the polymer at 1/4, 3/4, etc.

The very complex, though regular, crystal structure rationalizes in a general, though not in an analytic, fashion the large number of C-O stretching frequencies observed in the spectrum of the solid. It also offers a rationalization for the complexity of the infrared spectrum in the ν-CO region in non-polar solvents. The presence of oligomers and C_{2h} dimers, or dimers which do not have rigorous C_{2h} point symmetry in solution are consistent with the observed spectra. The formation of dimers or other higher oligomers by the compound $[(Me_5C_5)_2Yb][Co(CO)_4] \cdot THF$ would also explain the complexity of its υ-CO IR spectrum in noncoordinating solvents (see Table I).

In the discussion that follows, we will describe the discreteal dimeric and polymeric units with respect to their individual stereochemistry. An ORTEP view of the dimeric units is shown in Figure II, a portion of the polymeric unit in Figure III, positional parameters in Table II, and some bond lengths and bond angles in Tables III and IV, respectively. Crystal data are shown in Table V. As alluded to earlier, the Mn_2Yb_2 unit is not planar. The

angle between the two planes defined by Yb(2)Yb(3)Mn(2) and Yb(2)Yb(3)Mn(2') is 15.2°. The plane defined by Yb(2)Yb(3)Mn(2) is essentially co-planar with the equitorial carbonyl ligands on Mn(2). The distortion of the dimeric unit from planarity also may be described by reference to the Mn(2)Yb(2)Mn(2') and Mn(2)Yb(3)Mn(2) planes which form a dihedral angle of 11.8°. In addition, the dihedral angles formed by extension of the centroids of the Me_5C_5 rings CP(21) CP(31) and CP(22) CP(32) [see Table II for the definition of these symbols] are 17.5° and 51.6°, respectively.

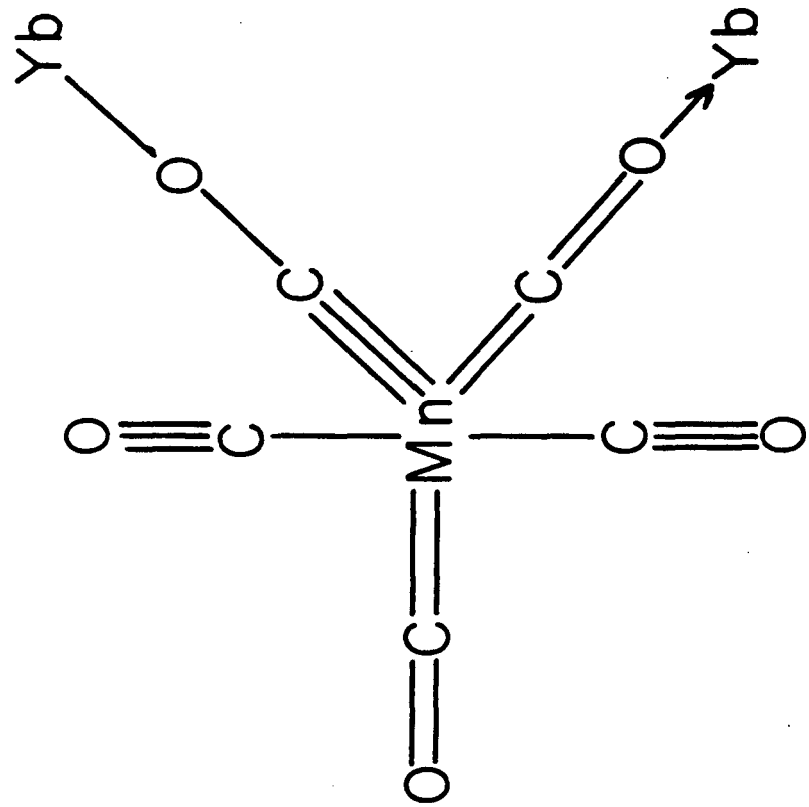
The averaged ytterbium-carbon length in the dimer is 2.574 ± 0.013Å and the averaged ytterbium-centroid distance is 2.281 ± 0.002Å. The centroid-Yb-centroid angle is 143.8°. These bond lengths are in the range found for other Yb(III) complexes in eight coordination[7,10,15c] and significantly shorter (0.17Å) than those found for a Yb(II) ion in eight coordination.[17] The averaged ytterbium-oxygen bond lengths is 2.271 ± 0.002Å and the averaged O-Yb-O angle is 85.63 ± 0.22°. These bond parameters in the dimer are very similar to those found in the polymer, even though the coordination numbers of ytterbium is nine in the latter, the only difference being the ytterbium oxygen bond lengths. In the polymer the averaged ytterbium-carbon bond length is 2.589 ± 0.015Å, the ytterbium-centroid distance is 2.304Å, the ytterbium-oxygen bond length are 2.389 ± 0.027Å, and the averaged O-Yb-O angle 69.43 ± 0.006°

The coordination geometry of the pentacarbonylmanganate fragment in the dimer and polymer are very similar, both being related to a trigonal bi-pyramid, as found in $[Ni(phen)_3][Mn(CO)_5]_2$.[18a] The most important feature, perhaps, of the ytterbium-manganese complex is the carbonyl groups that bridge the ytterbium and manganese atoms. In the dimer two equitorial carbonyl groups are bonded to two different ytterbium atoms and in the polymer all

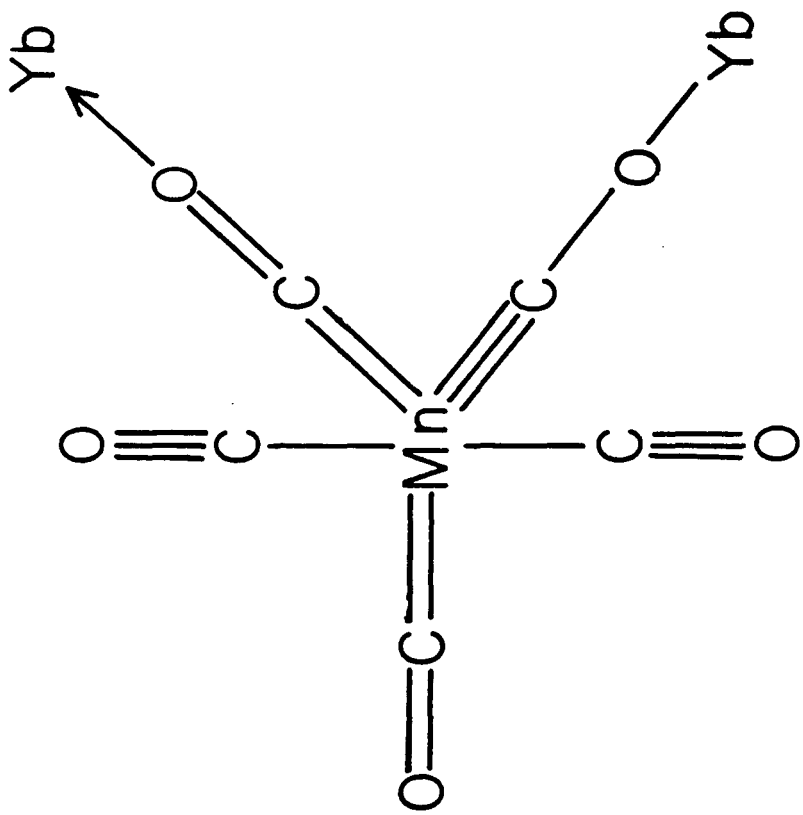
three equitorial carbonyl groups are bonded to three ytterbium atoms. In the dimer the averaged Yb-O-C and Mn-C-O angles are 171.6 ± 0.9° and 176.3 ± 0.4°, respectively. In the polymer, these averaged angles are 167.7 ± 0.5° and 178.9 ± 0.3°.

The averaged, terminal manganese-carbon bond lengths in the dimer and polymer are 1.833 ± 0.007Å and 1.820 ± 0.005 Å, respectively, whereas the bridging manganese-carbon distances are 1.748 ± 0.013Å and 1.791 ± 0.013Å, respectively. These distances may be compared with the averaged terminal manganese to carbon (equitorial) distance in $Mn_2(CO)_{10}$ of 1.856 ± 0.005Å[3b,c] and in a number of anionic $Mn(CO)_5$ fragments that range from 1.78 to 1.82Å.[18] In the ytterbium-manganese complex the short bridging manganese-carbon distance, relative to the terminal distance, is consistent with the view that electron-transfer into a neutral $Mn(CO)_5$ fragment puts electron density into molecular orbitals which are C-O antibonding and Mn-C bonding. The carbon-oxygen bond lengths are also consistent with this view (Table III) though these distances are not determined with high accuracy. The variation of the manganese-carbon and carbon-oxygen bond lengths suggest that the resonance structures I and II are important in the bonding in the contact ion-pair. Further, structures I and II emphasize that contact ion-pair formation tends to localize electron density into the manganese-carbon bonds that are part of the Mn-CO-Yb interaction.

[See drawing, next page.]



II.



I.

Experimental Section

All operations were carried out under nitrogen. Microanalyses were performed by the microanalytical laboratory of this laboratory of this department. The ^{1}H nuclear magnetic resonance spectra were measured at 89.56 MHz on a JEOL-FX90-Q instrument at 25°C in benzene-d_6 and are expressed in δ-values ($\delta Me_4Si = 0$). Infrared spectra were recoreded on a Perkin-Elmer 597 machine; solid spectra were measured as Nujol mulls and solution spectra were measured in matched NaCℓ cells, with spacings of either 0.5 mm or 0.1 mm. The magnetic susceptibility were made on a S.H.E. corporation model 905 Squid magnetometer. The sample containers were made from an alloy of aluminum with 3% silicon purchased from Varian. The sample containers were held together with a 2 cm. piece of 0.027 mm copper wire and sealed with silicon stopcock grease. The variation in the susceptibility of the container due to differing amounts of grease was less than 3%. The containers were designed by Dr. E. Gamp, and the design is available from the authors. The sample was loaded in a dry box, transported to the magnetometer in a Schlenk tube and suspended in the sample chamber by a piece of cotton thread attached to the copper wire. Sample measurements were made automatically at the following temperatures and magnetic field strengths: At 5 Kg magnetic field strength over a temperature range of 5-15 K a datum was measured every 2.5 K, at 15-50 K every 5 K, at 50-300 K every 10 K. At 40 Kg magnetic field strength over a temperature range of 5-30 K a datum was measured every 5 K, at 30-100 K every 10 K, and at 100-300 K every 20 K. All samples were corrected for container magnetism and compound diamagnetism using Pascal constants. Temperature independent paramagnetism was taken to be zero for ytterbium(III). The molar susceptibility was calculated and the molar susceptibility was plotted as a

function of the absolute temperature. A least squares fit to the line, using a program written by Dr. E. Gamp gave C_M where $\chi_M = C_M(T - \theta)$ and $\mu_{eff} = 2.8279[(\chi_M)(T - \theta)]^{1/2}$.

Mn(CO$_5$Yb(Me$_5$C$_5$)$_2$ · $^1/_4$ PhMe. Bis(pentamethylcyclopentadienyl) ytterbium-diethylether (1.0g, 0.0019 mol) in toluene (50 ml) was added to decacarbonyl-dimanganese (0.38 g, 0.000 97 mol) in toluune (20 ml). The dark blue solution was stirred for 12 h, filtered, and the filtrate was concentrated to ca. 40 ml. Cooling to -10°C yielded dark blue prisms which were collected and dried under reduced pressure. A second crop of blue prisms was isolated from the mother liquor. The combined yield was 1.0 g (82%). When heated in a sealed capillary the compound darkened at ca. 270°C and decomposed at ca. 320°C. Anal. Calcd for $C_{25}H_{30}MnO_5$: C, 48.6; h, 4.88. Found: C, 48.6, H, 4.70. ^{1}H NMR: δ 8.75 ($\upsilon^1/_2$ = 47Hz, 30H); 2.11 (0.75H); the aromatic hydrogens of the toluene of solvation were obscured by the residual benzene in benzene-d_6 solvent. IR: 2735 w, 1965 b,s, 1937 sh, 1928 sh, 1882 m, 1840 s, 1775 b,s, 1062 w, 1024 m, 800 w, 735 m, 728 m, 695 sh, 682s, 669s, 650 m, 645 m, 592 w, 555 s, 500 m, 463 m, 425 m, 395 m, 325 s, 285 w, cm^{-1}. A sample of the complex dissolved in benzene-d_6 and hydrolyzed with D_2O. Examination of an aliquot of the benzene layer by ^{1}H NMR spectroscopy showed resonances due to Me_5C_5D and PhMe in area ratio 8:1.

Re(CO)$_5$Yb(Me$_5$C$_5$)$_2$ · $^1/_4$ PhMe. Bis(pentamethylcyclopentadienyl)ytterbium-diethyl ether (0.21 g, 0.00040 mol) in toluene (25 ml) was added to deca-carbonyldirhenium (0.13 g, 0.00020 ml) in toluene (10 ml) and the solution was stirred for 48 h. The dark red solution was filtered and the filtrate was concentrated to ca. 5 ml and cooled (-10°C). The red microcrystals were

collected and dried under reduced pressure, yield was 0.17 g (53%), mp 315-320 (dec)°C. Anal. Calcd for $C_{25}H_{30}O_5Re_1Yb \cdot \frac{1}{4} C_7H_8$: C, 40.5; H, 4.07. Found: C, 40.4; H, 4.18. ^1H NMR: δ 9.56 ($\upsilon_{1/2}$ = 110Hz, 30H); 2.10 (0.75H); the aromatic protons of the solvated toluene were obscured by the residual benzene in the benzene-d_6 solvent. A sample of the complex in benzene-d_6 was hydrolyzed with D_2O. Examination of the benzene solution by ^1H NMR spectroscopy showed resonances due to Me_5C_5D and PhMe in area ratio 8:1. IR: 2720 w, 1982 sh, 1972 s, 1950 s, 1945 sh, 1750 b,s, 1015 w, 950 m, 795 w, 715 m, 625 w, and 585 s, cm^{-1}.

X-Ray Crystallography Crystals suitable for a X-ray study were grown from toluene, inserted into a quartz capillary, and the capillary flame sealed. Preliminary precession photographs indicated that the cell dimensions were large and suggested a monoclinic Laue symmetry. The derived cell dimensions were a = 18.0Å, b = 16.2Å, c = 18.9Å, and β = 80° with V = 5450Å^3. The crystal used for data collection was mounted on an Enrof-Nonius CAD4 automated diffractometer[19] and centered inthe beam. A first peak search follwed by automatic indexing gave a near-monoclinic cell with a = 9.44Å, b = 16.3Å, c = 18.1Å, β = 80°, and V = 2750Å. Location of additional peaks followed by automatic indexing gave a triclinic primitive cell with a volume of 5500Å^3, thesame as found in the primitive monoclinic cell from the precession work. Inspection of the Niggli values[20] f or this cell indicated that there were no cells of higher symmetry; the symmetry derived from the precession photographs were dismissed as 'pseudo-symmetry'. Accurate cell dimensions were obtained by centering the high angle reflections and data collection of a hemisphere of data was started, Table V.

After transfer and reduction of the first half of the data certain symmetries were noted in the Patterson and E-maps and a Delaunay reduction was performed on the cell. The program Tracer[21] immediately discovered the C-centered monoclinic unit cell which was confirmed by reduction and refinement of the data. The crystal parameters in Table V are for this monoclinic cell.

The 14401 raw intensity data were reduced to structure factor amplitudes with their esd's by corrections for scan speed, background, Lorentz and polarization effects. Analysis of the intensity check reflections showed a nearly linear and highly anisotropic decline in intensity over the data collection period (12 days). The relative intensities of three reflections at the end of the data collection period were 0.94, 0.82, and 0.78 for the $\bar{4}.18.3$, $10.14.\bar{2}$, and 2.4.10, respectively. An anisotropic, linear decay correction was applied to the data and then the data were transformed to correspond to the monoclinic cell. Inspection of the h0ℓ data showed no systematic absences apart from those generated by the centering operation, giving the choices of space group as C2, Cm or C2/m. The latter was confirmed by solution and refinement of the structure. Data were corrected for absorption by an empirical method based upon the observed intensities of the animuthal scan data. The maximum and minimum relative transmission factors were 1.00 and 0.919. Averaging of redundant and symmetry-equivalent data yielded 7442 unique reflections, (ave I) = 2.3%, R(ave F) = 17%.

Attempts to solve the structure were hampered by the strong pseudo-translation of $\frac{1}{2}$ a. The positions of the metal atoms were finally determined by a combination of vector analysis (Patterson map), direct methods (MULTAN 79), least-squares, and Fourier maps with different numbers and arrangements of atoms in different space groups. The discovery and refinement of the remainder of the atoms, including the toluene of solvation, proceeded

by normal least-squares and Fourier techniques. Given the large thermal motion of most of the methyl carbon atoms and the disorder of the toluene, no attempt was made to locate and refine the hydrogen atoms. The R-value for all 7442 data was 7.71%.

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SUPPLEMENTARY MATERIAL AVAILABLE

Listing of thermal parameters, carbon-carbon bond lengths, and observed structure factors (34 pages).

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(22) $R(avex) = \sum_i \left| |\bar{x}| - |x_i| \right| \Big/ \left[\sum_i x_i \right]^{-1}$

TABLE I. Infrared Spectra, υCO in cm^{-1}

Compound	medium	observed bands	reference
$Mn(CO)_5Yb(Me_5C_5)_2$	thf	2030w, 2010m, 1934s	this work
		1903s, 1770s	
	Nujol	1965s, 1937sh, 1928sh,	
		1882m, 1840s, 1775s	
	Cyclohexane	1984m, 1962s, 1955s,	
		1945m, 1778m, 1762s,	
		1750m, 1723m	
$LiMn(CO)_5$	thf	1895s, 1861s	16a
$NaMn(CO)_5$	thf	1902s, 1897s, 1875s,	16a
		1862s, 1829m	
$KMn(CO)_5$	thf	1896s, 1862s, 1830m	16b
$Mg(py)_4[Mn(CO)_5]_2$	PhMe	2031w, 1928s, 1904s,	16c
		1721s	
$Re(CO)_5Yb(Me_5C_5)_2$	Nujol	1982sh, 1972s, 1950s,	this work
		1945sh, 1785sh,	
		1770sh, 1750Brs	
$Co(CO)_4Yb(Me_5C_5)(thf)$	thf	2025m, 1935s, 1885w,	7 and
	Methyl-	2015s, 1975s, 1960sh, 1945s,	this work
	cyclohexane	1930s, 1825sh, 1810s, 1780s,	
		1715 brs	

TABLE II. Positional Parameters.

Atom	x	y	z
YB1	Ø.Ø573Ø(2)	Ø.252Ø3(1)	Ø.28381(2)
YB2	Ø.1Ø5Ø9(2)	Ø.ØØØØØ(Ø)	-Ø.197Ø9(2)
YB3	Ø.4Ø884(2)	Ø.ØØØØØ(Ø)	Ø.22843(2)
MN1	Ø.35154(6)	Ø.25Ø59(3)	Ø.42Ø52(6)
MN2	Ø.274Ø8(6)	Ø.Ø967Ø(3)	Ø.ØØ619(5)
O11	Ø.1919(3)	Ø.2511(1)	Ø.3235(3)
O12	Ø.39Ø2(3)	Ø.2517(1)	Ø.5853(3)
O13	Ø.4594(3)	Ø.2498(1)	Ø.3385(3)
O14	Ø.36Ø9(3)	Ø.3417(2)	Ø.4285(3)
O15	Ø.3513(3)	Ø.16ØØ(2)	Ø.43Ø6(3)
O21	Ø.179Ø(2)	Ø.Ø472(2)	-Ø.1183(2)
O22	Ø.3551(2)	Ø.Ø475(2)	Ø.1386(2)
O23	Ø.279Ø(5)	Ø.1869(2)	-Ø.Ø1Ø3(4)
O24	Ø.4Ø4Ø(3)	Ø.Ø9Ø3(2)	-Ø.Ø464(3)
O25	Ø.15ØØ(3)	Ø.1Ø79(2)	Ø.Ø668(3)
C11	Ø.2543(4)	Ø.2513(2)	Ø.3624(4)
C12	Ø.3749(4)	Ø.2514(2)	Ø.5189(4)
C13	Ø.4175(4)	Ø.2499(2)	Ø.371Ø(4)
C14	Ø.3564(4)	Ø.3Ø65(2)	Ø.424Ø(4)
C15	Ø.3515(4)	Ø.195Ø(2)	Ø.4258(4)
C21	Ø.2174(3)	Ø.Ø683(2)	-Ø.Ø691(3)
C22	Ø.3238(3)	Ø.Ø685(2)	Ø.Ø868(3)
C23	Ø.2781(5)	Ø.1522(2)	-Ø.ØØ39(5)
C24	Ø.3541(4)	Ø.Ø929(2)	-Ø.Ø273(4)
C25	Ø.1968(4)	Ø.1Ø42(2)	Ø.Ø426(4)
C1Ø1	Ø.Ø22Ø(4)	Ø.3113(2)	Ø.186Ø(4)
C212	Ø.1677(4)	Ø.Ø344(2)	-Ø.282Ø(3)
C213	Ø.1ØØØ(4)	Ø.Ø2Ø7(2)	-Ø.3286(3)
C214	Ø.2913(6)	Ø.ØØØØ(Ø)	-Ø.2ØØ2(7)
C215	Ø.1919(7)	Ø.Ø791(3)	-Ø.2724(5)
C216	Ø.Ø375(6)	Ø.Ø482(4)	-Ø.3835(5)
C3Ø1	Ø.2777(5)	Ø.ØØØØ(Ø)	Ø.2418(4)
C3Ø2	Ø.3151(3)	Ø.Ø349(2)	Ø.2812(3)
C3Ø3	Ø.375Ø(3)	Ø.Ø21Ø(2)	Ø.3443(3)
C3Ø4	Ø.2Ø88(5)	Ø.ØØØØ(Ø)	Ø.1714(5)
C3Ø5	Ø.2918(4)	Ø.Ø798(2)	Ø.2633(4)
C3Ø6	Ø.4224(5)	Ø.Ø491(3)	Ø.4Ø89(4)

Atom	x	y	z
C311	Ø.51Ø5(4)	Ø.ØØØØ(Ø)	Ø.1682(4)
C312	Ø.525Ø(3)	Ø.Ø349(2)	Ø.2142(3)
C313	Ø.5481(3)	Ø.Ø216(2)	Ø.2893(3)
C314	Ø.4887(6)	Ø.ØØØØ(Ø)	Ø.Ø835(5)
C315	Ø.5231(4)	Ø.Ø796(2)	Ø.189Ø(4)
C316	Ø.5841(4)	Ø.Ø488(3)	Ø.3594(4)
C1Ø2	-Ø.Ø224(4)	Ø.3165(2)	Ø.23Ø6(4)
C1Ø3	Ø.Ø263(4)	Ø.3273(2)	Ø.3Ø27(4)
C1Ø4	Ø.Ø994(4)	Ø.3283(2)	Ø.3Ø26(4)
C1Ø5	Ø.Ø97Ø(4)	Ø.3181(2)	Ø.2314(4)
C1Ø6	-Ø.ØØ81(6)	Ø.3Ø88(3)	Ø.Ø997(4)
C1Ø7	-Ø.1Ø87(4)	Ø.3163(3)	Ø.2Ø28(5)
C1Ø8	Ø.ØØ36(5)	Ø.34Ø1(3)	Ø.37Ø6(4)
C1Ø9	Ø.1687(5)	Ø.342Ø(2)	Ø.3695(5)
C11Ø	Ø.165Ø(5)	Ø.32ØØ(3)	Ø.2Ø14(5)
C111	Ø.ØØ48(6)	Ø.1994(3)	Ø.1751(4)
C112	-Ø.Ø276(5)	Ø.1887(3)	Ø.2277(4)
C113	Ø.Ø275(5)	Ø.1753(2)	Ø.2886(4)
C114	Ø.Ø951(4)	Ø.1767(2)	Ø.28Ø8(5)
C115	Ø.Ø844(5)	Ø.1915(3)	Ø.2Ø95(5)
C116	-Ø.Ø44Ø(11)	Ø.2Ø86(4)	Ø.Ø915(6)
C117	-Ø.1148(6)	Ø.1871(4)	Ø.2117(8)
C118	Ø.Ø175(6)	Ø.1577(3)	Ø.3622(5)
C119	Ø.1672(6)	Ø.1598(3)	Ø.3383(8)
C12Ø	Ø.141Ø(7)	Ø.1974(4)	Ø.1671(7)
C2Ø1	Ø.Ø377(5)	Ø.ØØØØ(Ø)	-Ø.1Ø17(4)
C2Ø2	Ø.Ø1Ø9(3)	Ø.Ø355(2)	-Ø.1462(3)
C2Ø3	-Ø.Ø332(3)	Ø.Ø213(2)	-Ø.2199(3)
C2Ø4	Ø.Ø862(6)	Ø.ØØØØ(Ø)	-Ø.Ø187(5)
C2Ø5	Ø.Ø199(4)	Ø.Ø8ØØ(3)	-Ø.1188(5)
C2Ø6	-Ø.Ø823(4)	Ø.Ø482(3)	-Ø.2819(4)
C211	Ø.21Ø7(5)	Ø.ØØØØ(Ø)	-Ø.2525(5)
C1	Ø.2198(6)	Ø.Ø668(4)	Ø.4919(6)
C2	Ø.2213(9)	Ø.Ø198(5)	Ø.4886(8)
C3	Ø.1959(7)	Ø.ØØØØ(Ø)	Ø.54ØØ(7)
C4	Ø.1974(1Ø)	Ø.Ø446(6)	Ø.5377(9)
C5	Ø.2434(9)	Ø.Ø453(5)	Ø.4458(8)
C6	Ø.2469(7)	Ø.ØØØØ(Ø)	Ø.44Ø8(6)

TABLE III. Selected Bond Lengths

YB1	O11		2.4Ø1(5)
YB1	O12		2.349(4)
YB1	O13		2.417(5)
YB1	C1Ø1		2.6Ø7(6)
YB1	C1Ø2		2.584(6)
YB1	C1Ø3		2.578(6)
YB1	C1Ø4		2.599(6)
YB1	C1Ø5		2.59Ø(6)
YB1	CP11	*	2.3Ø4
YB1	C111		2.61Ø(7)
YB1	C112		2.612(7)
YB1	C113		2.571(7)
YB1	C114		2.564(7)
YB1	C115		2.577(7)
YB1	CP12	*	2.3Ø5
YB2	O21		2.268(4)
YB2	C2Ø1		2.551(7)
YB2	C2Ø2		2.576(5)
YB2	C2Ø3		2.599(5)
YB2	CP21	**	2.279
YB2	C211		2.56Ø(9)
YB2	C212		2.565(6)
YB2	C213		2.563(5)
YB2	CP22	**	2.283
YB3	O22		2.273(4)
YB3	C3Ø1		2.582(8)
YB3	C3Ø2		2.582(5)
YB3	C3Ø3		2.59Ø(5)
YB3	CP31	**	2.292
YB3	C311		2.554(7)
YB3	C312		2.572(5)
YB3	C313		2.591(5)
YB3	CP32	**	2.28Ø

MN1	C11	1.796(7)
MN1	C12	1.771(8)
MN1	C13	1.8Ø5(8)
MN1	C14	1.825(7)
MN1	C15	1.814(7)
MN1	O11	2.957(5)
MN1	O12	2.968(5)
MN1	O13	2.963(5)
MN1	O14	2.974(5)
MN1	O15	2.959(5)
MN2	C21	1.735(6)
MN2	C22	1.761(6)
MN2	C23	1.823(8)
MN2	C24	1.839(8)
MN2	C25	1.838(8)
MN2	O21	2.924(4)
MN2	O22	2.94Ø(4)
MN2	O23	2.962(6)
MN2	O24	2.964(6)
MN2	O25	2.972(6)
C11	O11	1.161(7)
C12	O12	1.197(8)
C13	O13	1.159(8)
C14	O14	1.149(7)
C15	O15	1.145(7)
C21	O21	1.19Ø(6)
C22	O22	1.181(6)
C23	O23	1.139(8)
C24	O24	1.125(8)
C25	O25	1.135(8)

* CENTROID OF THE FIVE CARBONS ABOVE

** CENTROID OF CYCLOPENTADIENE RING GENERATED BY THE THREE CARBONS ABOVE

TABLE IV. Selected Bond Angles

MN1	C11	O11	178.2(5)
MN1	C12	O12	179.4(6)
MN1	C13	O13	179.1(5)
MN1	C14	O14	177.9(6)
MN1	C15	O15	178.6(6)
MN2	C21	O21	176.7(5)
MN2	C22	O22	175.9(5)
MN2	C23	O23	178.6(9)
MN2	C24	O24	178.6(6)
MN2	C25	O25	177.8(7)
YB1	O11	C11	160.4(5)
YB1	O12	C12	169.1(5)
YB1	O13	C13	173.7(5)
YB2	O21	C21	170.6(4)
YB3	O22	C22	172.5(4)
C11	MN1	C12	119.0(3)
C11	MN1	C13	115.2(3)
C11	MN1	C14	92.2(3)
C11	MN1	C15	91.5(3)
C12	MN1	C13	125.8(3)
C12	MN1	C14	87.4(3)
C12	MN1	C15	87.8(3)
C13	MN1	C14	89.8(3)
C13	MN1	C15	91.7(3)
C14	MN1	C15	174.9(3)
C21	MN2	C22	116.0(3)
C21	MN2	C23	118.6(3)
C21	MN2	C24	91.7(3)
C21	MN2	C25	91.9(3)
C22	MN2	C23	125.5(3)
C22	MN2	C24	90.4(3)
C22	MN2	C25	90.0(3)
C23	MN2	C24	87.8(4)
C23	MN2	C25	88.5(4)
C24	MN2	C25	175.7(3)
O11	YB1	O12	69.20(18)
O11	YB1	O13	138.85(17)
O12	YB1	O13	69.65(18)
CP11 *	YB1	O11	95.8
CP11	YB1	O12	107.9
CP11	YB1	O13	96.7
CP12	YB1	O11	97.5
CP12	YB1	O12	108.7
CP12	YB1	O13	95.4
CP11	YB1	CP12	143.4
O21	YB2	O21	85.41(24)
O21	YB2	CP21	103.5
O21	YB2	CP22	102.9
CP21	YB2	CP22	143.8
O22	YB3	O22	85.85(22)
O22	YB3	CP31	103.1
O22	YB3	CP32	103.2
CP31	YB3	CP32	143.8

* CP11,CP12, ETC. ARE THE CENTROIDS OF THE RING CARBONS OF THE PENTAMETHYLCYCLOPENTADINE LIGANDS

TABLE V. Crystal Data (25°) for $Mn(CO)_5Yb(Me_5C_5)_2 \cdot \frac{1}{4}$ PhMe

Space Group	C2/m
a(Å)	18.942(5)
b(Å)	32.591(5)
c(Å)	19.029(5)
β(deg)	109.92(2)
V(Å^3)	11045 (8)
Z	16
Formula Wt. (amu)	661.27
d(calc) g cm^{-3}	1.591
μ(calc) cm^{-1}	38.27
Size (mm)	0.18 x 0.19 x 0.42
Reflection, collected	14401
Reflections, unique	7442
Reflections, $F^2 > 3\sigma(F^2)$	5487
R(%)	2.79
Rw(%)	3.91
Variables	614
GOF	1.578
Monochromator	Highly oriented graphite
Radiation	MoK_α, λ = 0.71073Å
Scan Range, type	$3° \leq \theta \leq 45°$, θ-2θ
Scan Speed	0.575 - 6.7° min^{-1}
Scan width	$\Delta\theta = 0.45 + 0.347 \tan\theta$

FIGURE CAPTIONS

Figure I — A stereopair view oblique to the a-c plane.

Figure II — An ORTEP view of the dimeric molecule.

Figure III — An ORTEP view of a portion of the polymeric unit.

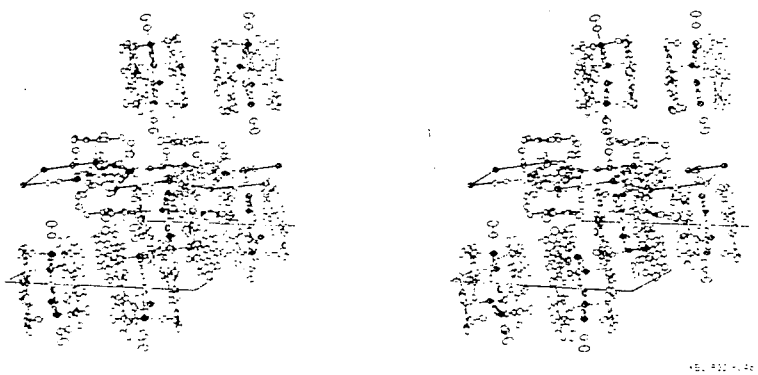
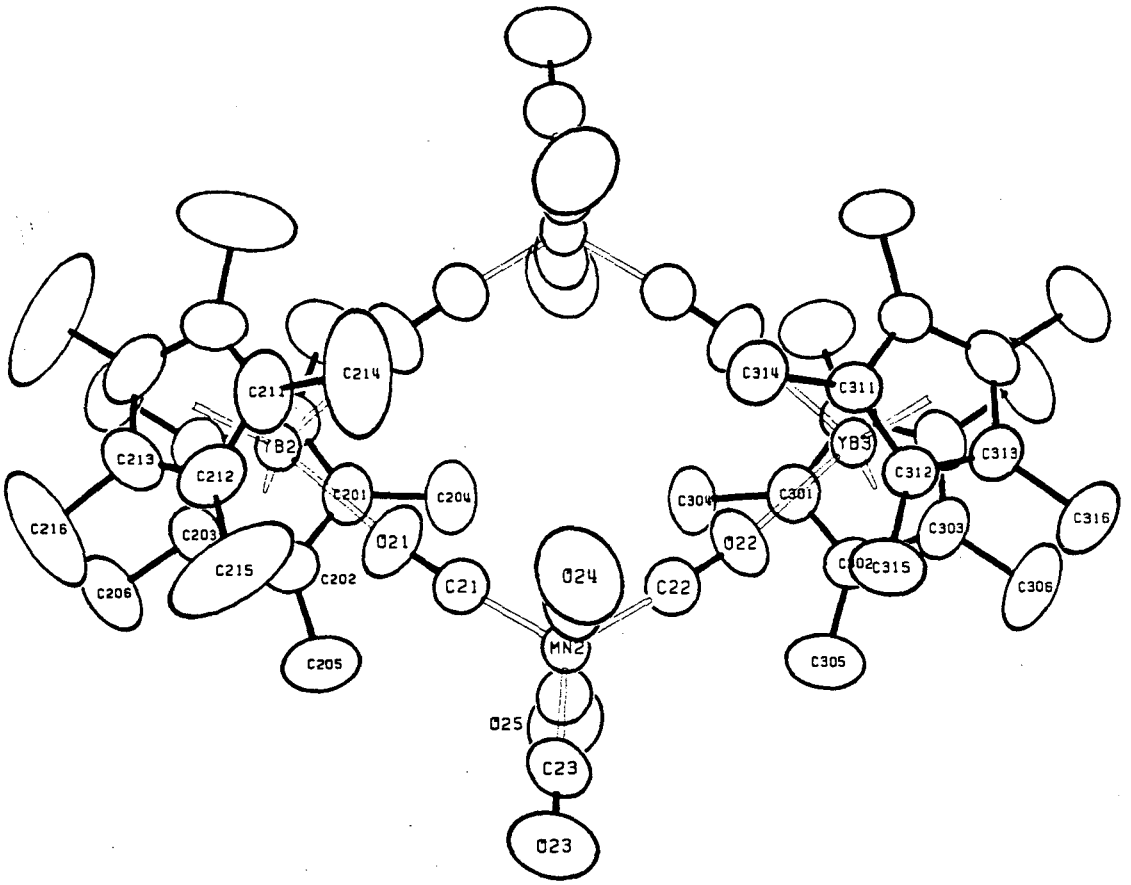


Figure 1



XBL 826-10530

Figure 2

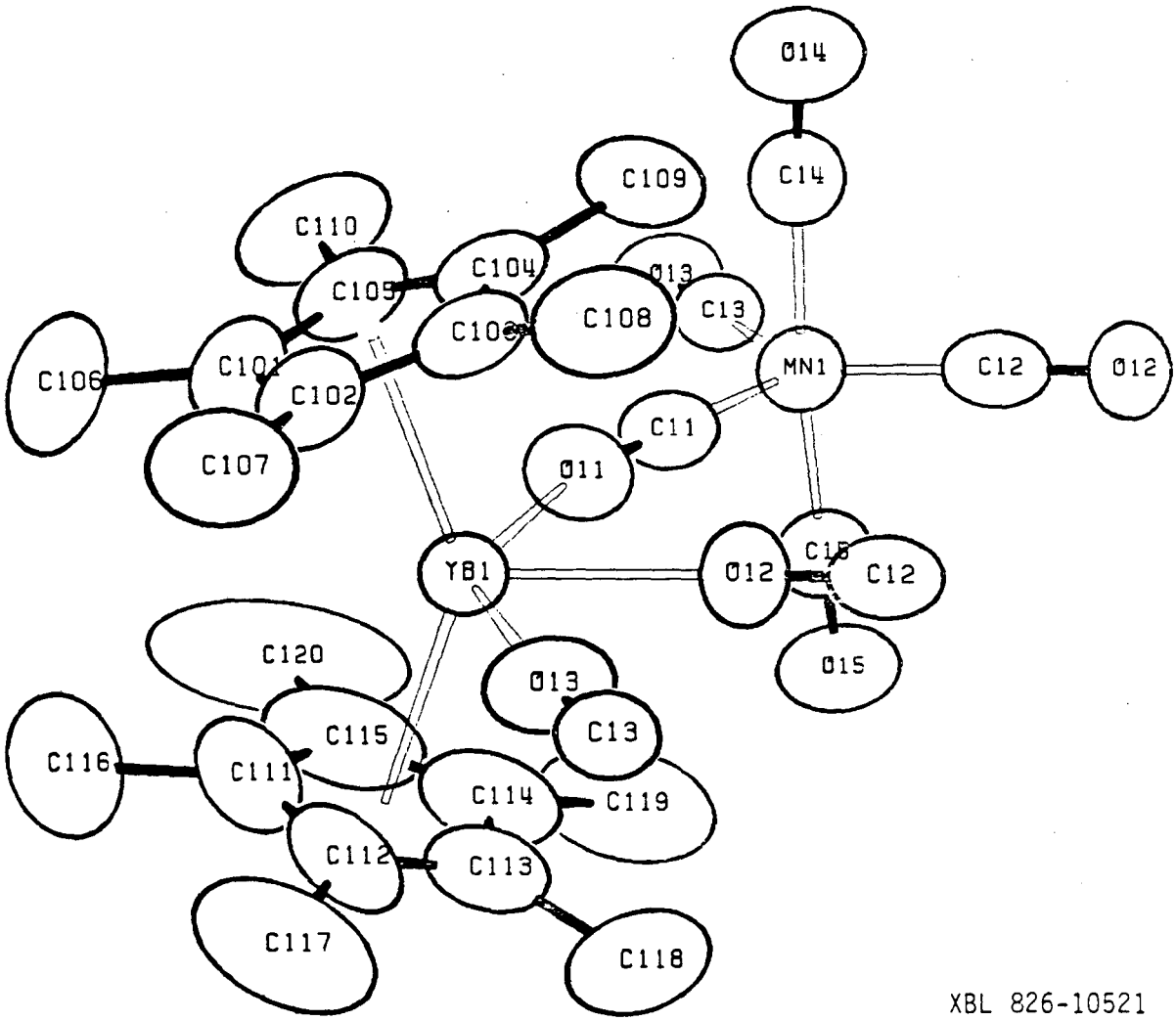

O14
C14
C109
C110
C104
O13
C105
C108
C13
C106
C101
C102
MN1
C12
O12
C11
C107
O11
YB1
O12
C15
C12
O15
C120
O13
C115
C13
C116
C111
C114
C119
C112
C113
C117
C118
XBL 826-10521

Figure 3

Supplementary Material for

Bis(Pentamethylcyclopentadienyl)Ytterbium(II) as a Lewis Acid and Electron-Transfer Ligand; Preparations and Crystal Structures of $[Yb(Me_5C_5)_2(\mu\text{-}CO)_xMn(CO)_{5-x}]_y$ where x and y are two and x is three and y is infinite.

James M. Boncella and Richard A. Andersen

Thermal Parameters

Atom	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
YB1	Ø.ØØ287(1)	Ø.ØØØ82(Ø)	Ø.ØØ33Ø(1)	Ø.ØØØØ8(1)	Ø.ØØ219(2)	-Ø.ØØØØ3(1)
YB2	Ø.ØØ211(1)	Ø.ØØØ86(Ø)	Ø.ØØ233(1)	Ø.ØØØØØ(Ø)	Ø.ØØ153(2)	Ø.ØØØØØ(Ø)
YB3	Ø.ØØ231(1)	Ø.ØØØ87(Ø)	Ø.ØØ21Ø(1)	Ø.ØØØØØ(Ø)	Ø.ØØ187(2)	Ø.ØØØØØ(Ø)
MN1	Ø.ØØ3Ø7(4)	Ø.ØØ1Ø1(1)	Ø.ØØ365(3)	Ø.ØØØ31(4)	Ø.ØØ26Ø(6)	Ø.ØØØØ9(3)
MN2	Ø.ØØ321(3)	Ø.ØØØ86(1)	Ø.ØØ276(3)	-Ø.ØØØØ5(4)	Ø.ØØØ74(5)	-Ø.ØØØØ6(3)
O11	Ø.ØØ27(2)	Ø.ØØ124(6	Ø.ØØ57(2)	Ø.ØØØ5(2)	Ø.ØØ21(3)	-Ø.ØØØØ(2)
O12	Ø.ØØ63(3)	Ø.ØØ132(6	Ø.ØØ32(1)	-Ø.ØØØ1(2)	Ø.ØØ24(3)	-Ø.ØØØØ(2)
O13	Ø.ØØ44(2)	Ø.ØØ117(6	Ø.ØØ65(2)	Ø.ØØØ2(2)	Ø.ØØ68(3)	Ø.ØØØØ(2)
O14	Ø.ØØ72(3)	Ø.ØØ117(6	Ø.ØØ82(3)	Ø.ØØØ2(2)	Ø.ØØ6Ø(4)	-Ø.ØØØØ(2)
O15	Ø.ØØ65(3)	Ø.ØØ1Ø6(6	Ø.ØØ79(3)	Ø.ØØØ1(2)	Ø.ØØ42(4)	Ø.ØØØ6(2)
O21	Ø.ØØ4Ø(2)	Ø.ØØ191(7	Ø.ØØ39(1)	-Ø.ØØ17(2)	Ø.ØØ33(2)	-Ø.ØØ21(2)
O22	Ø.ØØ38(2)	Ø.ØØ167(6	Ø.ØØ34(1)	Ø.ØØ14(2)	Ø.ØØ31(2)	Ø.ØØ19(2)
O23	Ø.Ø111(4)	Ø.ØØ114(7	Ø.Ø113(4)	-Ø.ØØØ6(3)	Ø.ØØØ5(7)	Ø.ØØ14(3)
O24	Ø.ØØ65(2)	Ø.ØØ3Ø5(11	Ø.ØØ71(2)	Ø.ØØØ4(3)	Ø.ØØ83(3)	Ø.ØØ24(3)
O25	Ø.ØØ52(2)	Ø.ØØ278(1Ø	Ø.ØØ72(2)	Ø.ØØ13(3)	Ø.ØØ6Ø(3)	-Ø.ØØ25(2)
C11	Ø.ØØ36(2)	Ø.ØØØ84(7	Ø.ØØ45(2)	Ø.ØØØ1(2)	Ø.ØØ43(4)	-Ø.ØØØ1(2)
C12	Ø.ØØ31(2)	Ø.ØØØ8Ø(7	Ø.ØØ57(3)	Ø.ØØØ3(2)	Ø.ØØ34(4)	-Ø.ØØØ1(2)
C13	Ø.ØØ34(3)	Ø.ØØØ85(7	Ø.ØØ41(2)	Ø.ØØØ2(2)	Ø.ØØ21(4)	Ø.ØØØØ(2)
C14	Ø.ØØ44(3)	Ø.ØØ121(9	Ø.ØØ44(2)	Ø.ØØØ5(3)	Ø.ØØ32(4)	-Ø.ØØØØ(3)
C15	Ø.ØØ44(3)	Ø.ØØ1Ø8(8	Ø.ØØ46(2)	Ø.ØØØ4(3)	Ø.ØØ3Ø(4)	Ø.ØØØ4(2)
C21	Ø.ØØ26(2)	Ø.ØØ113(8	Ø.ØØ36(2)	Ø.ØØØ1(2)	Ø.ØØ24(3)	-Ø.ØØØ4(2)
C22	Ø.ØØ29(2)	Ø.ØØ116(8	Ø.ØØ33(2)	-Ø.ØØØ1(2)	Ø.ØØ27(3)	-Ø.ØØØØ(2)
C23	Ø.ØØ6Ø(4)	Ø.ØØ1Ø4(9	Ø.ØØ6Ø(3)	Ø.ØØØØ(3)	-Ø.ØØØ7(6)	Ø.ØØØ7(3)
C24	Ø.ØØ43(3)	Ø.ØØ156(1Ø	Ø.ØØ35(2)	-Ø.ØØØ5(3)	Ø.ØØ21(4)	Ø.ØØ11(3)
C25	Ø.ØØ41(3)	Ø.ØØ134(9	Ø.ØØ43(3)	Ø.ØØØ7(3)	Ø.ØØØ8(5)	-Ø.ØØ1Ø(3)
C1Ø1	Ø.ØØ57(3)	Ø.ØØ128(9	Ø.ØØ39(2)	Ø.ØØØ7(3)	Ø.ØØ33(4)	Ø.ØØ12(2)
C1Ø2	Ø.ØØ38(3)	Ø.ØØ117(8	Ø.ØØ49(3)	Ø.ØØØ9(3)	Ø.ØØ22(4)	Ø.ØØ13(3)
C1Ø3	Ø.ØØ41(3)	Ø.ØØØ83(7	Ø.ØØ53(2)	Ø.ØØØ6(3)	Ø.ØØ4Ø(4)	Ø.ØØ14(2)
C1Ø4	Ø.ØØ36(3)	Ø.ØØØ77(7	Ø.ØØ56(2)	Ø.ØØØ4(2)	Ø.ØØ34(4)	Ø.ØØ15(2)
C1Ø5	Ø.ØØ38(2)	Ø.ØØ112(8	Ø.ØØ54(2)	Ø.ØØØ4(3)	Ø.ØØ48(4)	Ø.ØØ16(2)
C1Ø6	Ø.Ø1Ø7(6)	Ø.ØØ22Ø(14	Ø.ØØ42(3)	Ø.ØØ15(5)	Ø.ØØ3Ø(7)	Ø.ØØ15(4)
C1Ø7	Ø.ØØ3Ø(3)	Ø.ØØ155(11	Ø.ØØ96(5)	Ø.ØØØ8(3)	Ø.ØØ23(6)	Ø.ØØØ9(4)
C1Ø8	Ø.ØØ8Ø(4)	Ø.ØØ124(9	Ø.ØØ71(3)	Ø.ØØØ2(3)	Ø.ØØ97(4)	-Ø.ØØØ7(3)
C1Ø9	Ø.ØØ46(3)	Ø.ØØ1Ø4(9	Ø.ØØ71(4)	-Ø.ØØØ4(3)	Ø.ØØ13(6)	-Ø.ØØØ3(3)
C11Ø	Ø.ØØ69(3)	Ø.ØØ185(13	Ø.Ø1Ø6(4)	Ø.ØØØ3(4)	Ø.Ø112(5)	Ø.ØØ3Ø(4)
C111	Ø.Ø121(6)	Ø.ØØ161(11	Ø.ØØ43(3)	-Ø.ØØ19(5)	Ø.ØØ3Ø(7)	-Ø.ØØ26(3)
C112	Ø.ØØ57(4)	Ø.ØØ148(1Ø	Ø.ØØ57(3)	-Ø.ØØ1Ø(4)	Ø.ØØØ3(6)	-Ø.ØØ22(3)
C113	Ø.ØØ61(4)	Ø.ØØØ87(8	Ø.ØØ66(3)	-Ø.ØØØ8(3)	Ø.ØØ36(6)	-Ø.ØØ14(3)
C114	Ø.ØØ5Ø(3)	Ø.ØØ1ØØ(9	Ø.ØØ9Ø(4)	Ø.ØØØ3(3)	Ø.ØØ52(6)	-Ø.ØØ23(3)
C115	Ø.ØØ98(4)	Ø.ØØ163(1Ø	Ø.Ø1Ø3(3)	-Ø.ØØ27(4)	Ø.Ø144(5)	-Ø.ØØ52(3)

Thermal Parameters (continued)

C116	Ø.Ø269(14)	Ø.ØØ282(19	Ø.ØØ48(4)	-Ø.ØØ57(9)	Ø.ØØ14(14)	-Ø.ØØ22(5)
C117	Ø.ØØ42(4)	Ø.ØØ261(17	Ø.Ø149(8)	-Ø.ØØ14(5)	Ø.ØØ14(9)	-Ø.ØØ26(6)
C118	Ø.Ø123(6)	Ø.ØØ143(11	Ø.ØØ84(4)	-Ø.ØØ15(5)	Ø.ØØ92(8)	Ø.ØØØ6(4)
C119	Ø.ØØ58(5)	Ø.ØØ13Ø(11	Ø.Ø166(8)	Ø.ØØ19(4)	-Ø.ØØØ1(11)	-Ø.ØØØ4(6)
C12Ø	Ø.Ø247(6)	Ø.ØØ276(16	Ø.Ø284(5)	-Ø.ØØ84(5)	Ø.Ø462(6)	-Ø.Ø117(4)
C2Ø1	Ø.ØØ27(3)	Ø.ØØ152(13	Ø.ØØ27(3)	Ø.ØØØØ(Ø)	Ø.ØØ27(4)	Ø.ØØØØ(Ø)
C2Ø2	Ø.ØØ26(2)	Ø.ØØ112(8	Ø.ØØ41(2)	Ø.ØØØ1(2)	Ø.ØØ31(3)	-Ø.ØØØ7(2)
C2Ø3	Ø.ØØ22(2)	Ø.ØØ133(8	Ø.ØØ37(2)	Ø.ØØØ6(2)	Ø.ØØ22(3)	Ø.ØØØ6(2)
C2Ø4	Ø.ØØ33(4)	Ø.ØØ231(18	Ø.ØØ34(3)	Ø.ØØØØ(Ø)	Ø.ØØ24(5)	Ø.ØØØØ(Ø)
C2Ø5	Ø.ØØ43(3)	Ø.ØØ144(1Ø	Ø.ØØ8Ø(4)	Ø.ØØØ6(3)	Ø.ØØ51(5)	-Ø.ØØ18(3)
C2Ø6	Ø.ØØ35(3)	Ø.ØØ233(12	Ø.ØØ53(3)	Ø.ØØ24(4)	Ø.ØØ21(5)	Ø.ØØ24(3)
C211	Ø.ØØ27(3)	Ø.ØØ251(18	Ø.ØØ32(3)	Ø.ØØØØ(Ø)	Ø.ØØ36(4)	Ø.ØØØØ(Ø)
C212	Ø.ØØ6Ø(3)	Ø.ØØ1Ø8(8	Ø.ØØ37(2)	-Ø.ØØ16(3)	Ø.ØØ58(3)	-Ø.ØØØ2(2)
C213	Ø.ØØ51(3)	Ø.ØØ154(9	Ø.ØØ34(2)	Ø.ØØ22(3)	Ø.ØØ47(3)	Ø.ØØ15(2)
C214	Ø.ØØ24(4)	Ø.ØØ618(43	Ø.ØØ59(5)	Ø.ØØEØ(Ø)	Ø.ØØ28(7)	Ø.ØØØØ(Ø)
C215	Ø.Ø238(7)	Ø.ØØ214(13	Ø.Ø1Ø6(4)	-Ø.ØØ88(5)	Ø.Ø235(7)	-Ø.ØØ44(4)
C216	Ø.Ø1Ø4(5)	Ø.ØØ598(22	Ø.ØØ65(3)	Ø.Ø114(5)	Ø.ØØ9Ø(6)	Ø.ØØ76(5)
C3Ø1	Ø.ØØ28(3)	Ø.ØØ134(12	Ø.ØØ29(2)	Ø.ØØØØ(Ø)	Ø.ØØ36(4)	Ø.ØØØØ(Ø)
C3Ø2	Ø.ØØ35(2)	Ø.ØØØ99(7	Ø.ØØ32(2)	Ø.ØØØØ(2)	Ø.ØØ4Ø(3)	-Ø.ØØØ1(2)
C3Ø3	Ø.ØØ36(2)	Ø.ØØ143(8	Ø.ØØ25(2)	-Ø.ØØØ9(2)	Ø.ØØ31(3)	-Ø.ØØØ9(2)
C3Ø4	Ø.ØØ24(3)	Ø.ØØ196(16	Ø.ØØ34(3)	Ø.ØØØØ(Ø)	Ø.ØØ11(5)	Ø.ØØØØ(Ø)
C3Ø5	Ø.ØØ63(3)	Ø.ØØ126(1Ø	Ø.ØØ67(3)	Ø.ØØ11(3)	Ø.ØØ8Ø(4)	Ø.ØØØ4(3)
C3Ø6	Ø.ØØ51(3)	Ø.ØØ297(14	Ø.ØØ4Ø(2)	-Ø.ØØ23(4)	Ø.ØØ32(4)	-Ø.ØØ34(3)
C311	Ø.ØØ23(3)	Ø.ØØØ83(9	Ø.ØØ31(2)	Ø.ØØØØ(Ø)	Ø.ØØ29(4)	Ø.ØØØØ(Ø)
C312	Ø.ØØ26(2)	Ø.ØØØ83(6	Ø.ØØ32(2)	-Ø.ØØØ2(2)	Ø.ØØ23(3)	-Ø.ØØØ1(2)
C313	Ø.ØØ24(2)	Ø.ØØ1Ø2(7	Ø.ØØ35(2)	-Ø.ØØØ4(2)	Ø.ØØ16(3)	-Ø.ØØØ8(2)
C314	Ø.ØØ48(4)	Ø.ØØ134(12	Ø.ØØ28(2)	Ø.ØØØØ(Ø)	Ø.ØØ39(5)	Ø.ØØØØ(Ø)
C315	Ø.ØØ5Ø(3)	Ø.ØØØ85(8	Ø.ØØ61(3)	-Ø.ØØØ3(3)	Ø.ØØ45(5)	Ø.ØØØ9(3)
C316	Ø.ØØ47(3)	Ø.ØØ184(1Ø	Ø.ØØ48(3)	-Ø.ØØ11(3)	Ø.ØØ17(5)	-Ø.ØØ28(3)

Atom	$B, Å^2$	Atom	$B, Å^2$
C1	1Ø.9(3)	C4	7.4(4)
C2	7.3(4)	C5	6.4(4)
C3	8.1(3)	C6	7.1(3)

The form of the anisotropic thermal parameter is:

$\exp[-(B(1,1)*h^2 + B(2,2)*k^2 + B(3,3)*l^2 + B(1,2)*hk + B(1,3)*hl + B(2,3)*kl)]$.

Estimated standard deviations in the least significant digits are shown in parentheses

Carbon-Carbon Bond Lengths

INTERATOMIC DISTANCES IN PENTAMETHYL CYCLOPENTADIENIDE LIGANDS

ATOM 1	ATOM 2	DISTANCE
C1Ø1	C1Ø2	1.392(9)
C1Ø2	C1Ø3	1.414(9)
C1Ø3	C1Ø4	1.387(9)
C1Ø4	C1Ø5	1.38Ø(9)
C1Ø5	C1Ø1	1.4Ø6(9)
C1Ø1	C1Ø6	1.548(9)
C1Ø2	C1Ø7	1.537(9)
C1Ø3	C1Ø8	1.551(9)
C1Ø4	C1Ø9	1.55Ø(9)
C1Ø5	C11Ø	1.578(1Ø)

ATOM 1	ATOM 2	DISTANCE
C111	C112	1.386(13)
C112	C113	1.34Ø(1Ø)
C113	C114	1.339(11)
C114	C115	1.389(13)
C115	C111	1.446(14)
C111	C116	1.572(13)
C112	C117	1.575(12)
C113	C118	1.383(11)
C114	C119	1.532(12)
C115	C12Ø	1.559(14)

ATOM 1	ATOM 2	DISTANCE
C2Ø1	C2Ø2	1.421(7)
C2Ø2	C2Ø3	1.442(7)
C2Ø3	C2Ø3	1.388(11)
C2Ø1	C2Ø4	1.533(11)
C2Ø2	C2Ø5	1.533(9)
C2Ø3	C2Ø6	1.511(8)

ATOM 1	ATOM 2	DISTANCE
C211	C212	1.385(8)
C212	C213	1.362(9)
C213	C213	1.351(13)
C211	C214	1.512(13)
C212	C215	1.521(1Ø)
C213	C216	1.566(1Ø)

ATOM 1	ATOM 2	DISTANCE
C3Ø1	C3Ø2	1.414(7)
C3Ø2	C3Ø3	1.417(7)
C3Ø3	C3Ø3	1.369(11)
C3Ø1	C3Ø4	1.518(11)
C3Ø2	C3Ø5	1.533(9)
C3Ø3	C3Ø6	1.551(8)

ATOM 1	ATOM 2	DISTANCE
C311	C312	1.4Ø5(6)
C312	C313	1.414(7)
C313	C313	1.4Ø8(11)
C3Ø1	C3Ø4	1.518(11)
C3Ø2	C3Ø5	1.533(9)
C3Ø3	C3Ø6	1.551(8)

INTERATOMIC DISTANCE IN THE DISORDERED TOLUENE MOLECULE

ATOM 1	ATOM 2	DISTANCE
C1	C2	1.533(18)
C2	C3	1.387(16)
C3	C4	1.455(16)
C4	C1	1.3Ø9(17)
C1	C5	1.315(16)
C5	C6	1.481(15)
C6	C2	1.334(16)

Fobs and Fclc for Mn(CO)5 Yb (C5Me5)2 . 1/4(toluene) @ 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
Ø	Ø	2	1Ø54	1Ø23	2	Ø	1Ø	548	532	6	Ø	-2Ø	119	115	8	Ø	-1Ø	192	178	1Ø	Ø	2	2Ø8	2Ø4
Ø	Ø	3	3Ø2	316	2	Ø	11	86	83	6	Ø	-19	11Ø	1Ø2	8	Ø	-9	34Ø	343	1Ø	Ø	3	365	352
Ø	Ø	4	61Ø	671	2	Ø	12	3Ø6	313	6	Ø	-18	85	77	8	Ø	-8	314	316	1Ø	Ø	4	161	172
Ø	Ø	5	368	345	2	Ø	13	Ø*	24	6	Ø	-17	161	16Ø	8	Ø	-7	194	2Ø2	1Ø	Ø	5	3Ø5	31Ø
Ø	Ø	6	26Ø	247	2	Ø	14	6Ø	69	6	Ø	-16	17*	18	8	Ø	-6	6Ø5	6Ø9	1Ø	Ø	6	56	54
Ø	Ø	7	282	3Ø5	2	Ø	15	128	12Ø	6	Ø	-15	161	158	8	Ø	-5	768	758	1Ø	Ø	7	375	372
Ø	Ø	8	163	153	2	Ø	16	144	148	6	Ø	-14	281	283	8	Ø	-4	356	337	1Ø	Ø	8	113	1Ø1
Ø	Ø	9	66	67	2	Ø	17	136	133	6	Ø	-13	4Ø1	4Ø7	8	Ø	-3	1Ø53	1Ø59	1Ø	Ø	9	167	171
Ø	Ø	1Ø	458	455	2	Ø	18	36*	28	6	Ø	-12	387	379	8	Ø	-2	651	681	1Ø	Ø	1Ø	75	74
Ø	Ø	11	155	157	4	Ø	-2Ø	13*	6	6	Ø	-11	15Ø	149	8	Ø	-1	481	461	1Ø	Ø	11	58	55
Ø	Ø	12	175	172	4	Ø	-19	82	82	6	Ø	-1Ø	253	266	8	Ø	Ø	116	113	1Ø	Ø	12	119	1Ø9
Ø	Ø	13	111	112	4	Ø	-18	182	18Ø	6	Ø	-9	471	454	8	Ø	1	277	274	1Ø	Ø	13	18*	24
Ø	Ø	14	412	399	4	Ø	-17	6Ø	65	6	Ø	-8	13Ø	119	8	Ø	2	156	158	12	Ø	-19	Ø*	3Ø
Ø	Ø	15	Ø*	8	4	Ø	-16	29*	18	6	Ø	-7	313	328	8	Ø	3	142	156	12	Ø	-18	73	76
Ø	Ø	16	148	14Ø	4	Ø	-15	252	24Ø	6	Ø	-6	173	195	8	Ø	4	152	153	12	Ø	-17	178	181
Ø	Ø	17	151	143	4	Ø	-14	131	131	6	Ø	-5	53	41	8	Ø	5	378	373	12	Ø	-16	49	49
Ø	Ø	18	71	72	4	Ø	-13	51	58	6	Ø	-4	954	927	8	Ø	6	145	15Ø	12	Ø	-15	2Ø7	219
Ø	Ø	19	83	75	4	Ø	-12	339	343	6	Ø	-3	749	69Ø	8	Ø	7	3Ø3	3Ø4	12	Ø	-14	48	48
2	Ø	-19	74	71	4	Ø	-11	471	47Ø	6	Ø	-2	254	252	8	Ø	8	112	1Ø7	12	Ø	-13	342	349
2	Ø	-18	93	87	4	Ø	-1Ø	399	4Ø2	6	Ø	-1	628	582	8	Ø	9	236	239	12	Ø	-12	1Ø2	1Ø5
2	Ø	-17	91	94	4	Ø	-9	295	295	6	Ø	Ø	316	329	8	Ø	1Ø	34*	8	12	Ø	-11	467	462
2	Ø	-16	242	232	4	Ø	-8	1115	1163	6	Ø	1	737	748	8	Ø	11	237	24Ø	12	Ø	-1Ø	2ØØ	193
2	Ø	-15	63	7Ø	4	Ø	-7	34	34	6	Ø	2	569	614	8	Ø	12	135	137	12	Ø	-9	241	242
2	Ø	-14	13Ø	127	4	Ø	-6	632	565	6	Ø	3	245	236	8	Ø	13	54	54	12	Ø	-8	1Ø8	11Ø
2	Ø	-13	143	145	4	Ø	-5	7Ø	64	6	Ø	4	436	422	8	Ø	14	117	111	12	Ø	-7	192	188
2	Ø	-12	271	284	4	Ø	-4	548	538	6	Ø	5	217	237	1Ø	Ø	-2Ø	65	74	12	Ø	-6	4Ø	41
2	Ø	-11	174	175	4	Ø	-3	63	77	6	Ø	6	55	59	1Ø	Ø	-19	57	51	12	Ø	-5	8Ø	73
2	Ø	-1Ø	322	337	4	Ø	-2	186	2Ø2	6	Ø	7	47	51	1Ø	Ø	-18	73	75	12	Ø	-4	2Ø5	2Ø1
2	Ø	-9	148	134	4	Ø	-1	766	8Ø5	6	Ø	8	248	253	1Ø	Ø	-17	91	94	12	Ø	-3	378	37Ø
2	Ø	-8	28Ø	283	4	Ø	Ø	287	317	6	Ø	9	241	237	1Ø	Ø	-16	49	45	12	Ø	-2	171	174
2	Ø	-7	77	9Ø	4	Ø	1	7Ø	78	6	Ø	1Ø	67	65	1Ø	Ø	-15	Ø*	7	12	Ø	-1	347	36Ø
2	Ø	-6	6Ø6	616	4	Ø	2	583	541	6	Ø	11	222	22Ø	1Ø	Ø	-14	144	143	12	Ø	Ø	Ø*	3
2	Ø	-5	377	329	4	Ø	3	536	513	6	Ø	12	18*	17	1Ø	Ø	-13	211	211	12	Ø	1	358	354
2	Ø	-4	764	861	4	Ø	4	35Ø	323	6	Ø	13	127	128	1Ø	Ø	-12	161	162	12	Ø	2	114	117
2	Ø	-3	444	465	4	Ø	5	634	618	6	Ø	14	Ø*	12	1Ø	Ø	-11	213	214	12	Ø	3	454	448
2	Ø	-2	1223	1346	4	Ø	6	999	1Ø12	6	Ø	15	1Ø2	1Ø5	1Ø	Ø	-1Ø	6Ø	65	12	Ø	4	19*	9
2	Ø	-1	316	372	4	Ø	7	263	26Ø	6	Ø	16	65	62	1Ø	Ø	-9	386	372	12	Ø	5	186	188
2	Ø	Ø	613	553	4	Ø	8	33Ø	317	8	Ø	-2Ø	21*	46	1Ø	Ø	-8	1Ø3	98	12	Ø	6	1Ø6	1Ø5
2	Ø	1	143	126	4	Ø	9	41	38	8	Ø	-19	161	16Ø	1Ø	Ø	-7	734	73Ø	12	Ø	7	92	1ØØ
2	Ø	2	939	1ØØ3	4	Ø	1Ø	276	277	8	Ø	-18	67	7Ø	1Ø	Ø	-6	263	264	12	Ø	8	33*	35
2	Ø	3	2Ø8	175	4	Ø	11	98	1Ø2	8	Ø	-17	1Ø6	1Ø3	1Ø	Ø	-5	414	412	12	Ø	9	9*	2Ø
2	Ø	4	944	882	4	Ø	12	159	149	8	Ø	-16	3Ø2	293	1Ø	Ø	-4	67	74	12	Ø	1Ø	179	174
2	Ø	5	198	221	4	Ø	13	3Ø2	3Ø3	8	Ø	-15	68	78	1Ø	Ø	-3	319	321	12	Ø	11	65	63
2	Ø	6	154	18Ø	4	Ø	14	Ø*	46	8	Ø	-14	38	43	1Ø	Ø	-2	9Ø	9Ø	14	Ø	-18	72	77
2	Ø	7	235	227	4	Ø	15	17Ø	163	8	Ø	-13	9Ø	88	1Ø	Ø	-1	13Ø	133	14	Ø	-17	17Ø	169
2	Ø	8	565	56Ø	4	Ø	16	Ø*	41	8	Ø	-12	226	237	1Ø	Ø	Ø	Ø*	7	14	Ø	-16	55	59
2	Ø	9	359	363	4	Ø	17	7Ø	7Ø	8	Ø	-11	94	95	1Ø	Ø	1	4Ø1	4ØØ	14	Ø	-15	278	276

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
14	0	-14	29*	20	16	0	6	105	107	1	1	4	204	209	3	1	12	307	309	7	1	-16	128	131
14	0	-13	166	166	18	0	-15	156	153	1	1	5	226	206	3	1	13	103	100	7	1	-15	116	122
14	0	-12	153	152	18	0	-14	71	64	1	1	6	234	236	3	1	14	116	110	7	1	-14	139	138
14	0	-11	118	123	18	0	-13	128	126	1	1	7	184	174	3	1	15	84	88	7	1	-13	127	126
14	0	-10	117	116	18	0	-12	110	112	1	1	8	172	177	3	1	16	112	109	7	1	-12	218	215
14	0	-9	81	86	18	0	-11	230	232	1	1	9	277	276	3	1	17	137	137	7	1	-11	21*	10
14	0	-8	60	45	18	0	-10	245	234	1	1	10	27*	24	5	1	-20	119	116	7	1	-10	119	121
14	0	-7	422	422	18	0	-9	254	249	1	1	11	271	277	5	1	-19	29*	21	7	1	-9	89	80
14	0	-6	0*	26	18	0	-8	103	107	1	1	12	50	52	5	1	-18	154	157	7	1	-8	185	172
14	0	-5	305	309	18	0	-7	135	136	1	1	13	235	236	5	1	-17	140	139	7	1	-7	284	295
14	0	-4	63	61	18	0	-6	128	130	1	1	14	198	198	5	1	-16	145	151	7	1	-6	81	80
14	0	-3	384	373	18	0	-5	0*	17	1	1	15	76	74	5	1	-15	224	228	7	1	-5	99	97
14	0	-2	260	258	18	0	-4	0*	21	1	1	16	159	158	5	1	-14	24*	35	7	1	-4	211	195
14	0	-1	389	388	18	0	-3	15*	8	1	1	17	52	43	5	1	-13	239	234	7	1	-3	159	170
14	0	0	18*	19	18	0	-2	109	107	1	1	18	138	142	5	1	-12	28*	29	7	1	-2	14*	11
14	0	1	254	250	18	0	-1	170	170	3	1	-20	27*	31	5	1	-11	284	294	7	1	-1	43	53
14	0	2	125	131	18	0	0	112	114	3	1	-19	107	107	5	1	-10	245	242	7	1	0	134	141
14	0	3	42	43	18	0	1	71	76	3	1	-18	115	111	5	1	-9	83	84	7	1	1	137	135
14	0	4	36*	44	18	0	2	64	72	3	1	-17	134	131	5	1	-8	220	224	7	1	2	141	128
14	0	5	78	84	20	0	-10	0*	42	3	1	-16	210	208	5	1	-7	110	113	7	1	3	90	82
14	0	6	100	105	20	0	-9	38*	20	3	1	-15	38	36	5	1	-6	234	232	7	1	4	191	204
14	0	7	126	133	20	0	-8	43*	46	3	1	-14	225	225	5	1	-5	49	58	7	1	5	238	233
14	0	8	134	129	20	0	-7	0*	41	3	1	-13	94	90	5	1	-4	234	215	7	1	6	156	155
14	0	9	83	73	20	0	-6	143	140	3	1	-12	238	238	5	1	-3	194	198	7	1	7	156	160
16	0	-17	60	55	20	0	-5	92	96	3	1	-11	245	245	5	1	-2	22*	30	7	1	8	98	104
16	0	-16	25*	27	20	0	-4	97	102	3	1	-10	84	88	5	1	-1	182	159	7	1	9	295	297
16	0	-15	87	83	1	1	-19	127	125	3	1	-9	283	283	5	1	0	25*	25	7	1	10	145	145
16	0	-14	28*	29	1	1	-18	34*	36	3	1	-8	119	113	5	1	1	175	161	7	1	11	95	96
16	0	-13	35*	44	1	1	-17	177	175	3	1	-7	246	243	5	1	2	76	64	7	1	12	94	87
16	0	-12	0*	50	1	1	-16	24*	25	3	1	-6	52	51	5	1	3	63	88	7	1	13	118	113
16	0	-11	280	288	1	1	-15	256	264	3	1	-5	256	240	5	1	4	86	85	7	1	14	186	185
16	0	-10	9*	19	1	1	-14	107	109	3	1	-4	35	22	5	1	5	320	314	7	1	15	34*	21
16	0	-9	335	341	1	1	-13	160	163	3	1	-3	27*	34	5	1	6	320	322	9	1	-20	95	96
16	0	-8	186	183	1	1	-12	207	215	3	1	-2	41	44	5	1	7	81	80	9	1	-19	92	89
16	0	-7	381	390	1	1	-11	55	52	3	1	-1	26	34	5	1	8	215	211	9	1	-18	183	183
16	0	-6	258	256	1	1	-10	259	267	3	1	0	44	39	5	1	9	22*	30	9	1	-17	20*	23
16	0	-5	468	462	1	1	-9	46	48	3	1	1	155	152	5	1	10	317	322	9	1	-16	175	176
16	0	-4	135	134	1	1	-8	153	175	3	1	2	129	134	5	1	11	299	298	9	1	-15	52	57
16	0	-3	124	119	1	1	-7	64	86	3	1	3	317	294	5	1	12	0*	11	9	1	-14	175	175
16	0	-2	111	120	1	1	-6	101	101	3	1	4	55	44	5	1	13	131	131	9	1	-13	208	211
16	0	-1	113	113	1	1	-5	63	72	3	1	5	90	96	5	1	14	37	31	9	1	-12	30*	36
16	0	0	116	116	1	1	-4	114	129	3	1	6	81	79	5	1	15	184	180	9	1	-11	66	64
16	0	1	38*	59	1	1	-3	155	167	3	1	7	434	426	5	1	16	87	93	9	1	-10	20*	5
16	0	2	153	151	1	1	-2	8*	2	3	1	8	309	309	7	1	-20	23*	38	9	1	-9	172	169
16	0	3	105	114	1	1	1	32	24	3	1	9	80	80	7	1	-19	141	142	9	1	-8	246	244
16	0	4	33*	28	1	1	2	107	111	3	1	10	193	199	7	1	-18	16*	16	9	1	-7	81	77
16	0	5	154	162	1	1	3	124	136	3	1	11	130	127	7	1	-17	229	226	9	1	-6	6*	8

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
9	1	-5	143	148	11	1	8	74	80	15	1	-6	0*	4	19	1	-1	34*	46	2	2	7	322	323
9	1	-4	73	64	11	1	9	122	123	15	1	-5	71	69	19	1	0	82	86	2	2	8	81	88
9	1	-3	48	52	11	1	10	75	79	15	1	-4	0*	5	0	2	1	644	721	2	2	9	219	223
9	1	-2	141	136	11	1	11	164	164	15	1	-3	30*	31	0	2	2	11*	4	2	2	10	181	179
9	1	-1	209	212	11	1	12	23*	22	15	1	-2	104	100	0	2	3	621	668	2	2	11	36	38
9	1	0	0*	15	13	1	-19	89	92	15	1	-1	142	143	0	2	4	156	148	2	2	12	113	113
9	1	1	26*	36	13	1	-18	79	80	15	1	0	0*	2	0	2	5	468	443	2	2	13	103	98
9	1	2	99	101	13	1	-17	114	110	15	1	1	92	99	0	2	6	188	193	2	2	14	120	122
9	1	3	359	354	13	1	-16	155	160	15	1	2	34*	5	0	2	7	686	725	2	2	15	83	70
9	1	4	131	129	13	1	-15	39*	46	15	1	3	166	160	0	2	8	165	167	2	2	16	84	89
9	1	5	119	120	13	1	-14	190	192	15	1	4	131	133	0	2	9	446	444	2	2	17	122	118
9	1	6	86	78	13	1	-13	12*	13	15	1	5	56	55	0	2	10	89	82	2	2	18	29*	27
9	1	7	191	183	13	1	-12	142	142	15	1	6	94	93	0	2	11	188	184	4	2	-20	91	90
9	1	8	211	214	13	1	-11	98	98	15	1	7	48	45	0	2	12	9*	9	4	2	-19	22*	27
9	1	9	67	70	13	1	-10	33*	10	17	1	-16	38*	46	0	2	13	167	173	4	2	-18	102	101
9	1	10	126	127	13	1	-9	63	67	17	1	-15	81	82	0	2	14	153	150	4	2	-17	125	122
9	1	11	13*	26	13	1	-8	111	110	17	1	-14	102	105	0	2	15	90	81	4	2	-16	147	141
9	1	12	172	169	13	1	-7	102	102	17	1	-13	21*	6	0	2	16	133	127	4	2	-15	269	263
9	1	13	119	116	13	1	-6	57	56	17	1	-12	23*	38	0	2	17	73	62	4	2	-14	39	39
9	1	14	59	55	13	1	-5	40*	45	17	1	-11	41*	49	0	2	18	40	39	4	2	-13	222	218
11	1	-19	107	111	13	1	-4	36*	37	17	1	-10	86	84	0	2	19	30*	10	4	2	-12	142	148
11	1	-18	71	63	13	1	-3	0*	2	17	1	-9	27*	40	2	2	-19	23*	25	4	2	-11	273	266
11	1	-17	149	153	13	1	-2	7*	24	17	1	-8	26*	5	2	2	-18	198	191	4	2	-10	25*	21
11	1	-16	0*	18	13	1	-1	111	112	17	1	-7	0*	13	2	2	-17	46	49	4	2	-9	221	226
11	1	-15	255	265	13	1	0	202	202	17	1	-6	21*	2	2	2	-16	34*	35	4	2	-8	338	341
11	1	-14	93	94	13	1	1	84	79	17	1	-5	63	66	2	2	-15	135	134	4	2	-7	445	452
11	1	-13	128	131	13	1	2	103	95	17	1	-4	28*	18	2	2	-14	93	80	4	2	-6	92	83
11	1	-12	70	71	13	1	3	103	110	17	1	-3	120	119	2	2	-13	251	249	4	2	-5	349	371
11	1	-11	118	122	13	1	4	114	118	17	1	-2	81	89	2	2	-12	103	107	4	2	-4	56	46
11	1	-10	161	153	13	1	5	283	281	17	1	-1	58*	67	2	2	-11	635	636	4	2	-3	191	243
11	1	-9	135	140	13	1	6	24*	19	17	1	0	76	73	2	2	-10	10*	21	4	2	-2	682	728
11	1	-8	20*	29	13	1	7	145	148	17	1	1	61	62	2	2	-9	402	398	4	2	-1	794	850
11	1	-7	132	141	13	1	8	14*	28	17	1	2	120	121	2	2	-8	42	42	4	2	0	67	87
11	1	-6	200	194	13	1	9	132	132	17	1	3	38*	49	2	2	-7	412	422	4	2	1	211	211
11	1	-5	31	41	13	1	10	109	109	17	1	4	75	70	2	2	-6	165	142	4	2	2	349	354
11	1	-4	132	139	15	1	-18	130	125	19	1	-13	16*	7	2	2	-5	454	453	4	2	3	463	433
11	1	-3	89	83	15	1	-17	87	91	19	1	-12	71	75	2	2	-4	487	496	4	2	4	237	230
11	1	-2	24*	14	15	1	-16	73	72	19	1	-11	46	52	2	2	-3	550	569	4	2	5	341	339
11	1	-1	68	68	15	1	-15	104	106	19	1	-10	13*	4	2	2	-2	40	26	4	2	6	307	301
11	1	0	16*	12	15	1	-14	50	49	19	1	-9	12*	8	2	2	-1	882	909	4	2	7	262	250
11	1	1	254	254	15	1	-13	157	156	19	1	-8	15*	16	2	2	0	438	431	4	2	8	272	267
11	1	2	213	215	15	1	-12	24*	19	19	1	-7	19*	24	2	2	1	941	1007	4	2	9	283	277
11	1	3	26*	36	15	1	-11	53	51	19	1	-6	15*	4	2	2	2	433	446	4	2	10	121	115
11	1	4	171	164	15	1	-10	0*	21	19	1	-5	46*	47	2	2	3	936	996	4	2	11	113	115
11	1	5	0*	24	15	1	-9	47*	55	19	1	-4	83	83	2	2	4	178	164	4	2	12	217	221
11	1	6	259	263	15	1	-8	40*	51	19	1	-3	16*	9	2	2	5	668	638	4	2	13	156	150
11	1	7	202	206	15	1	-7	19*	11	19	1	-2	98	99	2	2	6	16*	10	4	2	14	19*	21

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
4	2	15	131	126	8	2	-13	44	39	10	2	-1	160	149	14	2	-17	20*	39	16	2	3	24*	29
4	2	16	67	58	8	2	-12	334	330	10	2	0	699	706	14	2	-16	20*	14	16	2	4	128	130
4	2	17	74	70	8	2	-11	159	148	10	2	1	305	315	14	2	-15	74	75	16	2	5	16*	8
6	2	-20	33*	31	8	2	-10	590	605	10	2	2	377	359	14	2	-14	207	216	16	2	6	11*	20
6	2	-19	125	123	8	2	-9	392	406	10	2	3	155	151	14	2	-13	26*	36	18	2	-15	26*	29
6	2	-18	19*	4	8	2	-8	424	425	10	2	4	191	198	14	2	-12	312	316	18	2	-14	45*	54
6	2	-17	66	64	8	2	-7	167	173	10	2	5	60	58	14	2	-11	0*	18	18	2	-13	78	73
6	2	-16	8*	20	8	2	-6	575	572	10	2	6	62	64	14	2	-10	450	454	18	2	-12	35*	50
6	2	-15	108	103	8	2	-5	92	87	10	2	7	125	130	14	2	-9	101	93	18	2	-11	37*	31
6	2	-14	15*	32	8	2	-4	249	266	10	2	8	127	125	14	2	-8	479	472	18	2	-10	24*	50
6	2	-13	73	78	8	2	-3	27*	62	10	2	9	34*	34	14	2	-7	18*	8	18	2	-9	105	105
6	2	-12	333	337	8	2	-2	405	418	10	2	10	102	102	14	2	-6	211	221	18	2	-8	202	212
6	2	-11	238	232	8	2	-1	406	421	10	2	11	10*	23	14	2	-5	84	76	18	2	-7	124	125
6	2	-10	221	221	8	2	0	288	286	10	2	12	55	59	14	2	-4	143	145	18	2	-6	237	247
6	2	-9	361	368	8	2	1	314	301	10	2	13	0*	22	14	2	-3	96	93	18	2	-5	180	179
6	2	-8	422	418	8	2	2	395	410	12	2	-19	20*	4	14	2	-2	69	71	18	2	-4	205	213
6	2	-7	582	563	8	2	3	301	290	12	2	-18	180	183	14	2	-1	111	106	18	2	-3	212	203
6	2	-6	628	642	8	2	4	553	560	12	2	-17	91	90	14	2	0	207	210	18	2	-2	227	223
6	2	-5	984	967	8	2	5	431	433	12	2	-16	135	137	14	2	1	43	42	18	2	-1	79	77
6	2	-4	533	530	8	2	6	237	229	12	2	-15	17*	34	14	2	2	274	283	18	2	0	83	80
6	2	-3	194	209	8	2	7	160	156	12	2	-14	145	146	14	2	3	80	78	18	2	1	25*	25
6	2	-2	300	292	8	2	8	92	102	12	2	-13	34*	49	14	2	4	189	199	18	2	2	30*	35
6	2	-1	45	49	8	2	9	45	45	12	2	-12	20*	1	14	2	5	87	84	20	2	-10	127	135
6	2	0	255	240	8	2	10	124	128	12	2	-11	13*	2	14	2	6	233	239	20	2	-9	150	154
6	2	1	262	233	8	2	11	164	154	12	2	-10	292	294	14	2	7	31*	15	20	2	-8	137	142
6	2	2	332	334	8	2	12	93	85	12	2	-9	186	178	14	2	8	72	70	20	2	-7	206	203
6	2	3	238	254	8	2	13	79	80	12	2	-8	337	326	14	2	9	45	44	20	2	-6	136	142
6	2	4	296	300	8	2	14	92	88	12	2	-7	15*	16	16	2	-17	28*	29	20	2	-5	108	100
6	2	5	302	295	10	2	-20	106	106	12	2	-6	407	409	16	2	-16	120	116	20	2	-4	7*	47
6	2	6	384	389	10	2	-19	34*	30	12	2	-5	63	61	16	2	-15	86	86	1	3	-19	109	105
6	2	7	167	173	10	2	-18	106	105	12	2	-4	565	579	16	2	-14	236	234	1	3	-18	58	58
6	2	8	489	476	10	2	-17	63	62	12	2	-3	166	164	16	2	-13	130	136	1	3	-17	190	184
6	2	9	345	331	10	2	-16	235	235	12	2	-2	238	240	16	2	-12	318	320	1	3	-16	13*	1
6	2	10	147	156	10	2	-15	128	130	12	2	-1	70	62	16	2	-11	87	90	1	3	-15	221	216
6	2	11	184	186	10	2	-14	305	312	12	2	0	197	184	16	2	-10	190	183	1	3	-14	90	91
6	2	12	0*	12	10	2	-13	281	281	12	2	1	56	54	16	2	-9	152	146	1	3	-13	177	177
6	2	13	91	92	10	2	-12	188	187	12	2	2	95	89	16	2	-8	69	61	1	3	-12	243	251
6	2	14	43*	50	10	2	-11	144	142	12	2	3	154	151	16	2	-7	79	74	1	3	-11	72	74
6	2	15	112	112	10	2	-10	238	242	12	2	4	179	178	16	2	-6	34*	40	1	3	-10	320	320
6	2	16	98	97	10	2	-9	130	129	12	2	5	72	75	16	2	-5	100	99	1	3	-9	81	76
8	2	-20	12*	28	10	2	-8	160	163	12	2	6	161	158	16	2	-4	295	299	1	3	-8	183	193
8	2	-19	94	91	10	2	-7	16*	24	12	2	7	48*	63	16	2	-3	74	74	1	3	-7	113	118
8	2	-18	89	84	10	2	-6	275	291	12	2	8	152	148	16	2	-2	250	256	1	3	-6	204	202
8	2	-17	12*	36	10	2	-5	281	280	12	2	9	58	66	16	2	-1	125	124	1	3	-5	173	167
8	2	-16	137	136	10	2	-4	332	344	12	2	10	141	143	16	2	0	259	268	1	3	-4	70	71
8	2	-15	168	166	10	2	-3	269	262	12	2	11	71	66	16	2	1	190	192	1	3	-3	105	116
8	2	-14	168	166	10	2	-2	503	500	14	2	-18	29*	14	16	2	2	239	242	1	3	-2	22	21

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
1	3	-1	69	73	3	3	8	149	144	7	3	-2Ø	27*	43	9	3	-9	118	115	11	3	4	257	254
1	3	Ø	57	51	3	3	9	179	183	7	3	-19	145	147	9	3	-8	1Ø2	1Ø1	11	3	5	25*	44
1	3	1	6Ø	59	3	3	1Ø	284	282	7	3	-18	38	41	9	3	-7	159	159	11	3	6	169	168
1	3	2	179	177	3	3	11	23*	26	7	3	-17	184	185	9	3	-6	139	145	11	3	7	82	83
1	3	3	13*	1	3	3	12	239	243	7	3	-16	134	136	9	3	-5	23*	24	11	3	8	135	131
1	3	4	85	89	3	3	13	3Ø*	31	7	3	-15	16Ø	167	9	3	-4	15*	2Ø	11	3	9	142	144
1	3	5	14*	4Ø	3	3	14	182	181	7	3	-14	21Ø	214	9	3	-3	1Ø3	1Ø2	11	3	1Ø	Ø*	28
1	3	6	249	241	3	3	15	113	118	7	3	-13	68	63	9	3	-2	16*	7	11	3	11	127	131
1	3	7	2Ø7	211	3	3	16	93	94	7	3	-12	164	161	9	3	-1	14*	13	11	3	12	19*	4
1	3	8	14Ø	143	3	3	17	121	115	7	3	-11	Ø*	2Ø	9	3	Ø	171	165	13	3	-19	1Ø8	1Ø5
1	3	9	2Ø5	219	5	3	-2Ø	126	124	7	3	-1Ø	198	2Ø3	9	3	1	184	188	13	3	-18	93	98
1	3	1Ø	9Ø	87	5	3	-19	2Ø*	11	7	3	-9	169	166	9	3	2	Ø*	4	13	3	-17	8Ø	78
1	3	11	27Ø	273	5	3	-18	158	159	7	3	-8	1Ø2	96	9	3	3	181	175	13	3	-16	14Ø	144
1	3	12	65	64	5	3	-17	134	13Ø	7	3	-7	1Ø2	1ØØ	9	3	4	22*	25	13	3	-15	23*	19
1	3	13	189	186	5	3	-16	125	125	7	3	-6	42	47	9	3	5	212	218	13	3	-14	222	216
1	3	14	185	188	5	3	-15	21Ø	21Ø	7	3	-5	115	113	9	3	6	176	174	13	3	-13	24*	17
1	3	15	1Ø3	93	5	3	-14	6Ø	62	7	3	-4	91	87	9	3	7	13Ø	127	13	3	-12	137	137
1	3	16	199	199	5	3	-13	243	248	7	3	-3	126	114	9	3	8	149	151	13	3	-11	27*	28
1	3	17	28*	22	5	3	-12	56	55	7	3	-2	1ØØ	1Ø1	9	3	9	31*	41	13	3	-1Ø	45	48
1	3	18	133	134	5	3	-11	2Ø5	2Ø4	7	3	-1	92	88	9	3	1Ø	191	192	13	3	-9	31*	37
3	3	-19	112	112	5	3	-1Ø	155	151	7	3	Ø	21*	14	9	3	11	48*	54	13	3	-8	Ø*	2
3	3	-18	127	122	5	3	-9	131	131	7	3	1	55	59	9	3	12	133	129	13	3	-7	28*	16
3	3	-17	1Ø4	1Ø6	5	3	-8	324	315	7	3	2	3Ø6	295	9	3	13	8Ø	75	13	3	-6	46	45
3	3	-16	2Ø8	211	5	3	-7	49	51	7	3	3	62	59	9	3	14	93	88	13	3	-5	35*	37
3	3	-15	3Ø*	33	5	3	-6	21Ø	192	7	3	4	134	134	11	3	-19	97	94	13	3	-4	Ø*	2Ø
3	3	-14	229	233	5	3	-5	158	139	7	3	5	193	183	11	3	-18	85	88	13	3	-3	85	81
3	3	-13	8Ø	82	5	3	-4	24*	7	7	3	6	268	256	11	3	-17	145	148	13	3	-2	115	112
3	3	-12	251	249	5	3	-3	Ø*	1Ø	7	3	7	289	284	11	3	-16	Ø*	5	13	3	-1	21*	27
3	3	-11	251	26Ø	5	3	-2	174	161	7	3	8	26*	6	11	3	-15	173	17Ø	13	3	Ø	113	117
3	3	-1Ø	115	118	5	3	-1	Ø*	12	7	3	9	22Ø	22Ø	11	3	-14	56	55	13	3	1	3Ø*	3Ø
3	3	-9	211	218	5	3	Ø	179	168	7	3	1Ø	86	88	11	3	-13	145	148	13	3	2	162	165
3	3	-8	16*	8	5	3	1	117	1Ø4	7	3	11	2Ø3	196	11	3	-12	149	151	13	3	3	177	177
3	3	-7	292	296	5	3	2	76	68	7	3	12	178	175	11	3	-11	8*	15	13	3	4	5Ø	54
3	3	-6	16Ø	141	5	3	3	135	142	7	3	13	64	6Ø	11	3	-1Ø	96	87	13	3	5	177	183
3	3	-5	13Ø	12Ø	5	3	4	146	154	7	3	14	136	134	11	3	-9	Ø*	19	13	3	6	19*	12
3	3	-4	41	43	5	3	5	138	13Ø	7	3	15	3Ø*	24	11	3	-8	1Ø1	1Ø4	13	3	7	183	188
3	3	-3	64	6Ø	5	3	6	197	2Ø1	9	3	-2Ø	12Ø	115	11	3	-7	18*	8	13	3	8	76	84
3	3	-2	96	89	5	3	7	19*	17	9	3	-19	7Ø	69	11	3	-6	Ø*	21	13	3	9	98	1ØØ
3	3	-1	8*	11	5	3	8	343	342	9	3	-18	167	169	11	3	-5	4Ø*	34	13	3	1Ø	89	91
3	3	Ø	126	119	5	3	9	184	183	9	3	-17	13*	23	11	3	-4	21*	11	15	3	-18	119	114
3	3	1	41	39	5	3	1Ø	176	181	9	3	-16	234	239	11	3	-3	25*	22	15	3	-17	67	71
3	3	2	2Ø*	26	5	3	11	158	155	9	3	-15	83	86	11	3	-2	8Ø	79	15	3	-16	1Ø4	1Ø8
3	3	3	184	165	5	3	12	1Ø5	1Ø3	9	3	-14	175	175	11	3	-1	164	164	15	3	-15	126	128
3	3	4	212	199	5	3	13	2Ø3	199	9	3	-13	116	114	11	3	Ø	54	47	15	3	-14	35*	34
3	3	5	335	329	5	3	14	12*	26	9	3	-12	129	133	11	3	1	1Ø7	1Ø9	15	3	-13	131	128
3	3	6	64	63	5	3	15	133	131	9	3	-11	169	171	11	3	2	1Ø8	1Ø8	15	3	-12	26*	13
3	3	7	238	25Ø	5	3	16	47*	52	9	3	-1Ø	78	86	11	3	3	81	85	15	3	-11	46	45

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
15	3	-10	43*	60	19	3	-5	38*	35	2	4	2	86	86	4	4	10	111	111	8	4	-18	124	127
15	3	-9	0*	12	19	3	-4	78	77	2	4	3	452	421	4	4	11	12*	39	8	4	-17	191	190
15	3	-8	50	46	19	3	-3	33*	4	2	4	4	18*	21	4	4	12	185	183	8	4	-16	156	145
15	3	-7	0*	7	19	3	-2	106	108	2	4	5	16*	18	4	4	13	198	198	8	4	-15	50	54
15	3	-6	17*	24	19	3	-1	49*	54	2	4	6	603	613	4	4	14	0*	18	8	4	-14	114	122
15	3	-5	33*	36	19	3	0	88	88	2	4	7	236	239	4	4	15	191	183	8	4	-13	198	202
15	3	-4	66	58	0	4	0	1362	1551	2	4	8	364	350	4	4	16	27*	6	8	4	-12	117	114
15	3	-3	51*	57	0	4	1	516	558	2	4	9	125	129	4	4	17	50	49	8	4	-11	0*	3
15	3	-2	75	68	0	4	2	1091	1197	2	4	10	533	537	6	4	-20	43	35	8	4	-10	97	91
15	3	-1	87	82	0	4	3	322	281	2	4	11	98	95	6	4	-19	177	172	8	4	-9	239	233
15	3	0	80	77	0	4	4	266	255	2	4	12	190	188	6	4	-18	15*	21	8	4	-8	311	308
15	3	1	138	138	0	4	5	101	96	2	4	13	87	84	6	4	-17	86	91	8	4	-7	413	407
15	3	2	42*	51	0	4	6	341	334	2	4	14	164	168	6	4	-16	104	105	8	4	-6	319	313
15	3	3	124	120	0	4	7	82	76	2	4	15	51	48	6	4	-15	266	261	8	4	-5	647	642
15	3	4	97	95	0	4	8	260	258	2	4	16	105	105	6	4	-14	195	196	8	4	-4	465	463
15	3	5	96	96	0	4	9	98	102	2	4	17	155	147	6	4	-13	226	232	8	4	-3	935	954
15	3	6	134	132	0	4	10	261	260	2	4	18	73	66	6	4	-12	444	452	8	4	-2	515	533
15	3	7	20*	19	0	4	11	0*	6	4	4	-20	43*	56	6	4	-11	198	195	8	4	-1	392	389
17	3	-16	48*	62	0	4	12	240	241	4	4	-19	19*	19	6	4	-10	179	186	8	4	0	304	295
17	3	-15	40*	52	0	4	13	174	180	4	4	-18	101	93	6	4	-9	230	221	8	4	1	321	310
17	3	-14	52*	66	0	4	14	244	242	4	4	-17	165	164	6	4	-8	279	271	8	4	2	107	113
17	3	-13	31*	26	0	4	15	50	47	4	4	-16	118	119	6	4	-7	348	358	8	4	3	122	115
17	3	-12	58*	77	0	4	16	216	213	4	4	-15	121	115	6	4	-6	65	55	8	4	4	131	130
17	3	-11	24*	1	0	4	17	80	74	4	4	-14	188	190	6	4	-5	185	194	8	4	5	208	211
17	3	-10	52	49	0	4	18	31*	36	4	4	-13	175	179	6	4	-4	169	187	8	4	6	91	91
17	3	-9	20*	44	0	4	19	110	107	4	4	-12	154	152	6	4	-3	512	480	8	4	7	286	289
17	3	-8	33*	36	2	4	-19	17*	7	4	4	-11	216	213	6	4	-2	599	585	8	4	8	100	101
17	3	-7	0*	4	2	4	-18	144	143	4	4	-10	600	598	6	4	-1	738	718	8	4	9	180	177
17	3	-6	12*	5	2	4	-17	19*	32	4	4	-9	368	372	6	4	0	574	549	8	4	10	64	68
17	3	-5	59	62	2	4	-16	127	124	4	4	-8	604	626	6	4	1	535	542	8	4	11	207	208
17	3	-4	0*	16	2	4	-15	96	95	4	4	-7	49	55	6	4	2	552	572	8	4	12	141	135
17	3	-3	67	70	2	4	-14	239	238	4	4	-6	722	696	6	4	3	419	416	8	4	13	58	63
17	3	-2	48	59	2	4	-13	0*	20	4	4	-5	251	240	6	4	4	296	299	8	4	14	114	111
17	3	-1	80	86	2	4	-12	29*	32	4	4	-4	280	256	6	4	5	176	189	10	4	-20	95	98
17	3	0	96	95	2	4	-11	236	241	4	4	-3	18*	12	6	4	6	170	176	10	4	-19	79	79
17	3	1	27*	34	2	4	-10	125	133	4	4	-2	253	232	6	4	7	110	110	10	4	-18	61	63
17	3	2	99	99	2	4	-9	55	43	4	4	-1	206	204	6	4	8	136	133	10	4	-17	64	68
17	3	3	24*	28	2	4	-8	474	485	4	4	0	426	420	6	4	9	224	221	10	4	-16	101	99
17	3	4	103	96	2	4	-7	187	194	4	4	1	216	202	6	4	10	0*	10	10	4	-15	38*	44
19	3	-13	33*	43	2	4	-6	726	713	4	4	2	384	352	6	4	11	195	189	10	4	-14	68	60
19	3	-12	35*	50	2	4	-5	89	75	4	4	3	217	224	6	4	12	77	70	10	4	-13	232	231
19	3	-11	24*	41	2	4	-4	900	886	4	4	4	535	522	6	4	13	141	143	10	4	-12	78	72
19	3	-10	19*	29	2	4	-3	145	146	4	4	5	637	652	6	4	14	6*	16	10	4	-11	216	219
19	3	-9	8*	20	2	4	-2	548	582	4	4	6	511	523	6	4	15	83	80	10	4	-10	170	173
19	3	-8	6*	13	2	4	-1	43	52	4	4	7	158	157	6	4	16	62	55	10	4	-9	512	513
19	3	-7	0*	25	2	4	0	742	729	4	4	8	487	493	8	4	-20	20*	15	10	4	-8	168	162
19	3	-6	0*	26	2	4	1	643	642	4	4	9	131	131	8	4	-19	113	112	10	4	-7	625	634

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
10	4	-6	309	315	12	4	8	92	94	16	4	-2	120	119	1	5	-4	88	92	3	5	5	257	264
10	4	-5	541	535	12	4	9	33*	38	16	4	-1	32*	38	1	5	-3	165	162	3	5	6	185	177
10	4	-4	159	160	12	4	10	136	134	16	4	0	20*	22	1	5	-2	30	26	3	5	7	91	97
10	4	-3	322	310	12	4	11	83	80	16	4	1	36*	6	1	5	-1	60	59	3	5	8	68	60
10	4	-2	49	45	14	4	-18	39*	56	16	4	2	79	75	1	5	0	36	34	3	5	9	291	299
10	4	-1	120	124	14	4	-17	171	174	16	4	3	172	173	1	5	1	160	165	3	5	10	331	330
10	4	0	22*	26	14	4	-16	44*	47	16	4	4	111	115	1	5	2	205	214	3	5	11	16*	14
10	4	1	276	279	14	4	-15	276	279	16	4	5	97	96	1	5	3	45	38	3	5	12	169	166
10	4	2	102	100	14	4	-14	0*	5	16	4	6	45	42	1	5	4	59	63	3	5	13	20*	7
10	4	3	379	379	14	4	-13	202	203	18	4	-14	41*	47	1	5	5	169	143	3	5	14	200	194
10	4	4	114	114	14	4	-12	79	81	18	4	-13	168	169	1	5	6	326	314	3	5	15	129	128
10	4	5	298	298	14	4	-11	160	158	18	4	-12	167	167	1	5	7	193	195	3	5	16	72	71
10	4	6	12*	17	14	4	-10	36*	31	18	4	-11	188	189	1	5	8	115	124	3	5	17	95	98
10	4	7	334	331	14	4	-9	54	59	18	4	-10	198	201	1	5	9	203	207	5	5	-20	123	123
10	4	8	88	83	14	4	-8	66	62	18	4	-9	272	274	1	5	10	68	64	5	5	-19	23*	32
10	4	9	132	130	14	4	-7	307	305	18	4	-8	167	162	1	5	11	312	308	5	5	-18	148	149
10	4	10	122	116	14	4	-6	32*	20	18	4	-7	126	127	1	5	12	125	130	5	5	-17	143	147
10	4	11	55	55	14	4	-5	377	379	18	4	-6	81	76	1	5	13	164	165	5	5	-16	119	122
10	4	12	109	105	14	4	-4	106	107	18	4	-5	26*	42	1	5	14	137	138	5	5	-15	206	211
10	4	13	6*	9	14	4	-3	348	349	18	4	-4	13*	19	1	5	15	146	146	5	5	-14	60	62
12	4	-19	25*	31	14	4	-2	139	136	18	4	-3	43*	54	1	5	16	203	200	5	5	-13	263	264
12	4	-18	78	78	14	4	-1	492	489	18	4	-2	131	133	1	5	17	25*	12	5	5	-12	58	63
12	4	-17	134	134	14	4	0	74	75	18	4	-1	128	133	1	5	18	128	124	5	5	-11	200	199
12	4	-16	0*	20	14	4	1	247	243	18	4	0	81	81	3	5	-19	120	119	5	5	-10	142	148
12	4	-15	206	207	14	4	2	42	31	18	4	1	134	139	3	5	-18	120	119	5	5	-9	131	139
12	4	-14	20*	14	14	4	3	128	132	18	4	2	133	135	3	5	-17	84	81	5	5	-8	191	193
12	4	-13	365	363	14	4	4	6*	5	20	4	-9	0*	33	3	5	-16	170	170	5	5	-7	18*	17
12	4	-12	87	85	14	4	5	13*	2	20	4	-8	0*	2	3	5	-15	30*	37	5	5	-6	17*	24
12	4	-11	461	466	14	4	6	140	142	20	4	-7	25*	13	3	5	-14	228	228	5	5	-5	72	72
12	4	-10	140	142	14	4	7	58*	71	20	4	-6	85	90	3	5	-13	93	89	5	5	-4	60	59
12	4	-9	282	276	14	4	8	78	76	20	4	-5	136	139	3	5	-12	199	199	5	5	-3	88	84
12	4	-8	18*	20	14	4	9	117	115	20	4	-4	144	141	3	5	-11	222	214	5	5	-2	27*	48
12	4	-7	199	196	16	4	-17	77	78	1	5	-19	105	103	3	5	-10	116	118	5	5	-1	23*	19
12	4	-6	0*	20	16	4	-16	19*	42	1	5	-18	78	78	3	5	-9	291	292	5	5	0	47	38
12	4	-5	63	63	16	4	-15	68	66	1	5	-17	208	208	3	5	-8	51	49	5	5	1	160	152
12	4	-4	79	75	16	4	-14	27*	3	1	5	-16	22*	35	3	5	-7	279	283	5	5	2	126	117
12	4	-3	339	342	16	4	-13	24*	24	1	5	-15	189	192	3	5	-6	17*	6	5	5	3	132	142
12	4	-2	33*	29	16	4	-12	42*	48	1	5	-14	39*	51	3	5	-5	203	185	5	5	4	291	293
12	4	-1	351	354	16	4	-11	240	250	1	5	-13	218	224	3	5	-4	48	43	5	5	5	60	59
12	4	0	11*	8	16	4	-10	63	57	1	5	-12	202	205	3	5	-3	49	41	5	5	6	207	200
12	4	1	435	440	16	4	-9	296	301	1	5	-11	43	40	3	5	-2	24	19	5	5	7	108	112
12	4	2	97	95	16	4	-8	176	171	1	5	-10	239	239	3	5	-1	63	56	5	5	8	396	394
12	4	3	398	404	16	4	-7	376	382	1	5	-9	37	32	3	5	0	136	129	5	5	9	202	203
12	4	4	83	85	16	4	-6	241	236	1	5	-8	239	248	3	5	1	92	69	5	5	10	115	119
12	4	5	244	246	16	4	-5	402	409	1	5	-7	125	125	3	5	2	8*	12	5	5	11	69	75
12	4	6	72	69	16	4	-4	83	79	1	5	-6	199	182	3	5	3	39*	55	5	5	12	167	170
12	4	7	20*	26	16	4	-3	204	199	1	5	-5	208	197	3	5	4	122	127	5	5	13	251	254

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	5	14	56	63	9	5	-12	125	123	11	5	2	59	57	15	5	-10	82	79	19	5	-4	50	58
5	5	15	101	100	9	5	-11	238	241	11	5	3	98	101	15	5	-9	16*	2	19	5	-3	26*	1
5	5	16	34*	39	9	5	-10	95	93	11	5	4	280	279	15	5	-8	0*	2	19	5	-2	81	93
7	5	-20	52	57	9	5	-9	88	94	11	5	5	101	101	15	5	-7	56	46	19	5	-1	30*	50
7	5	-19	162	159	9	5	-8	45	46	11	5	6	143	144	15	5	-6	34*	45	0	6	0	100	82
7	5	-18	22*	29	9	5	-7	224	226	11	5	7	70	74	15	5	-5	10*	4	0	6	1	119	108
7	5	-17	185	182	9	5	-6	135	134	11	5	8	178	178	15	5	-4	72	73	0	6	2	590	591
7	5	-16	80	83	9	5	-5	63	70	11	5	9	195	189	15	5	-3	118	115	0	6	3	771	800
7	5	-15	185	189	9	5	-4	119	119	11	5	10	34*	31	15	5	-2	23*	27	0	6	4	33	57
7	5	-14	180	180	9	5	-3	116	119	11	5	11	123	124	15	5	-1	62*	65	0	6	5	734	707
7	5	-13	65	62	9	5	-2	17*	19	11	5	12	19*	8	15	5	0	80	76	0	6	6	50	49
7	5	-12	135	139	9	5	-1	11*	16	13	5	-18	98	96	15	5	1	188	188	0	6	7	790	801
7	5	-11	43*	40	9	5	0	203	205	13	5	-17	81	80	15	5	2	73	80	0	6	8	107	95
7	5	-10	178	179	9	5	1	179	176	13	5	-16	117	123	15	5	3	83	81	0	6	9	520	514
7	5	-9	196	191	9	5	2	21*	26	13	5	-15	70	69	15	5	4	51*	56	0	6	10	53	61
7	5	-8	29*	37	9	5	3	107	107	13	5	-14	161	160	15	5	5	106	105	0	6	11	242	236
7	5	-7	94	92	9	5	4	50	49	13	5	-13	26*	10	15	5	6	137	139	0	6	12	29*	34
7	5	-6	89	82	9	5	5	244	245	13	5	-12	67	74	15	5	7	0*	7	0	6	13	128	131
7	5	-5	176	177	9	5	6	210	207	13	5	-11	20*	16	17	5	-16	84	86	0	6	14	198	196
7	5	-4	73	76	9	5	7	30*	27	13	5	-10	102	100	17	5	-15	41	50	0	6	15	62	61
7	5	-3	113	113	9	5	8	128	126	13	5	-9	113	114	17	5	-14	36*	48	0	6	16	106	104
7	5	-2	183	177	9	5	9	28*	33	13	5	-8	78	78	17	5	-13	77	82	0	6	17	73	67
7	5	-1	117	113	9	5	10	214	212	13	5	-7	25*	33	17	5	-12	112	112	0	6	18	67	71
7	5	0	6*	17	9	5	11	87	89	13	5	-6	80	76	17	5	-11	22*	18	2	6	-19	22*	34
7	5	1	87	89	9	5	12	120	119	13	5	-5	115	113	17	5	-10	18*	16	2	6	-18	123	120
7	5	2	256	264	9	5	13	78	74	13	5	-4	65	60	17	5	-9	25*	17	2	6	-17	101	102
7	5	3	84	88	11	5	-19	78	78	13	5	-3	117	119	17	5	-8	29*	6	2	6	-16	123	121
7	5	4	190	179	11	5	-18	86	84	13	5	-2	143	146	17	5	-7	31*	14	2	6	-15	98	102
7	5	5	135	133	11	5	-17	183	186	13	5	-1	58	56	17	5	-6	24*	15	2	6	-14	18*	12
7	5	6	217	207	11	5	-16	16*	15	13	5	0	87	90	17	5	-5	49*	65	2	6	-13	342	341
7	5	7	258	257	11	5	-15	196	199	13	5	1	29*	20	17	5	-4	25*	27	2	6	-12	129	134
7	5	8	33*	38	11	5	-14	5*	25	13	5	2	198	189	17	5	-3	81	80	2	6	-11	369	378
7	5	9	123	126	11	5	-13	220	220	13	5	3	214	214	17	5	-2	0*	21	2	6	-10	53	48
7	5	10	19*	6	11	5	-12	179	178	13	5	4	41	36	17	5	-1	100	106	2	6	-9	480	486
7	5	11	227	228	11	5	-11	20*	25	13	5	5	152	149	17	5	0	95	97	2	6	-8	139	148
7	5	12	195	198	11	5	-10	12*	16	13	5	6	85	82	17	5	1	20*	19	2	6	-7	487	484
7	5	13	33*	25	11	5	-9	119	118	13	5	7	220	215	17	5	2	79	84	2	6	-6	43	37
7	5	14	120	115	11	5	-8	196	197	13	5	8	78	81	17	5	3	18*	10	2	6	-5	47	28
7	5	15	35*	40	11	5	-7	120	122	13	5	9	92	89	17	5	4	105	103	2	6	-4	100	92
9	5	-20	110	106	11	5	-6	41	37	13	5	10	86	80	19	5	-12	0*	17	2	6	-3	390	357
9	5	-19	54	50	11	5	-5	116	120	15	5	-17	37*	41	19	5	-11	28*	4	2	6	-2	30*	13
9	5	-18	126	126	11	5	-4	18*	18	15	5	-16	111	107	19	5	-10	24*	27	2	6	-1	344	347
9	5	-17	22*	24	11	5	-3	31*	30	15	5	-15	128	130	19	5	-9	18*	20	2	6	0	225	221
9	5	-16	230	228	11	5	-2	59	50	15	5	-14	26*	15	19	5	-8	29*	17	2	6	1	807	852
9	5	-15	136	138	11	5	-1	171	175	15	5	-13	93	92	19	5	-7	23*	36	2	6	2	318	290
9	5	-14	83	87	11	5	0	110	114	15	5	-12	24*	6	19	5	-6	27*	28	2	6	3	575	590
9	5	-13	113	114	11	5	1	44	40	15	5	-11	102	104	19	5	-5	20*	15	2	6	4	63	83

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	6	5	716	732	4	6	14	73	69	8	6	-14	86	92	1Ø	6	-1	148	148	14	6	-17	9*	26
2	6	6	146	15Ø	4	6	15	12Ø	112	8	6	-13	167	166	1Ø	6	Ø	667	674	14	6	-16	19*	15
2	6	7	199	199	4	6	16	71	7Ø	8	6	-12	348	355	1Ø	6	1	159	161	14	6	-15	45*	5Ø
2	6	8	9*	9	4	6	17	79	78	8	6	-11	25Ø	244	1Ø	6	2	431	423	14	6	-14	199	2Ø4
2	6	9	217	214	6	6	-2Ø	79	77	8	6	-1Ø	437	444	1Ø	6	3	12Ø	119	14	6	-13	28*	22
2	6	1Ø	Ø*	18	6	6	-19	42*	49	8	6	-9	4Ø9	4Ø3	1Ø	6	4	124	122	14	6	-12	3Ø3	298
2	6	11	72	72	6	6	-18	28*	36	8	6	-8	461	468	1Ø	6	5	17*	34	14	6	-11	81	85
2	6	12	2Ø8	2Ø8	6	6	-17	17Ø	164	8	6	-7	222	215	1Ø	6	6	5*	4	14	6	-1Ø	424	432
2	6	13	34	28	6	6	-16	72	69	8	6	-6	3Ø7	3Ø5	1Ø	6	7	59	56	14	6	-9	9Ø	87
2	6	14	93	95	6	6	-15	95	94	8	6	-5	286	286	1Ø	6	8	159	164	14	6	-8	438	435
2	6	15	82	81	6	6	-14	67	71	8	6	-4	2Ø4	2Ø1	1Ø	6	9	58	59	14	6	-7	27*	22
2	6	16	92	91	6	6	-13	93	92	8	6	-3	32	49	1Ø	6	1Ø	129	127	14	6	-6	291	288
2	6	17	8Ø	79	6	6	-12	116	113	8	6	-2	418	439	1Ø	6	11	15*	16	14	6	-5	111	1Ø7
2	6	18	16*	26	6	6	-11	317	314	8	6	-1	273	281	1Ø	6	12	93	91	14	6	-4	91	82
4	6	-19	38	41	6	6	-1Ø	222	214	8	6	Ø	466	459	1Ø	6	13	34*	15	14	6	-3	39*	38
4	6	-18	155	153	6	6	-9	353	357	8	6	1	367	37Ø	12	6	-19	15*	16	14	6	-2	28*	15
4	6	-17	95	97	6	6	-8	284	276	8	6	2	516	5Ø8	12	6	-18	165	167	14	6	-1	97	87
4	6	-16	24*	22	6	6	-7	572	559	8	6	3	243	241	12	6	-17	92	96	14	6	Ø	273	279
4	6	-15	354	349	6	6	-6	654	67Ø	8	6	4	462	462	12	6	-16	146	152	14	6	1	123	124
4	6	-14	62	58	6	6	-5	445	463	8	6	5	251	248	12	6	-15	34*	44	14	6	2	285	289
4	6	-13	181	185	6	6	-4	484	474	8	6	6	288	279	12	6	-14	148	152	14	6	3	29*	28
4	6	-12	14*	17	6	6	-3	642	646	8	6	7	129	133	12	6	-13	59	58	14	6	4	271	273
4	6	-11	311	318	6	6	-2	371	381	8	6	8	69	74	12	6	-12	23*	23	14	6	5	88	93
4	6	-1Ø	19*	24	6	6	-1	142	139	8	6	9	76	78	12	6	-11	11*	2Ø	14	6	6	188	191
4	6	-9	69	54	6	6	Ø	19*	22	8	6	1Ø	43*	37	12	6	-1Ø	288	288	14	6	7	31*	35
4	6	-8	2Ø1	216	6	6	1	152	129	8	6	11	145	139	12	6	-9	96	98	14	6	8	111	113
4	6	-7	299	3Ø6	6	6	2	1Ø7	1Ø5	8	6	12	91	89	12	6	-8	372	37Ø	16	6	-16	147	147
4	6	-6	1Ø2	97	6	6	3	223	226	8	6	13	63	65	12	6	-7	87	89	16	6	-15	1Ø2	1Ø1
4	6	-5	649	632	6	6	4	259	252	8	6	14	115	1Ø8	12	6	-6	531	531	16	6	-14	241	239
4	6	-4	361	335	6	6	5	2Ø3	2Ø3	1Ø	6	-19	Ø*	16	12	6	-5	9*	2	16	6	-13	13Ø	129
4	6	-3	611	542	6	6	6	333	339	1Ø	6	-18	131	127	12	6	-4	615	618	16	6	-12	3Ø3	3Ø5
4	6	-2	389	37Ø	6	6	7	155	159	1Ø	6	-17	13*	11	12	6	-3	76	77	16	6	-11	115	11Ø
4	6	-1	9Ø4	839	6	6	8	382	383	1Ø	6	-16	21Ø	2Ø3	12	6	-2	346	341	16	6	-1Ø	2Ø2	2Ø1
4	6	Ø	367	336	6	6	9	269	264	1Ø	6	-15	11Ø	1Ø5	12	6	-1	21*	14	16	6	-9	122	126
4	6	1	574	535	6	6	1Ø	128	132	1Ø	6	-14	335	336	12	6	Ø	212	2Ø7	16	6	-8	112	1Ø7
4	6	2	481	467	6	6	11	222	215	1Ø	6	-13	16Ø	154	12	6	1	Ø*	8	16	6	-7	62	57
4	6	3	354	358	6	6	12	23*	16	1Ø	6	-12	2Ø7	2Ø8	12	6	2	Ø*	4	16	6	-6	58	57
4	6	4	262	255	6	6	13	97	97	1Ø	6	-11	141	141	12	6	3	131	132	16	6	-5	1Ø4	97
4	6	5	115	126	6	6	14	59	62	1Ø	6	-1Ø	25Ø	253	12	6	4	171	173	16	6	-4	282	293
4	6	6	232	228	6	6	15	95	93	1Ø	6	-9	24*	5	12	6	5	49	46	16	6	-3	73	71
4	6	7	85	81	6	6	16	1ØØ	89	1Ø	6	-8	79	64	12	6	6	261	263	16	6	-2	338	344
4	6	8	181	186	8	6	-2Ø	24*	35	1Ø	6	-7	4Ø*	4Ø	12	6	7	59	62	16	6	-1	165	162
4	6	9	3Ø2	3Ø3	8	6	-19	139	137	1Ø	6	-6	246	253	12	6	8	151	148	16	6	Ø	252	25Ø
4	6	1Ø	2Ø1	2Ø4	8	6	-18	54	46	1Ø	6	-5	194	2Ø5	12	6	9	Ø*	27	16	6	1	1Ø9	112
4	6	11	1Ø6	98	8	6	-17	17*	1Ø	1Ø	6	-4	53Ø	526	12	6	1Ø	158	155	16	6	2	279	272
4	6	12	191	188	8	6	-16	181	18Ø	1Ø	6	-3	194	2ØØ	12	6	11	44*	45	16	6	3	69	7Ø
4	6	13	177	171	8	6	-15	36*	41	1Ø	6	-2	614	599	14	6	-18	35*	44	16	6	4	87	86

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
16	6	5	46	46	1	7	6	218	212	3	7	15	128	124	7	7	-12	196	195	9	7	0	78	75
18	6	-14	86	86	1	7	7	159	165	3	7	16	98	95	7	7	-11	0*	18	9	7	1	108	110
18	6	-13	108	102	1	7	8	151	154	3	7	17	134	132	7	7	-10	166	169	9	7	2	9*	5
18	6	-12	20*	19	1	7	9	224	224	5	7	-19	20*	23	7	7	-9	112	116	9	7	3	155	154
18	6	-11	26*	17	1	7	10	61	62	5	7	-18	142	142	7	7	-8	85	88	9	7	4	0*	4
18	6	-10	23*	32	1	7	11	280	279	5	7	-17	108	109	7	7	-7	59	52	9	7	5	230	226
18	6	-9	76	72	1	7	12	66	71	5	7	-16	123	125	7	7	-6	94	91	9	7	6	141	144
18	6	-8	196	204	1	7	13	185	184	5	7	-15	174	174	7	7	-5	139	142	9	7	7	100	100
18	6	-7	160	162	1	7	14	119	120	5	7	-14	43*	56	7	7	-4	54	55	9	7	8	142	139
18	6	-6	226	233	1	7	15	135	133	5	7	-13	196	195	7	7	-3	113	116	9	7	9	77	76
18	6	-5	167	163	1	7	16	177	177	5	7	-12	74	74	7	7	-2	16*	24	9	7	10	188	189
18	6	-4	237	241	1	7	17	11*	7	5	7	-11	185	179	7	7	-1	102	98	9	7	11	40*	47
18	6	-3	191	182	1	7	18	136	135	5	7	-10	174	179	7	7	0	26*	32	9	7	12	143	136
18	6	-2	182	182	3	7	-19	121	122	5	7	-9	156	158	7	7	1	74	79	9	7	13	92	92
18	6	-1	40*	49	3	7	-18	129	126	5	7	-8	174	175	7	7	2	190	186	11	7	-19	76	78
18	6	0	97	94	3	7	-17	85	80	5	7	-7	26	33	7	7	3	93	89	11	7	-18	91	91
18	6	1	32*	48	3	7	-16	188	187	5	7	-6	111	123	7	7	4	198	188	11	7	-17	147	148
18	6	2	10*	12	3	7	-15	53	49	5	7	-5	28*	16	7	7	5	141	142	11	7	-16	0*	15
20	6	-8	105	110	3	7	-14	238	242	5	7	-4	110	101	7	7	6	151	151	11	7	-15	162	167
20	6	-7	166	170	3	7	-13	32*	30	5	7	-3	45	47	7	7	7	285	285	11	7	-14	39	38
20	6	-6	145	142	3	7	-12	202	202	5	7	-2	7*	6	7	7	8	20*	29	11	7	-13	138	141
20	6	-5	131	122	3	7	-11	179	171	5	7	-1	128	124	7	7	9	207	208	11	7	-12	120	112
1	7	-19	104	102	3	7	-10	119	115	5	7	0	57	53	7	7	10	47	41	11	7	-11	25*	32
1	7	-18	54	54	3	7	-9	292	282	5	7	1	196	202	7	7	11	221	220	11	7	-10	88	90
1	7	-17	185	183	3	7	-8	28*	25	5	7	2	141	134	7	7	12	160	162	11	7	-9	28*	40
1	7	-16	52	52	3	7	-7	246	257	5	7	3	138	148	7	7	13	79	75	11	7	-8	177	177
1	7	-15	196	196	3	7	-6	37	45	5	7	4	252	243	7	7	14	143	139	11	7	-7	103	105
1	7	-14	86	86	3	7	-5	169	169	5	7	5	78	72	7	7	15	8*	12	11	7	-6	39	36
1	7	-13	235	236	3	7	-4	151	150	5	7	6	232	221	9	7	-19	41*	52	11	7	-5	54	53
1	7	-12	222	222	3	7	-3	83	83	5	7	7	60	57	9	7	-18	149	147	11	7	-4	21*	30
1	7	-11	68	69	3	7	-2	121	101	5	7	8	278	279	9	7	-17	31*	14	11	7	-3	83	87
1	7	-10	261	255	3	7	-1	72	69	5	7	9	165	164	9	7	-16	235	230	11	7	-2	42*	47
1	7	-9	26*	15	3	7	0	124	115	5	7	10	111	105	9	7	-15	102	104	11	7	-1	147	146
1	7	-8	265	269	3	7	1	173	160	5	7	11	134	133	9	7	-14	170	175	11	7	0	95	89
1	7	-7	97	98	3	7	2	47	52	5	7	12	116	116	9	7	-13	136	134	11	7	1	78	80
1	7	-6	200	186	3	7	3	123	139	5	7	13	225	224	9	7	-12	112	111	11	7	2	106	106
1	7	-5	215	209	3	7	4	100	105	5	7	14	22*	13	9	7	-11	194	196	11	7	3	87	89
1	7	-4	85	77	3	7	5	244	255	5	7	15	144	145	9	7	-10	27*	28	11	7	4	198	199
1	7	-3	19*	27	3	7	6	105	98	5	7	16	61	63	9	7	-9	114	113	11	7	5	0*	22
1	7	-2	25	21	3	7	7	189	198	7	7	-20	44	44	9	7	-8	55	50	11	7	6	124	127
1	7	-1	47	50	3	7	8	149	138	7	7	-19	138	139	9	7	-7	124	125	11	7	7	47	52
1	7	0	12*	15	3	7	9	210	211	7	7	-18	29*	27	9	7	-6	149	146	11	7	8	138	139
1	7	1	47	51	3	7	10	206	203	7	7	-17	157	158	9	7	-5	99	101	11	7	9	146	145
1	7	2	119	121	3	7	11	22*	27	7	7	-16	125	128	9	7	-4	23*	16	11	7	10	0*	35
1	7	3	14*	17	3	7	12	159	158	7	7	-15	142	143	9	7	-3	0*	26	11	7	11	133	135
1	7	4	163	156	3	7	13	0*	16	7	7	-14	205	205	9	7	-2	27*	44	13	7	-18	76	79
1	7	5	20*	9	3	7	14	172	179	7	7	-13	62	58	9	7	-1	15*	4	13	7	-17	65	66

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
13	7	-16	126	125	15	7	4	92	86	Ø	8	11	58	47	4	8	-17	118	116	6	8	-6	65	77
13	7	-15	29*	31	15	7	5	98	1Ø1	Ø	8	12	163	16Ø	4	8	-16	69	69	6	8	-5	175	178
13	7	-14	144	141	15	7	6	147	147	Ø	8	13	1Ø9	11Ø	4	8	-15	146	154	6	8	-4	152	154
13	7	-13	2Ø*	24	15	7	7	9*	22	Ø	8	14	23Ø	228	4	8	-14	72	72	6	8	-3	267	277
13	7	-12	11Ø	1Ø8	17	7	-15	65	65	Ø	8	15	1Ø*	8	4	8	-13	67	72	6	8	-2	5Ø4	5Ø6
13	7	-11	8Ø	73	17	7	-14	31*	47	Ø	8	16	136	141	4	8	-12	168	17Ø	6	8	-1	443	46Ø
13	7	-1Ø	1Ø1	99	17	7	-13	62	58	Ø	8	17	95	88	4	8	-11	239	236	6	8	Ø	574	581
13	7	-9	117	117	17	7	-12	92	95	Ø	8	18	48	51	4	8	-1Ø	45Ø	445	6	8	1	649	658
13	7	-8	Ø*	15	17	7	-11	39*	34	2	8	-19	17*	33	4	8	-9	226	233	6	8	2	518	537
13	7	-7	26*	8	17	7	-1Ø	27*	5	2	8	-18	98	1ØØ	4	8	-8	692	695	6	8	3	452	443
13	7	-6	47	43	17	7	-9	25*	14	2	8	-17	63	64	4	8	-7	126	134	6	8	4	329	33Ø
13	7	-5	18*	2	17	7	-8	19*	12	2	8	-16	128	124	4	8	-6	399	413	6	8	5	214	221
13	7	-4	38*	51	17	7	-7	11*	9	2	8	-15	73	75	4	8	-5	162	172	6	8	6	129	129
13	7	-3	86	88	17	7	-6	Ø*	9	2	8	-14	157	156	4	8	-4	112	116	6	8	7	67	69
13	7	-2	153	15Ø	17	7	-5	26*	16	2	8	-13	99	97	4	8	-3	138	145	6	8	8	158	152
13	7	-1	22*	3	17	7	-4	4*	27	2	8	-12	11Ø	112	4	8	-2	287	272	6	8	9	146	137
13	7	Ø	116	119	17	7	-3	38*	59	2	8	-11	138	14Ø	4	8	-1	26*	28	6	8	1Ø	24*	18
13	7	1	7*	3Ø	17	7	-2	47	47	2	8	-1Ø	21Ø	2Ø9	4	8	Ø	37Ø	367	6	8	11	184	188
13	7	2	139	137	17	7	-1	76	77	2	8	-9	1Ø9	1Ø6	4	8	1	24*	21	6	8	12	62	61
13	7	3	163	164	17	7	Ø	89	9Ø	2	8	-8	438	431	4	8	2	4Ø6	4Ø3	6	8	13	122	121
13	7	4	32*	41	17	7	1	32*	33	2	8	-7	98	1Ø5	4	8	3	331	338	6	8	14	2Ø*	32
13	7	5	134	136	17	7	2	1Ø7	1Ø7	2	8	-6	745	744	4	8	4	325	341	6	8	15	72	68
13	7	6	28*	3Ø	17	7	3	23*	8	2	8	-5	259	264	4	8	5	475	465	8	8	-19	136	134
13	7	7	179	178	17	7	4	12Ø	119	2	8	-4	848	828	4	8	6	521	528	8	8	-18	84	89
13	7	8	87	9Ø	19	7	-12	25*	21	2	8	-3	341	325	4	8	7	286	279	8	8	-17	133	129
13	7	9	1Ø5	1Ø6	19	7	-11	Ø*	3Ø	2	8	-2	415	397	4	8	8	341	341	8	8	-16	16Ø	157
15	7	-17	68	68	19	7	-1Ø	29*	18	2	8	-1	191	189	4	8	9	5Ø	48	8	8	-15	123	131
15	7	-16	1Ø4	1Ø3	19	7	-9	Ø*	19	2	8	Ø	264	282	4	8	1Ø	1Ø8	113	8	8	-14	51	5Ø
15	7	-15	114	115	19	7	-8	9*	5	2	8	1	181	181	4	8	11	11*	8	8	8	-13	196	2Ø1
15	7	-14	31*	42	19	7	-7	27*	1Ø	2	8	2	124	126	4	8	12	123	123	8	8	-12	112	1Ø7
15	7	-13	1Ø2	1ØØ	19	7	-6	53	5Ø	2	8	3	22*	11	4	8	13	155	145	8	8	-11	84	81
15	7	-12	Ø*	25	19	7	-5	Ø*	5	2	8	4	2Ø4	229	4	8	14	34*	4Ø	8	8	-1Ø	24*	17
15	7	-11	1Ø7	1Ø5	19	7	-4	76	78	2	8	5	266	272	4	8	15	138	134	8	8	-9	313	31Ø
15	7	-1Ø	44*	62	19	7	-3	25*	4	2	8	6	468	471	4	8	16	Ø*	11	8	8	-8	23Ø	227
15	7	-9	22*	17	19	7	-2	95	93	2	8	7	218	21Ø	6	8	-19	142	143	8	8	-7	425	42Ø
15	7	-8	32*	3	19	7	-1	14*	37	2	8	8	4Ø5	398	6	8	-18	Ø*	12	8	8	-6	241	233
15	7	-7	31*	29	Ø	8	Ø	562	669	2	8	9	2Ø7	2Ø2	6	8	-17	13Ø	133	8	8	-5	578	574
15	7	-6	9*	7	Ø	8	1	323	323	2	8	1Ø	378	372	6	8	-16	64	6Ø	8	8	-4	33Ø	319
15	7	-5	19*	19	Ø	8	2	454	491	2	8	11	56	58	6	8	-15	188	192	8	8	-3	684	691
15	7	-4	59	49	Ø	8	3	259	256	2	8	12	2Ø3	2Ø2	6	8	-14	2Ø7	198	8	8	-2	543	549
15	7	-3	36*	27	Ø	8	4	394	384	2	8	13	24*	26	6	8	-13	238	242	8	8	-1	47Ø	459
15	7	-2	59	55	Ø	8	5	51	55	2	8	14	151	151	6	8	-12	372	366	8	8	Ø	261	253
15	7	-1	72	66	Ø	8	6	117	134	2	8	15	6Ø	58	6	8	-11	122	12Ø	8	8	1	37Ø	369
15	7	Ø	33*	41	Ø	8	7	1Ø2	114	2	8	16	114	111	6	8	-1Ø	3Ø8	3Ø5	8	8	2	163	153
15	7	1	155	15Ø	Ø	8	8	169	172	2	8	17	112	112	6	8	-9	267	267	8	8	3	137	129
15	7	2	79	74	Ø	8	9	62	64	4	8	-19	31*	38	6	8	-8	15Ø	148	8	8	4	14Ø	142
15	7	3	99	99	Ø	8	1Ø	2Ø8	216	4	8	-18	1Ø1	93	6	8	-7	4*	39	8	8	5	17Ø	173

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
8	8	6	77	79	12	8	-13	389	393	14	8	5	27*	34	1	9	-13	144	143	3	9	-4	53	49
8	8	7	213	207	12	8	-12	39	35	14	8	6	114	107	1	9	-12	166	165	3	9	-3	22*	26
8	8	8	119	121	12	8	-11	409	411	14	8	7	84	87	1	9	-11	55	53	3	9	-2	73	70
8	8	9	123	126	12	8	-10	109	112	14	8	8	90	92	1	9	-10	270	271	3	9	-1	89	85
8	8	10	51	53	12	8	-9	296	285	16	8	-16	31*	38	1	9	-9	120	115	3	9	0	120	120
8	8	11	171	170	12	8	-8	0*	1	16	8	-15	67	69	1	9	-8	281	275	3	9	1	19*	16
8	8	12	128	120	12	8	-7	243	241	16	8	-14	11*	2	1	9	-7	198	198	3	9	2	181	177
8	8	13	52	64	12	8	-6	31*	24	16	8	-13	16*	28	1	9	-6	268	252	3	9	3	163	173
8	8	14	120	118	12	8	-5	63	55	16	8	-12	86	88	1	9	-5	263	262	3	9	4	47	51
10	8	-19	54	55	12	8	-4	57	58	16	8	-11	184	186	1	9	-4	108	103	3	9	5	97	99
10	8	-18	95	97	12	8	-3	307	311	16	8	-10	73	75	1	9	-3	108	104	3	9	6	15*	20
10	8	-17	78	84	12	8	-2	23*	30	16	8	-9	271	273	1	9	-2	99	90	3	9	7	240	242
10	8	-16	87	87	12	8	-1	355	358	16	8	-8	157	153	1	9	-1	68	70	3	9	8	284	285
10	8	-15	0*	8	12	8	0	20*	39	16	8	-7	328	331	1	9	0	65	54	3	9	9	68	70
10	8	-14	72*	70	12	8	1	387	394	16	8	-6	188	187	1	9	1	50	55	3	9	10	162	162
10	8	-13	163	159	12	8	2	65	64	16	8	-5	364	372	1	9	2	78	71	3	9	11	107	105
10	8	-12	135	129	12	8	3	386	389	16	8	-4	87	84	1	9	3	199	187	3	9	12	273	272
10	8	-11	295	290	12	8	4	65	64	16	8	-3	185	181	1	9	4	298	288	3	9	13	46	48
10	8	-10	136	129	12	8	5	224	225	16	8	-2	74	63	1	9	5	25*	14	3	9	14	177	176
10	8	-9	497	488	12	8	6	79	74	16	8	-1	87	82	1	9	6	95	94	3	9	15	58	57
10	8	-8	193	195	12	8	7	65	66	16	8	0	6*	13	1	9	7	17*	34	3	9	16	132	129
10	8	-7	562	563	12	8	8	77	76	16	8	1	15*	19	1	9	8	156	164	3	9	17	130	131
10	8	-6	339	348	12	8	9	6*	9	16	8	2	121	120	1	9	9	196	209	5	9	-19	27*	38
10	8	-5	505	504	12	8	10	142	144	16	8	3	112	113	1	9	10	19*	13	5	9	-18	137	140
10	8	-4	202	202	14	8	-18	15*	34	16	8	4	101	100	1	9	11	191	187	5	9	-17	130	129
10	8	-3	349	340	14	8	-17	171	176	16	8	5	108	115	1	9	12	85	86	5	9	-16	115	116
10	8	-2	61	61	14	8	-16	38*	40	18	8	-14	75	75	1	9	13	192	189	5	9	-15	221	222
10	8	-1	85	94	14	8	-15	275	268	18	8	-13	144	142	1	9	14	187	183	5	9	-14	65	62
10	8	0	89	91	14	8	-14	20*	2	18	8	-12	142	147	1	9	15	103	104	5	9	-13	213	220
10	8	1	225	225	14	8	-13	217	208	18	8	-11	201	205	1	9	16	171	174	5	9	-12	20*	19
10	8	2	57	58	14	8	-12	28*	25	18	8	-10	213	211	1	9	17	59	48	5	9	-11	213	211
10	8	3	329	326	14	8	-11	166	157	18	8	-9	226	223	1	9	18	172	170	5	9	-10	111	110
10	8	4	106	102	14	8	-10	0*	12	18	8	-8	139	133	3	9	-19	103	105	5	9	-9	87	93
10	8	5	297	306	14	8	-9	29*	15	18	8	-7	126	130	3	9	-18	95	97	5	9	-8	97	99
10	8	6	0*	29	14	8	-8	36*	39	18	8	-6	80	74	3	9	-17	68	62	5	9	-7	14*	7
10	8	7	268	270	14	8	-7	244	241	18	8	-5	8*	17	3	9	-16	173	175	5	9	-6	152	153
10	8	8	103	104	14	8	-6	28*	36	18	8	-4	0*	2	3	9	-15	23*	17	5	9	-5	101	100
10	8	9	122	118	14	8	-5	348	349	18	8	-3	32*	45	3	9	-14	195	194	5	9	-4	38	32
10	8	10	115	109	14	8	-4	19*	32	18	8	-2	118	115	3	9	-13	69	63	5	9	-3	53	51
10	8	11	34*	37	14	8	-3	395	398	18	8	-1	136	142	3	9	-12	227	228	5	9	-2	34	30
10	8	12	117	115	14	8	-2	142	130	18	8	0	111	115	3	9	-11	231	231	5	9	-1	15*	34
12	8	-19	13*	18	14	8	-1	422	430	18	8	1	129	135	3	9	-10	168	166	5	9	0	69	69
12	8	-18	70	73	14	8	0	27*	15	1	9	-18	64	63	3	9	-9	313	320	5	9	1	109	110
12	8	-17	109	107	14	8	1	289	292	1	9	-17	149	144	3	9	-8	91	90	5	9	2	159	152
12	8	-16	8*	2	14	8	2	31*	33	1	9	-16	0*	5	3	9	-7	222	226	5	9	3	106	102
12	8	-15	203	198	14	8	3	118	120	1	9	-15	176	175	3	9	-6	8*	13	5	9	4	247	241
12	8	-14	10*	29	14	8	4	60*	52	1	9	-14	93	92	3	9	-5	46	62	5	9	5	94	93

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	9	6	353	342	9	9-17		11*	4	11	9	-3	17Ø	169	15	9-13		97	97	19	9	-3	2Ø*	9
5	9	7	63	62	9	9-16		173	171	11	9	-2	27*	26	15	9-12		Ø*	27	19	9	-2	57	59
5	9	8	2Ø1	2Ø5	9	9-15		64	68	11	9	-1	62	57	15	9-11		6Ø	67	Ø	1Ø	Ø	1Ø2	111
5	9	9	28*	16	9	9-14		176	179	11	9	Ø	24*	17	15	9-1Ø		86	88	Ø	1Ø	1	1Ø24	961
5	9	1Ø	246	25Ø	9	9-13		194	188	11	9	1	76	75	15	9 -9		Ø*	9	Ø	1Ø	2	26*	47
5	9	11	158	163	9	9-12		12*	8	11	9	2	168	173	15	9 -8		59	63	Ø	1Ø	3	654	614
5	9	12	51	51	9	9-11		152	151	11	9	3	35	29	15	9 -7		41*	34	Ø	1Ø	4	445	436
5	9	13	127	127	9	9-1Ø		2Ø*	23	11	9	4	132	136	15	9 -6		42	4Ø	Ø	1Ø	5	799	8Ø1
5	9	14	33*	31	9	9 -9		254	25Ø	11	9	5	Ø*	11	15	9 -5		56	6Ø	Ø	1Ø	6	2Ø2	21Ø
5	9	15	169	166	9	9 -8		66	63	11	9	6	222	216	15	9 -4		6*	6	Ø	1Ø	7	675	68Ø
5	9	16	114	111	9	9 -7		1Ø6	1Ø7	11	9	7	1Ø4	1ØØ	15	9 -3		34*	34	Ø	1Ø	8	15*	1Ø
7	9-19		141	14Ø	9	9 -6		46	52	11	9	8	125	124	15	9 -2		115	117	Ø	1Ø	9	512	511
7	9-18		6*	6	9	9 -5		36*	29	11	9	9	1Ø8	117	15	9 -1		138	134	Ø	1Ø	1Ø	5Ø	45
7	9-17		184	182	9	9 -4		7*	1	11	9	1Ø	77	73	15	9 Ø		12*	27	Ø	1Ø	11	12Ø	1Ø7
7	9-16		134	135	9	9 -3		24*	27	11	9	11	156	16Ø	15	9 1		116	113	Ø	1Ø	12	124	126
7	9-15		137	137	9	9 -2		228	224	13	9-18		54*	6Ø	15	9 2		1Ø*	3	Ø	1Ø	13	18Ø	179
7	9-14		13Ø	131	9	9 -1		1Ø9	115	13	9-17		98	98	15	9 3		143	141	Ø	1Ø	14	172	173
7	9-13		94	93	9	9 Ø		46	46	13	9-16		13Ø	13Ø	15	9 4		79	8Ø	Ø	1Ø	15	Ø*	25
7	9-12		166	162	9	9 1		18*	28	13	9-15		4Ø	37	15	9 5		61	61	Ø	1Ø	16	15Ø	151
7	9-11		93	86	9	9 2		137	131	13	9-14		119	122	15	9 6		1Ø4	1Ø7	Ø	1Ø	17	33*	27
7	9-1Ø		112	113	9	9 3		166	167	13	9-13		39*	34	17	9-15		93	91	Ø	1Ø	18	27*	31
7	9 -9		1Ø4	1Ø2	9	9 4		57	62	13	9-12		136	14Ø	17	9-14		98	96	2	1Ø-19		Ø*	17
7	9 -8		121	13Ø	9	9 5		84	85	13	9-11		56*	58	17	9-13		36*	25	2	1Ø-18		151	152
7	9 -7		181	176	9	9 6		91	96	13	9-1Ø		5*	21	17	9-12		77	74	2	1Ø-17		9*	3Ø
7	9 -6		33	37	9	9 7		111	114	13	9 -9		31*	38	17	9-11		Ø*	2	2	1Ø-16		53	55
7	9 -5		113	113	9	9 8		2Ø7	2Ø6	13	9 -8		25*	11	17	9-1Ø		27*	44	2	1Ø-15		171	172
7	9 -4		16*	36	9	9 9		23*	22	13	9 -7		93	96	17	9 -9		3Ø*	25	2	1Ø-14		168	173
7	9 -3		62	54	9	9 1Ø		174	176	13	9 -6		85	84	17	9 -8		11*	17	2	1Ø-13		165	169
7	9 -2		24*	3Ø	9	9 11		25*	16	13	9 -5		46	47	17	9 -7		37*	44	2	1Ø-12		34*	33
7	9 -1		99	96	9	9 12		18Ø	177	13	9 -4		111	112	17	9 -6		6*	13	2	1Ø-11		489	5Ø3
7	9 Ø		219	221	9	9 13		125	127	13	9 -3		22*	27	17	9 -5		38*	35	2	1Ø-1Ø		Ø*	9
7	9 1		38	38	11	9-19		91	89	13	9 -2		65	62	17	9 -4		Ø*	9	2	1Ø -9		356	361
7	9 2		217	2Ø8	11	9-18		54	59	13	9 -1		14*	24	17	9 -3		78	78	2	1Ø -8		18*	26
7	9 3		56	51	11	9-17		128	128	13	9 Ø		163	164	17	9 -2		Ø*	34	2	1Ø -7		464	472
7	9 4		293	284	11	9-16		29*	31	13	9 1		135	139	17	9 -1		46*	43	2	1Ø -6		165	17Ø
7	9 5		166	164	11	9-15		2Ø2	198	13	9 2		114	115	17	9 Ø		3Ø*	37	2	1Ø -5		11*	15
7	9 6		151	15Ø	11	9-14		99	99	13	9 3		122	118	17	9 1		35*	41	2	1Ø -4		322	3Ø2
7	9 7		159	155	11	9-13		111	11Ø	13	9 4		134	132	17	9 2		1Ø4	11Ø	2	1Ø -3		197	213
7	9 8		63	55	11	9-12		93	9Ø	13	9 5		164	163	17	9 3		18*	33	2	1Ø -2		75	6Ø
7	9 9		214	21Ø	11	9-11		152	148	13	9 6		Ø*	12	19	9-11		27*	37	2	1Ø -1		528	53Ø
7	9 1Ø		1Ø3	1Ø4	11	9-1Ø		184	184	13	9 7		14Ø	141	19	9-1Ø		Ø*	9	2	1Ø Ø		18Ø	185
7	9 11		133	132	11	9 -9		25*	1	13	9 8		33*	43	19	9 -9		31*	26	2	1Ø 1		694	643
7	9 12		117	117	11	9 -8		32*	6	13	9 9		116	115	19	9 -8		24*	14	2	1Ø 2		23*	23
7	9 13		111	1Ø9	11	9 -7		Ø*	7	15	9-17		66	7Ø	19	9 -7		26*	19	2	1Ø 3		1233	122Ø
7	9 14		2Ø2	197	11	9 -6		15*	22	15	9-16		59	59	19	9 -6		21*	19	2	1Ø 4		24Ø	237
9	9-19		79	75	11	9 -5		82	85	15	9-15		47*	61	19	9 -5		27*	27	2	1Ø 5		327	339
9	9-18		145	147	11	9 -4		114	114	15	9-14		53	55	19	9 -4		31*	54	2	1Ø 6		18*	23

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	1Ø	7	376	373	6	1Ø	-19	115	116	8	1Ø	-7	278	273	1Ø	1Ø	6	Ø*	2Ø	14	1Ø	-6	24Ø	235
2	1Ø	8	224	224	6	1Ø	-18	26*	29	8	1Ø	-6	3Ø7	3Ø3	1Ø	1Ø	7	8Ø	77	14	1Ø	-5	85	83
2	1Ø	9	121	119	6	1Ø	-17	77	8Ø	8	1Ø	-5	131	122	1Ø	1Ø	8	129	134	14	1Ø	-4	139	126
2	1Ø	1Ø	177	184	6	1Ø	-16	38	34	8	1Ø	-4	131	138	1Ø	1Ø	9	54	51	14	1Ø	-3	11Ø	11Ø
2	1Ø	11	3Ø*	35	6	1Ø	-15	187	195	8	1Ø	-3	126	134	1Ø	1Ø	1Ø	14Ø	143	14	1Ø	-2	12*	25
2	1Ø	12	116	121	6	1Ø	-14	74	67	8	1Ø	-2	296	3Ø2	1Ø	1Ø	11	33*	53	14	1Ø	-1	1Ø8	1Ø3
2	1Ø	13	125	121	6	1Ø	-13	19*	25	8	1Ø	-1	383	39Ø	1Ø	1Ø	12	72	7Ø	14	1Ø	Ø	173	174
2	1Ø	14	129	13Ø	6	1Ø	-12	166	169	8	1Ø	Ø	458	447	12	1Ø	-18	173	174	14	1Ø	1	29*	3Ø
2	1Ø	15	45	41	6	1Ø	-11	211	2Ø6	8	1Ø	1	256	25Ø	12	1Ø	-17	96	9Ø	14	1Ø	2	259	257
2	1Ø	16	48	47	6	1Ø	-1Ø	79	84	8	1Ø	2	458	453	12	1Ø	-16	129	132	14	1Ø	3	1Ø1	1Ø4
2	1Ø	17	96	93	6	1Ø	-9	462	469	8	1Ø	3	23Ø	236	12	1Ø	-15	41*	38	14	1Ø	4	166	165
4	1Ø	-19	7*	3	6	1Ø	-8	459	464	8	1Ø	4	481	484	12	1Ø	-14	111	114	14	1Ø	5	59	57
4	1Ø	-18	86	85	6	1Ø	-7	393	387	8	1Ø	5	257	265	12	1Ø	-13	28*	1Ø	14	1Ø	6	226	226
4	1Ø	-17	178	18Ø	6	1Ø	-6	463	464	8	1Ø	6	184	188	12	1Ø	-12	5Ø*	63	14	1Ø	7	Ø*	5
4	1Ø	-16	138	134	6	1Ø	-5	718	724	8	1Ø	7	138	138	12	1Ø	-11	1Ø*	9	14	1Ø	8	78	75
4	1Ø	-15	232	231	6	1Ø	-4	484	485	8	1Ø	8	55	44	12	1Ø	-1Ø	26Ø	255	16	1Ø	-16	13Ø	129
4	1Ø	-14	33*	3Ø	6	1Ø	-3	324	3Ø5	8	1Ø	9	79	89	12	1Ø	-9	144	149	16	1Ø	-15	77	83
4	1Ø	-13	285	29Ø	6	1Ø	-2	237	243	8	1Ø	1Ø	Ø*	8	12	1Ø	-8	3Ø5	3Ø5	16	1Ø	-14	22Ø	214
4	1Ø	-12	147	152	6	1Ø	-1	28Ø	273	8	1Ø	11	151	151	12	1Ø	-7	61	57	16	1Ø	-13	111	11Ø
4	1Ø	-11	189	19Ø	6	1Ø	Ø	265	27Ø	8	1Ø	12	11Ø	1Ø8	12	1Ø	-6	457	454	16	1Ø	-12	246	248
4	1Ø	-1Ø	111	111	6	1Ø	1	2Ø*	29	8	1Ø	13	81	86	12	1Ø	-5	14*	1Ø	16	1Ø	-11	61	53
4	1Ø	-9	19Ø	2Ø3	6	1Ø	2	2Ø5	212	8	1Ø	14	85	82	12	1Ø	-4	592	585	16	1Ø	-1Ø	173	174
4	1Ø	-8	98	1ØØ	6	1Ø	3	149	162	1Ø	1Ø	-19	Ø*	22	12	1Ø	-3	129	133	16	1Ø	-9	129	132
4	1Ø	-7	57Ø	571	6	1Ø	4	264	261	1Ø	1Ø	-18	96	95	12	1Ø	-2	275	271	16	1Ø	-8	66	74
4	1Ø	-6	213	2Ø3	6	1Ø	5	24Ø	241	1Ø	1Ø	-17	44	42	12	1Ø	-1	44*	51	16	1Ø	-7	45*	54
4	1Ø	-5	483	474	6	1Ø	6	368	377	1Ø	1Ø	-16	215	215	12	1Ø	Ø	118	114	16	1Ø	-6	41*	39
4	1Ø	-4	24Ø	229	6	1Ø	7	1Ø5	1Ø5	1Ø	1Ø	-15	46*	67	12	1Ø	1	31*	33	16	1Ø	-5	67*	59
4	1Ø	-3	512	511	6	1Ø	8	271	265	1Ø	1Ø	-14	267	27Ø	12	1Ø	2	38*	4Ø	16	1Ø	-4	297	3Ø4
4	1Ø	-2	412	423	6	1Ø	9	297	296	1Ø	1Ø	-13	219	223	12	1Ø	3	72	75	16	1Ø	-3	8Ø	73
4	1Ø	-1	784	8ØØ	6	1Ø	1Ø	1Ø4	1Ø6	1Ø	1Ø	-12	241	247	12	1Ø	4	175	172	16	1Ø	-2	235	238
4	1Ø	Ø	73	78	6	1Ø	11	178	179	1Ø	1Ø	-11	2Ø*	9	12	1Ø	5	74	73	16	1Ø	-1	96	96
4	1Ø	1	6ØØ	599	6	1Ø	12	Ø*	1	1Ø	1Ø	-1Ø	135	133	12	1Ø	6	193	191	16	1Ø	Ø	267	269
4	1Ø	2	514	513	6	1Ø	13	111	112	1Ø	1Ø	-9	39*	48	12	1Ø	7	Ø*	17	16	1Ø	1	18Ø	181
4	1Ø	3	241	241	6	1Ø	14	48	44	1Ø	1Ø	-8	44	41	12	1Ø	8	191	189	16	1Ø	2	179	181
4	1Ø	4	94	86	6	1Ø	15	1ØØ	99	1Ø	1Ø	-7	58*	56	12	1Ø	9	62	59	16	1Ø	3	24*	8
4	1Ø	5	266	276	8	1Ø	-19	85	82	1Ø	1Ø	-6	284	28Ø	12	1Ø	1Ø	134	13Ø	16	1Ø	4	12Ø	12Ø
4	1Ø	6	216	216	8	1Ø	-18	125	124	1Ø	1Ø	-5	143	14Ø	14	1Ø	-17	Ø*	25	16	1Ø	5	11*	3
4	1Ø	7	253	254	8	1Ø	-17	111	113	1Ø	1Ø	-4	4Ø3	4ØØ	14	1Ø	-16	Ø*	16	18	1Ø	-13	58	58
4	1Ø	8	266	263	8	1Ø	-16	98	92	1Ø	1Ø	-3	214	221	14	1Ø	-15	36*	4Ø	18	1Ø	-12	43*	53
4	1Ø	9	175	176	8	1Ø	-15	135	125	1Ø	1Ø	-2	579	573	14	1Ø	-14	2Ø4	21Ø	18	1Ø	-11	44*	43
4	1Ø	1Ø	91	96	8	1Ø	-14	15Ø	15Ø	1Ø	1Ø	-1	94	93	14	1Ø	-13	Ø*	1Ø	18	1Ø	-1Ø	47*	61
4	1Ø	11	195	191	8	1Ø	-13	69	68	1Ø	1Ø	Ø	627	624	14	1Ø	-12	266	266	18	1Ø	-9	1Ø3	1Ø2
4	1Ø	12	24Ø	247	8	1Ø	-12	229	229	1Ø	1Ø	1	166	167	14	1Ø	-11	65	64	18	1Ø	-8	15Ø	153
4	1Ø	13	185	174	8	1Ø	-11	271	269	1Ø	1Ø	2	331	317	14	1Ø	-1Ø	359	37Ø	18	1Ø	-7	113	1Ø9
4	1Ø	14	25*	28	8	1Ø	-1Ø	53Ø	53Ø	1Ø	1Ø	3	75	76	14	1Ø	-9	8Ø	76	18	1Ø	-6	215	218
4	1Ø	15	141	143	8	1Ø	-9	311	3Ø9	1Ø	1Ø	4	127	134	14	1Ø	-8	445	438	18	1Ø	-5	175	177
4	1Ø	16	37*	49	8	1Ø	-8	249	25Ø	1Ø	1Ø	5	7*	3Ø	14	1Ø	-7	22*	35	18	1Ø	-4	177	179

Reflections flagged with an asterisk were considered unobserved.

Fobs and Fcalc for Mn(CO)5 Yb (C5Me5)2 . 1/4(toluene) @ 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
18	10	-3	172	166	3	11	-14	208	207	5	11	-3	82	80	7	11	9	276	281	11	11	-10	192	192
18	10	-2	199	194	3	11	-13	6*	14	5	11	-2	80	74	7	11	10	104	102	11	11	-9	81	86
18	10	-1	97	93	3	11	-12	195	200	5	11	-1	22*	26	7	11	11	140	141	11	11	-8	31*	34
18	10	0	40*	49	3	11	-11	158	154	5	11	0	151	153	7	11	12	73	76	11	11	-7	16*	12
18	10	1	15*	24	3	11	-10	78	78	5	11	1	273	272	7	11	13	139	136	11	11	-6	139	140
1	11	-18	22*	28	3	11	-9	256	253	5	11	2	114	114	7	11	14	157	162	11	11	-5	116	119
1	11	-17	134	137	3	11	-8	10*	22	5	11	3	160	155	9	11	-19	54	58	11	11	-4	72	68
1	11	-16	34*	25	3	11	-7	182	181	5	11	4	115	109	9	11	-18	168	165	11	11	-3	181	185
1	11	-15	212	215	3	11	-6	120	117	5	11	5	205	199	9	11	-17	39*	37	11	11	-2	124	121
1	11	-14	153	154	3	11	-5	124	128	5	11	6	280	289	9	11	-16	172	170	11	11	-1	98	94
1	11	-13	173	176	3	11	-4	216	220	5	11	7	81	77	9	11	-15	74	82	11	11	0	40	43
1	11	-12	171	173	3	11	-3	5*	8	5	11	8	92	90	9	11	-14	182	182	11	11	1	153	149
1	11	-11	122	117	3	11	-2	38	30	5	11	9	12*	12	9	11	-13	181	186	11	11	2	201	209
1	11	-10	222	221	3	11	-1	30	36	5	11	10	214	208	9	11	-12	0*	13	11	11	3	15*	12
1	11	-9	0*	8	3	11	0	0*	9	5	11	11	249	246	9	11	-11	89	84	11	11	4	85	89
1	11	-8	197	197	3	11	1	27*	11	5	11	12	12*	21	9	11	-10	53	52	11	11	5	83	81
1	11	-7	92	91	3	11	2	227	223	5	11	13	163	159	9	11	-9	165	166	11	11	6	198	196
1	11	-6	89	90	3	11	3	311	309	5	11	14	37*	31	9	11	-8	88	93	11	11	7	111	108
1	11	-5	82	84	3	11	4	68	63	5	11	15	198	197	9	11	-7	55	50	11	11	8	73	73
1	11	-4	18*	12	3	11	5	157	146	7	11	-19	112	112	9	11	-6	0*	25	11	11	9	109	106
1	11	-3	62	63	3	11	6	25*	21	7	11	-18	22*	7	9	11	-5	22*	18	11	11	10	32*	47
1	11	-2	80	88	3	11	7	320	316	7	11	-17	143	145	9	11	-4	95	98	11	11	11	162	163
1	11	-1	44	50	3	11	8	211	213	7	11	-16	137	137	9	11	-3	117	117	13	11	-17	85	86
1	11	0	71	64	3	11	9	67	58	7	11	-15	86	83	9	11	-2	144	151	13	11	-16	102	104
1	11	1	71	69	3	11	10	66	65	7	11	-14	150	149	9	11	-1	150	151	13	11	-15	10*	26
1	11	2	24*	21	3	11	11	97	98	7	11	-13	99	95	9	11	0	80	85	13	11	-14	107	109
1	11	3	8*	24	3	11	12	209	200	7	11	-12	200	201	9	11	1	38*	52	13	11	-13	14*	4
1	11	4	199	198	3	11	13	83	80	7	11	-11	39*	34	9	11	2	25*	32	13	11	-12	154	158
1	11	5	108	109	3	11	14	122	122	7	11	-10	147	141	9	11	3	243	244	13	11	-11	127	127
1	11	6	143	152	3	11	15	94	90	7	11	-9	20*	16	9	11	4	131	133	13	11	-10	53	56
1	11	7	196	190	3	11	16	105	102	7	11	-8	219	221	9	11	5	94	91	13	11	-9	61	61
1	11	8	123	118	5	11	-19	13*	18	7	11	-7	108	117	9	11	6	59	59	13	11	-8	88	88
1	11	9	265	259	5	11	-18	145	146	7	11	-6	0*	5	9	11	7	186	182	13	11	-7	115	117
1	11	10	26*	38	5	11	-17	86	91	7	11	-5	51	52	9	11	8	218	215	13	11	-6	19*	24
1	11	11	217	217	5	11	-16	100	105	7	11	-4	112	122	9	11	9	16*	27	13	11	-5	88	89
1	11	12	0*	9	5	11	-15	153	152	7	11	-3	63	63	9	11	10	120	123	13	11	-4	144	140
1	11	13	222	224	5	11	-14	32*	35	7	11	-2	88	84	9	11	11	19*	2	13	11	-3	10*	16
1	11	14	118	120	5	11	-13	156	154	7	11	-1	199	196	9	11	12	144	141	13	11	-2	66	60
1	11	14	118	120	5	11	-12	6*	14	7	11	0	101	103	9	11	13	120	117	13	11	-1	102	103
1	11	15	91	92	5	11	-11	213	224	7	11	1	42	49	11	11	-18	89	85	13	11	0	181	174
1	11	16	116	117	5	11	-10	202	206	7	11	2	45	49	11	11	-17	116	122	13	11	1	82	79
1	11	17	11*	26	5	11	-9	111	106	7	11	3	17*	12	11	11	-16	70	72	13	11	2	68	65
3	11	-19	113	117	5	11	-8	145	143	7	11	4	195	199	11	11	-15	189	190	13	11	3	41	43
3	11	-18	109	109	5	11	-7	101	95	7	11	5	179	175	11	11	-14	72	76	13	11	4	114	113
3	11	-17	100	98	5	11	-6	218	216	7	11	6	16*	29	11	11	-13	77	83	13	11	5	160	158
3	11	-16	182	179	5	11	-5	90	93	7	11	7	140	140	11	11	-12	72	74	13	11	6	24*	35
3	11	-15	28*	37	5	11	-4	84	79	7	11	8	79	77	11	11	-11	109	104	13	11	7	126	123

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
13	11	8	58	64	19	11	-5	12*	19	2	12	7	9Ø	87	4	12	16	12*	25	8	12	-8	166	164
13	11	9	135	132	19	11	-4	85	82	2	12	8	419	42Ø	6	12	-19	1Ø8	1Ø8	8	12	-7	259	266
15	11	-16	63	57	19	11	-3	18*	3	2	12	9	233	234	6	12	-18	48*	5Ø	8	12	-6	252	247
15	11	-15	67	66	Ø	12	Ø	1471	1471	2	12	1Ø	333	343	6	12	-17	123	13Ø	8	12	-5	458	455
15	11	-14	86	84	Ø	12	1	215	215	2	12	11	22*	15	6	12	-16	41	43	8	12	-4	262	245
15	11	-13	129	126	Ø	12	2	631	613	2	12	12	248	248	6	12	-15	122	125	8	12	-3	67Ø	666
15	11	-12	12*	2	Ø	12	3	287	285	2	12	13	13*	6	6	12	-14	223	219	8	12	-2	474	486
15	11	-11	83	78	Ø	12	4	549	53Ø	2	12	14	96	98	6	12	-13	274	274	8	12	-1	436	423
15	11	-1Ø	18*	5	Ø	12	5	152	162	2	12	15	8Ø	81	6	12	-12	361	352	8	12	Ø	131	132
15	11	-9	26*	39	Ø	12	6	17Ø	174	2	12	16	88	93	6	12	-11	158	166	8	12	1	323	323
15	11	-8	6*	8	Ø	12	7	122	126	2	12	17	121	125	6	12	-1Ø	266	27Ø	8	12	2	119	123
15	11	-7	28*	32	Ø	12	8	148	146	4	12	-19	14*	26	6	12	-9	281	279	8	12	3	134	129
15	11	-6	65	62	Ø	12	9	13*	12	4	12	-18	98	97	6	12	-8	148	138	8	12	4	95	94
15	11	-5	33*	42	Ø	12	1Ø	279	283	4	12	-17	24*	48	6	12	-7	77	82	8	12	5	234	241
15	11	-4	13*	11	Ø	12	11	95	96	4	12	-16	23*	12	6	12	-6	113	12Ø	8	12	6	94	1ØØ
15	11	-3	26*	2	Ø	12	12	131	127	4	12	-16	Ø*	12	6	12	-5	124	121	8	12	7	196	195
15	11	-2	54	53	Ø	12	13	68	76	4	12	-15	169	17Ø	6	12	-4	436	434	8	12	8	75	7Ø
15	11	-1	1ØØ	96	Ø	12	14	231	227	4	12	-14	71	66	6	12	-3	255	246	8	12	9	125	128
15	11	Ø	27*	4Ø	Ø	12	15	6*	26	4	12	-13	29*	41	6	12	-2	361	358	8	12	1Ø	25*	14
15	11	1	76	76	Ø	12	16	81	86	4	12	-12	19Ø	184	6	12	-1	28Ø	282	8	12	11	175	176
15	11	2	17*	23	Ø	12	17	1ØØ	99	4	12	-11	225	229	6	12	Ø	473	466	8	12	12	67*	75
15	11	3	149	146	Ø	12	18	Ø*	34	4	12	-1Ø	4ØØ	395	6	12	1	629	652	8	12	13	43*	47
15	11	4	127	133	2	12	-18	96	92	4	12	-9	277	288	6	12	2	523	521	1Ø	12	-18	78	78
15	11	5	54	61	2	12	-17	51	52	4	12	-8	783	79Ø	6	12	3	3Ø4	3Ø9	1Ø	12	-17	35*	44
15	11	6	111	117	2	12	-16	124	123	4	12	-7	153	144	6	12	4	321	311	1Ø	12	-16	81	84
17	11	-14	67	68	2	12	-15	Ø*	12	4	12	-6	331	33Ø	6	12	5	152	152	1Ø	12	-15	28*	6
17	11	-13	9*	3	2	12	-14	95	91	4	12	-5	115	111	6	12	6	122	119	1Ø	12	-14	47*	45
17	11	-12	3Ø*	15	2	12	-13	124	121	4	12	-4	226	242	6	12	7	Ø*	6	1Ø	12	-13	189	191
17	11	-11	21*	7	2	12	-12	192	199	4	12	-3	263	276	6	12	8	187	186	1Ø	12	-12	138	138
17	11	-1Ø	25*	27	2	12	-11	157	16Ø	4	12	-2	2ØØ	194	6	12	9	188	187	1Ø	12	-11	262	256
17	11	-9	57*	6Ø	2	12	-1Ø	186	188	4	12	-1	2Ø8	2Ø9	6	12	1Ø	9*	3	1Ø	12	-1Ø	61	59
17	11	-8	6Ø	55	2	12	-9	94	92	4	12	Ø	246	265	6	12	11	161	164	1Ø	12	-9	36Ø	359
17	11	-7	19*	1Ø	2	12	-8	344	333	4	12	1	19*	23	6	12	12	16*	44	1Ø	12	-8	127	125
17	11	-6	Ø*	1Ø	2	12	-7	122	124	4	12	2	393	391	6	12	13	95	98	1Ø	12	-7	5ØØ	5Ø9
17	11	-5	19*	14	2	12	-6	678	676	4	12	3	359	348	6	12	14	21*	33	1Ø	12	-6	217	228
17	11	-4	29*	29	2	12	-5	4Ø4	394	4	12	4	383	383	6	12	15	7Ø	73	1Ø	12	-5	316	325
17	11	-3	51	49	2	12	-4	763	796	4	12	5	552	546	8	12	-19	113	116	1Ø	12	-4	77	79
17	11	-2	76	72	2	12	-3	48	41	4	12	6	586	585	8	12	-18	62*	64	1Ø	12	-3	252	254
17	11	-1	33*	32	2	12	-2	662	669	4	12	7	218	214	8	12	-17	62	64	1Ø	12	-2	52	46
17	11	Ø	71	73	2	12	-1	126	137	4	12	8	277	281	8	12	-16	198	198	1Ø	12	-1	81	82
17	11	1	63	58	2	12	Ø	316	324	4	12	9	21*	14	8	12	-15	77	83	1Ø	12	Ø	Ø*	5
17	11	2	14Ø	143	2	12	1	17*	9	4	12	1Ø	155	155	8	12	-14	63	63	1Ø	12	1	281	288
19	11	-1Ø	32*	2Ø	2	12	2	3Ø8	3Ø5	4	12	11	64	7Ø	8	12	-13	172	173	1Ø	12	2	92	1Ø1
19	11	-9	3Ø*	5	2	12	3	1Ø9	1Ø9	4	12	12	91	91	8	12	-12	126	129	1Ø	12	3	3Ø6	3Ø4
19	11	-8	23*	25	2	12	4	413	411	4	12	13	132	127	8	12	-11	124	126	1Ø	12	4	1Ø7	1Ø5
19	11	-7	Ø*	3	2	12	5	219	212	4	12	14	Ø*	33	8	12	-1Ø	21*	37	1Ø	12	5	283	293
19	11	-6	26*	33	2	12	6	41Ø	4Ø2	4	12	15	1Ø6	1Ø4	8	12	-9	282	284	1Ø	12	6	37*	19

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
10	12	7	293	294	14	12	-3	338	337	1	13	-16	0*	3	3	13	-6	61	59	5	13	6	278	276
10	12	8	79	77	14	12	-2	160	151	1	13	-15	163	159	3	13	-5	18*	37	5	13	7	21*	0
10	12	9	122	123	14	12	-1	353	357	1	13	-14	90	90	3	13	-4	37	27	5	13	8	217	211
10	12	10	53*	62	14	12	0	0*	26	1	13	-13	134	130	3	13	-3	8*	24	5	13	9	51	49
10	12	11	39*	35	14	12	1	220	227	1	13	-12	146	149	3	13	-2	14*	7	5	13	10	169	166
12	12	-18	38*	52	14	12	2	16*	32	1	13	-11	50	49	3	13	-1	36	32	5	13	11	130	125
12	12	-17	116	117	14	12	3	65	69	1	13	-10	231	236	3	13	0	65	64	5	13	12	84	85
12	12	-16	21*	33	14	12	4	49	50	1	13	-9	123	123	3	13	1	98	97	5	13	13	155	155
12	12	-15	208	207	14	12	5	31*	55	1	13	-8	219	219	3	13	2	169	168	5	13	14	24*	15
12	12	-14	35*	29	14	12	6	93	90	1	13	-7	185	181	3	13	3	121	121	5	13	15	105	106
12	12	-13	324	330	14	12	7	76	80	1	13	-6	117	119	3	13	4	46	48	7	13	-18	0*	7
12	12	-12	60	64	16	12	-15	50	53	1	13	-5	140	142	3	13	5	178	180	7	13	-17	160	162
12	12	-11	394	392	16	12	-14	13*	7	1	13	-4	137	136	3	13	6	157	151	7	13	-16	90	92
12	12	-10	86	82	16	12	-13	0*	17	1	13	-3	134	142	3	13	7	149	145	7	13	-15	117	115
12	12	-9	243	245	16	12	-12	74	73	1	13	-2	72	68	3	13	8	185	194	7	13	-14	133	144
12	12	-8	70	68	16	12	-11	181	182	1	13	-1	50	47	3	13	9	116	119	7	13	-13	35*	29
12	12	-7	209	212	16	12	-10	11*	33	1	13	0	88	97	3	13	10	192	191	7	13	-12	124	125
12	12	-6	45*	55	16	12	-9	249	256	1	13	1	54	56	3	13	11	75	75	7	13	-11	21*	11
12	12	-5	88	86	16	12	-8	125	126	1	13	2	172	168	3	13	12	216	214	7	13	-10	105	106
12	12	-4	34*	38	16	12	-7	283	287	1	13	3	41	41	3	13	13	19*	14	7	13	-9	74	68
12	12	-3	288	296	16	12	-6	177	172	1	13	4	143	154	3	13	14	188	186	7	13	-8	78	71
12	12	-2	111	107	16	12	-5	351	345	1	13	5	16*	36	3	13	15	87	88	7	13	-7	165	168
12	12	-1	277	292	16	12	-4	117	114	1	13	6	175	185	3	13	16	84	83	7	13	-6	21*	24
12	12	0	13*	24	16	12	-3	142	143	1	13	7	122	116	5	13	-18	136	137	7	13	-5	129	130
12	12	1	296	296	16	12	-2	97	91	1	13	8	44	45	5	13	-17	126	127	7	13	-4	20*	15
12	12	2	89	86	16	12	-1	93	92	1	13	9	118	113	5	13	-16	99	102	7	13	-3	38	37
12	12	3	360	356	16	12	0	67	50	1	13	10	16*	17	5	13	-15	180	177	7	13	-2	72	71
12	12	4	0*	7	16	12	1	0*	25	1	13	11	188	188	5	13	-14	69	60	7	13	-1	0*	15
12	12	5	195	198	16	12	2	114	118	1	13	12	78	80	5	13	-13	196	190	7	13	0	95	98
12	12	6	46*	44	16	12	3	84	83	1	13	13	209	210	5	13	-12	17*	19	7	13	1	26*	34
12	12	7	104	105	16	12	4	72	73	1	13	14	152	152	5	13	-11	216	216	7	13	2	242	240
12	12	8	25*	37	18	12	-12	118	118	1	13	15	108	105	5	13	-10	66	70	7	13	3	68	62
12	12	9	24*	30	18	12	-11	187	184	1	13	16	170	164	5	13	-9	151	152	7	13	4	204	209
14	12	-17	150	154	18	12	-10	185	178	1	13	17	13*	17	5	13	-8	110	111	7	13	5	98	95
14	12	-16	32*	30	18	12	-9	196	193	3	13	-18	85	89	5	13	-7	17*	4	7	13	6	143	142
14	12	-15	233	237	18	12	-8	99	95	3	13	-17	66	66	5	13	-6	53	48	7	13	7	148	154
14	12	-14	20*	7	18	12	-7	101	97	3	13	-16	148	150	5	13	-5	130	128	7	13	8	53	50
14	12	-13	150	152	18	12	-6	81	77	3	13	-16	148	150	5	13	-4	69	63	7	13	9	207	210
14	12	-12	52	46	18	12	-5	0*	2	3	13	-15	26*	16	5	13	-3	100	97	7	13	10	66	69
14	12	-11	98	97	18	12	-4	0*	1	3	13	-14	183	183	5	13	-2	17*	17	7	13	11	134	138
14	12	-10	15*	32	18	12	-3	25*	28	3	13	-13	77	73	5	13	-1	8*	2	7	13	12	140	139
14	12	-9	37*	28	18	12	-2	99	95	3	13	-12	212	220	5	13	0	18*	24	7	13	13	50	44
14	12	-8	27*	28	18	12	-1	141	148	3	13	-11	202	194	5	13	1	63	60	7	13	14	134	134
14	12	-7	288	280	18	12	0	116	119	3	13	-10	130	133	5	13	2	96	95	9	13	-18	118	119
14	12	-6	48	45	1	13	-18	75	76	3	13	-9	294	289	5	13	3	117	111	9	13	-17	9*	9
14	12	-5	295	302	1	13	-18	75	75	3	13	-8	60	60	5	13	4	257	253	9	13	-16	151	150
14	12	-4	20*	16	1	13	-17	139	143	3	13	-7	267	261	5	13	5	108	112	9	13	-15	93	98

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
9	13	-14	101	105	11	13	2	103	102	15	13	-4	26*	61	2	14	-15	82	82	4	14	-4	280	265
9	13	-13	170	172	11	13	3	14*	11	15	13	-3	85	83	2	14	-14	102	104	4	14	-3	496	475
9	13	-12	200*	39	11	13	4	117	115	15	13	-2	34*	45	2	14	-13	210	216	4	14	-2	392	396
9	13	-11	202	205	11	13	5	0*	13	15	13	-1	91	87	2	14	-13	216	216	4	14	-1	801	798
9	13	-10	23*	32	11	13	6	161	162	15	13	0	36*	42	2	14	-12	132	136	4	14	0	173	167
9	13	-9	159	160	11	13	7	100	100	15	13	1	132	136	2	14	-11	332	340	4	14	1	395	393
9	13	-8	35	33	11	13	8	129	127	15	13	2	26*	7	2	14	-10	76	79	4	14	2	184	188
9	13	-7	93	93	11	13	9	136	131	15	13	3	136	135	2	14	-9	423	421	4	14	3	365	369
9	13	-6	21*	27	11	13	10	53	54	15	13	4	66	70	2	14	-8	119	116	4	14	4	174	180
9	13	-5	20*	21	13	13	-17	97	91	15	13	5	61	63	2	14	-7	272	266	4	14	5	70	89
9	13	-4	0*	40	13	13	-16	96	92	17	13	-13	18*	22	2	14	-6	48	47	4	14	6	321	311
9	13	-3	19*	24	13	13	-15	76	75	17	13	-12	62	57	2	14	-5	82	93	4	14	7	80	76
9	13	-2	101	104	13	13	-14	109	111	17	13	-11	17*	16	2	14	-4	208	209	4	14	8	164	166
9	13	-1	29*	32	13	13	-13	12*	10	17	13	-10	39*	47	2	14	-3	398	398	4	14	9	245	249
9	13	0	129	129	13	13	-12	88	89	17	13	-9	6*	11	2	14	-2	211	202	4	14	10	153	164
9	13	1	101	104	13	13	-11	75	75	17	13	-8	0*	20	2	14	-1	403	406	4	14	11	153	156
9	13	2	20*	12	13	13	-10	39*	41	17	13	-7	30*	27	2	14	0	171	166	4	14	12	183	190
9	13	3	96	98	13	13	-9	69	65	17	13	-6	15*	22	2	14	1	797	787	4	14	13	199	200
9	13	4	20*	16	13	13	-8	0*	18	17	13	-5	56	55	2	14	2	506	497	4	14	14	19*	39
9	13	5	100	101	13	13	-7	26*	38	17	13	-4	0*	15	2	14	3	649	660	4	14	15	116	120
9	13	6	72	69	13	13	-6	0*	16	17	13	-3	35*	47	2	14	4	91	67	6	14	-18	19*	15
9	13	7	121	120	13	13	-5	23*	5	17	13	-2	9*	6	2	14	5	610	621	6	14	-17	104	106
9	13	8	180	181	13	13	-4	25*	18	17	13	-1	35*	50	2	14	6	197	185	6	14	-16	16*	26
9	13	9	23*	25	13	13	-3	27*	40	17	13	0	45*	45	2	14	7	158	162	6	14	-15	106	113
9	13	10	188	186	13	13	-2	93	95	17	13	1	20*	31	2	14	8	0*	17	6	14	-14	31*	41
9	13	11	57	51	13	13	-1	25*	34	17	13	2	93	99	2	14	9	150	155	6	14	-13	111	116
9	13	12	135	132	13	13	0	116	121	0	14	0	583	582	2	14	10	108	117	6	14	-12	100	105
11	13	-18	60	57	13	13	1	90	83	0	14	1	321	311	2	14	11	117	121	6	14	-11	246	243
11	13	-17	126	123	13	13	2	125	131	0	14	2	67	63	2	14	12	127	136	6	14	-11	255	243
11	13	-16	0*	5	13	13	3	107	113	0	14	3	654	647	2	14	13	86	89	6	14	-10	161	170
11	13	-15	178	174	13	13	4	100	102	0	14	4	129	114	2	14	14	68	70	6	14	-9	212	207
11	13	-14	52	50	13	13	5	153	151	0	14	5	413	412	2	14	15	74	78	6	14	-8	250	243
11	13	-13	156	158	13	13	6	24*	20	0	14	6	41*	44	2	14	16	82	81	6	14	-7	408	406
11	13	-12	121	123	13	13	7	136	135	0	14	7	701	703	4	14	-18	124	126	6	14	-6	519	518
11	13	-11	94	86	13	13	8	13*	53	0	14	8	7*	8	4	14	-17	111	116	6	14	-5	516	510
11	13	-10	101	97	15	13	-16	66	67	0	14	9	305	308	4	14	-16	87	86	6	14	-4	409	389
11	13	-9	29*	13	15	13	-15	52	60	0	14	10	107	114	4	14	-15	261	265	6	14	-3	427	418
11	13	-8	39	45	15	13	-14	16*	29	0	14	11	129	136	4	14	-14	42	43	6	14	-2	310	298
11	13	-7	24*	9	15	13	-13	79	78	0	14	12	66	74	4	14	-13	171	173	6	14	-1	215	211
11	13	-6	14*	6	15	13	-12	37*	40	0	14	13	97	105	4	14	-12	25*	37	6	14	0	154	154
11	13	-5	20*	13	15	13	-11	71	67	0	14	14	196	203	4	14	-11	308	315	6	14	1	101	108
11	13	-4	68	73	15	13	-10	72	68	0	14	15	6*	0	4	14	-10	38	32	6	14	2	112	109
11	13	-3	64	63	15	13	-9	42	40	0	14	16	107	116	4	14	-9	36*	36	6	14	3	230	230
11	13	-2	50	56	15	13	-8	8*	43	0	14	17	81	77	4	14	-8	267	278	6	14	4	281	279
11	13	-1	85	83	15	13	-7	25*	9	2	14	-18	98	102	4	14	-7	268	275	6	14	5	169	167
11	13	0	69	70	15	13	-6	0*	10	2	14	-17	68	65	4	14	-6	94	92	6	14	6	236	237
11	13	1	26*	40	15	13	-5	0*	16	2	14	-16	91	96	4	14	-5	503	492	6	14	7	150	164

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
6	14	8	304	296	10	14	-10	213	213	12	14	7	0*	37	18	14	-7	139	140	3	15	-12	180	183
6	14	9	241	243	10	14	-9	24*	23	12	14	8	123	125	18	14	-6	160	161	3	15	-11	101	103
6	14	10	92	96	10	14	-8	72	72	12	14	9	34*	26	18	14	-5	146	144	3	15	-10	92	98
6	14	11	175	185	10	14	-7	33*	42	14	14	-16	24*	4	18	14	-4	172	174	3	15	-9	158	158
6	14	12	21*	18	10	14	-6	188	184	14	14	-15	46*	36	18	14	-3	180	180	3	15	-8	39	35
6	14	13	87	90	10	14	-5	140	134	14	14	-14	158	159	18	14	-2	150	150	3	15	-7	161	159
6	14	14	22*	27	10	14	-4	312	310	14	14	-13	0*	15	1	15	-17	146	146	3	15	-6	189	180
8	14	-18	71	76	10	14	-3	151	157	14	14	-12	210	209	1	15	-16	46	40	3	15	-5	71	68
8	14	-17	37*	41	10	14	-2	406	398	14	14	-11	22*	24	1	15	-15	144	145	3	15	-4	145	146
8	14	-16	153	152	10	14	-1	100	104	14	14	-10	336	334	1	15	-14	111	110	3	15	-3	61	60
8	14	-15	60	54	10	14	0	492	504	14	14	-9	39*	47	1	15	-13	180	178	3	15	-2	113	108
8	14	-14	88	96	10	14	1	145	154	14	14	-8	397	386	1	15	-12	223	221	3	15	-1	38	32
8	14	-13	133	138	10	14	2	270	271	14	14	-7	17*	7	1	15	-11	105	111	3	15	0	62	62
8	14	-12	325	326	10	14	3	69	72	14	14	-6	233	233	1	15	-10	214	216	3	15	1	166	169
8	14	-11	144	143	10	14	4	125	132	14	14	-5	104	105	1	15	-9	20*	29	3	15	2	18*	22
8	14	-10	397	398	10	14	5	22*	12	14	14	-4	130	128	1	15	-8	182	178	3	15	3	164	162
8	14	-9	303	301	10	14	6	61	63	14	14	-3	78	78	1	15	-7	84	79	3	15	4	150	150
8	14	-8	284	286	10	14	7	77	77	14	14	-2	87	90	1	15	-6	87	88	3	15	5	331	326
8	14	-7	151	147	10	14	8	112	114	14	14	-1	37*	31	1	15	-5	93	88	3	15	6	95	92
8	14	-6	251	251	10	14	9	71	68	14	14	0	159	150	1	15	-4	25*	22	3	15	7	121	121
8	14	-5	109	113	10	14	10	92	90	14	14	1	61*	60	1	15	-3	65	67	3	15	8	16*	20
8	14	-4	136	143	10	14	11	13*	36	14	14	2	163	161	1	15	-2	105	102	3	15	9	173	170
8	14	-3	18*	33	12	14	-17	73	78	14	14	3	17*	40	1	15	-1	61	63	3	15	10	159	159
8	14	-2	324	330	12	14	-17	81	78	14	14	4	154	158	1	15	0	115	117	3	15	11	23*	5
8	14	-1	263	269	12	14	-16	115	119	14	14	5	81	77	1	15	1	0*	1	3	15	12	134	133
8	14	0	265	262	12	14	-15	13*	8	14	14	6	157	158	1	15	2	22*	34	3	15	13	11*	19
8	14	1	293	289	12	14	-14	83	82	16	14	-14	167	164	1	15	3	89	83	3	15	14	170	164
8	14	2	354	355	12	14	-13	23*	29	16	14	-13	79	73	1	15	4	16*	27	3	15	15	143	140
8	14	3	196	203	12	14	-12	0*	21	16	14	-12	220	222	1	15	5	26*	12	3	15	16	32*	38
8	14	4	397	406	12	14	-11	34*	29	16	14	-11	44*	48	1	15	6	216	225	5	15	-18	149	149
8	14	5	275	284	12	14	-10	259	252	16	14	-10	124	121	1	15	7	203	205	5	15	-17	82	83
8	14	6	197	197	12	14	-9	146	146	16	14	-9	81	79	1	15	8	96	100	5	15	-16	72	78
8	14	7	170	173	12	14	-8	269	271	16	14	-8	73	71	1	15	9	160	164	5	15	-15	115	117
8	14	8	31*	34	12	14	-7	66	61	16	14	-7	36*	43	1	15	10	106	109	5	15	-14	30*	29
8	14	9	109	116	12	14	-6	360	362	16	14	-6	13*	30	1	15	11	235	235	5	15	-14	37	29
8	14	10	22*	32	12	14	-5	19*	9	16	14	-5	98*	90	1	15	12	17*	22	5	15	-13	156	157
8	14	11	141	144	12	14	-4	490	482	16	14	-4	209	211	1	15	13	158	154	5	15	-12	62	65
8	14	12	83	82	12	14	-3	73	67	16	14	-3	45	42	1	15	14	91	88	5	15	-11	126	131
8	14	13	66	71	12	14	-2	220	222	16	14	-2	215	216	1	15	15	93	95	5	15	-10	128	120
10	14	-18	89	96	12	14	-1	31*	32	16	14	-1	117	122	1	15	16	148	149	5	15	-9	133	122
10	14	-17	0*	6	12	14	0	144	143	16	14	0	177	179	3	15	-18	112	114	5	15	-8	222	222
10	14	-16	147	148	12	14	1	28*	33	16	14	1	115	119	3	15	-17	77	79	5	15	-7	0*	5
10	14	-15	111	112	12	14	2	23*	36	16	14	2	187	183	3	15	-16	155	153	5	15	-6	156	149
10	14	-14	296	301	12	14	3	106	102	16	14	3	29*	39	3	15	-15	18*	26	5	15	-5	41	48
10	14	-13	145	141	12	14	4	126	124	18	14	-10	0*	21	3	15	-15	28*	26	5	15	-4	151	151
10	14	-12	164	166	12	14	5	26*	27	18	14	-9	77	76	3	15	-14	193	189	5	15	-3	0*	5
10	14	-11	84	83	12	14	6	181	184	18	14	-8	155	156	3	15	-13	24*	19	5	15	-2	24*	21

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	15	-1	97	95	7	15	12	155	156	11	15	-4	76	69	15	15	-7	27*	7	2	16	-14	121	121
5	15	Ø	24*	18	7	15	13	39	39	11	15	-3	15*	1Ø	15	15	-6	2Ø*	2	2	16	-13	32*	36
5	15	1	148	148	9	15	-18	13Ø	132	11	15	-2	13*	35	15	15	-5	47*	61	2	16	-12	13*	8
5	15	2	55	54	9	15	-18	135	132	11	15	-1	2Ø5	2Ø1	15	15	-4	86	85	2	16	-11	2Ø3	2Ø8
5	15	3	241	238	9	15	-17	16*	16	11	15	Ø	154	156	15	15	-3	15*	44	2	16	-1Ø	72	72
5	15	4	171	172	9	15	-16	2Ø1	2Ø4	11	15	1	25*	46	15	15	-2	23*	13	2	16	-9	Ø*	4
5	15	5	34*	27	9	15	-15	1Ø8	111	11	15	2	67	65	15	15	-1	Ø*	22	2	16	-8	389	381
5	15	6	68	75	9	15	-14	113	114	11	15	3	129	138	15	15	Ø	33*	34	2	16	-7	223	222
5	15	7	44	44	9	15	-13	8Ø	86	11	15	4	179	173	15	15	1	13Ø	129	2	16	-6	536	525
5	15	8	2Ø5	2Ø8	9	15	-12	121	124	11	15	5	16*	14	15	15	2	77	75	2	16	-5	76	82
5	15	9	154	152	9	15	-11	167	16Ø	11	15	6	1Ø1	1Ø1	15	15	3	89	9Ø	2	16	-4	778	785
5	15	1Ø	69	68	9	15	-1Ø	5Ø	53	11	15	7	1Ø*	27	15	15	4	93	94	2	16	-3	99	1ØØ
5	15	11	118	12Ø	9	15	-9	Ø*	2Ø	11	15	8	111	1Ø7	17	15	-12	34*	39	2	16	-2	512	5Ø4
5	15	12	111	112	9	15	-8	29*	28	11	15	9	14Ø	138	17	15	-11	28*	31	2	16	-1	6*	17
5	15	13	224	227	9	15	-7	41*	48	11	15	1Ø	11*	23	17	15	-1Ø	Ø*	1	2	16	Ø	441	447
5	15	14	61	6Ø	9	15	-6	1Ø5	1Ø9	13	15	-16	38*	51	17	15	-9	18*	29	2	16	1	211	227
5	15	15	96	97	9	15	-5	96	95	13	15	-15	35*	38	17	15	-8	18*	9	2	16	2	89	94
7	15	-18	Ø*	25	9	15	-4	39	39	13	15	-14	144	141	17	15	-7	28*	29	2	16	3	257	256
7	15	-17	1Ø6	112	9	15	-3	49	55	13	15	-13	53	51	17	15	-6	24*	19	2	16	4	73	71
7	15	-16	1Ø1	1Ø1	9	15	-2	51	52	13	15	-12	11Ø	1Ø9	17	15	-5	37*	37	2	16	5	28*	36
7	15	-15	1ØØ	99	9	15	-1	32*	44	13	15	-11	23*	51	17	15	-4	19*	31	2	16	6	466	47Ø
7	15	-14	212	211	9	15	Ø	91	9Ø	13	15	-1Ø	119	113	17	15	-3	9*	6	2	16	7	178	174
7	15	-13	34*	13	9	15	1	2Ø2	2ØØ	13	15	-9	1Ø3	1Ø4	17	15	-2	27*	32	2	16	8	249	246
7	15	-12	154	15Ø	9	15	2	94	95	13	15	-8	35*	23	17	15	-1	38*	51	2	16	9	98	1ØØ
7	15	-11	22*	27	9	15	3	1Ø3	1Ø2	13	15	-7	8*	Ø	17	15	Ø	1Ø3	99	2	16	1Ø	4ØØ	399
7	15	-1Ø	238	239	9	15	4	13*	1Ø	13	15	-6	99	98	Ø	16	Ø	862	88Ø	2	16	11	119	118
7	15	-9	76	75	9	15	5	211	21Ø	13	15	-5	34*	43	Ø	16	1	197	187	2	16	12	158	16Ø
7	15	-8	92	9Ø	9	15	6	158	159	13	15	-4	26*	18	Ø	16	2	7Ø6	732	2	16	13	39	36
7	15	-7	13*	3Ø	9	15	7	121	12Ø	13	15	-3	131	131	Ø	16	3	217	223	2	16	13	33*	36
7	15	-6	8Ø	76	9	15	8	133	134	13	15	-2	164	166	Ø	16	4	287	282	2	16	14	123	127
7	15	-5	11*	29	9	15	9	95	93	13	15	-1	Ø*	22	Ø	16	5	16*	18	2	16	15	29*	43
7	15	-4	62	68	9	15	1Ø	171	168	13	15	Ø	63	67	Ø	16	6	313	3Ø5	2	16	16	58	66
7	15	-3	1Ø9	113	9	15	11	39*	58	13	15	1	26*	23	Ø	16	7	52	45	4	16	-18	58*	58
7	15	-2	61	62	9	15	12	47*	57	13	15	2	147	148	Ø	16	8	2Ø4	218	4	16	-17	82	82
7	15	-1	12*	1Ø	11	15	-17	117	119	13	15	3	96	95	Ø	16	9	99	1Ø1	4	16	-16	65	67
7	15	Ø	85	87	11	15	-16	13*	35	13	15	4	34*	27	Ø	16	1Ø	176	18Ø	4	16	-15	67	66
7	15	1	1Ø2	112	11	15	-15	86	87	13	15	5	79	81	Ø	16	11	16*	6	4	16	-14	18Ø	172
7	15	2	169	177	11	15	-14	19*	13	13	15	6	Ø*	1	Ø	16	12	168	161	4	16	-13	126	122
7	15	3	1Ø3	1Ø9	11	15	-13	122	122	13	15	7	148	152	Ø	16	13	119	124	4	16	-12	119	119
7	15	4	11*	41	11	15	-12	175	18Ø	15	15	-15	1Ø2	1Ø2	Ø	16	14	137	141	4	16	-11	1Ø4	1Ø2
7	15	5	97	1Ø3	11	15	-11	24*	28	15	15	-14	9*	28	Ø	16	15	54	56	4	16	-1Ø	443	434
7	15	6	119	118	11	15	-1Ø	98	95	15	15	-13	67	64	Ø	16	16	126	125	4	16	-9	288	282
7	15	7	26Ø	256	11	15	-9	23*	19	15	15	-12	38*	35	Ø	16	17	49*	62	4	16	-8	429	417
7	15	8	14*	29	11	15	-8	148	151	15	15	-11	59	55	2	16	-17	Ø*	14	4	16	-7	41	21
7	15	9	188	188	11	15	-7	96	92	15	15	-1Ø	26*	2Ø	2	16	-17	Ø*	14	4	16	-6	449	441
7	15	1Ø	21*	22	11	15	-6	11*	17	15	15	-9	23*	9	2	16	-16	65	69	4	16	-5	333	332
7	15	11	217	217	11	15	-5	33*	38	15	15	-8	2Ø*	15	2	16	-15	67	67	4	16	-4	153	153

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
4	16	-3	193	189	6	16	9	176	174	10	16	-9	401	408	14	16	-13	129	131	1	17	-11	47*	42
4	16	-2	132	139	6	16	10	25*	35	10	16	-8	82	84	14	16	-12	27*	37	1	17	-10	162	161
4	16	-1	10*	21	6	16	11	143	142	10	16	-7	409	429	14	16	-11	108	111	1	17	-9	35	37
4	16	0	321	326	6	16	12	60	54	10	16	-6	175	173	14	16	-10	22*	36	1	17	-8	168	163
4	16	1	128	123	6	16	13	84	91	10	16	-5	299	304	14	16	-9	62	63	1	17	-8	167	163
4	16	2	282	281	6	16	14	23*	25	10	16	-4	30*	25	14	16	-8	33*	17	1	17	-7	137	135
4	16	3	180	178	6	16	14	14*	25	10	16	-3	167	155	14	16	-7	241	236	1	17	-6	113	118
4	16	4	407	404	8	16	-18	67	68	10	16	-2	24*	28	14	16	-6	50	52	1	17	-5	176	175
4	16	5	457	466	8	16	-17	94	100	10	16	-1	38*	41	14	16	-5	306	309	1	17	-4	34*	26
4	16	6	397	389	8	16	-17	107	100	10	16	0	19*	1	14	16	-4	68	65	1	17	-3	16*	20
4	16	7	110	111	8	16	-16	110	110	10	16	1	249	258	14	16	-3	276	278	1	17	-2	129	128
4	16	8	320	330	8	16	-15	0*	12	10	16	2	71	71	14	16	-2	111	103	1	17	-1	14*	5
4	16	9	80	75	8	16	-14	129	131	10	16	3	325	330	14	16	-1	371	361	1	17	0	90	100
4	16	10	78	77	8	16	-13	184	180	10	16	4	93	88	14	16	0	43*	44	1	17	1	69	72
4	16	11	27*	30	8	16	-12	66	67	10	16	5	273	280	14	16	1	164	161	1	17	2	167	170
4	16	12	116	115	8	16	-11	13*	21	10	16	6	0*	16	14	16	2	31*	36	1	17	3	26*	30
4	16	13	80	84	8	16	-10	104	108	10	16	7	271	270	14	16	3	80	76	1	17	4	85	88
4	16	14	0*	9	8	16	-9	101	100	10	16	8	21*	42	14	16	4	10*	5	1	17	5	22*	34
4	16	14	30*	9	8	16	-8	172	169	10	16	9	91	90	14	16	5	16*	4	1	17	6	134	138
4	16	15	125	128	8	16	-7	232	230	10	16	10	56*	64	14	16	6	106	101	1	17	7	84	83
6	16	-18	20*	2	8	16	-6	141	135	12	16	-16	31*	30	16	16	-13	15*	12	1	17	8	85	85
6	16	-17	42*	48	8	16	-5	365	369	12	16	-15	153	155	16	16	-12	37*	45	1	17	9	132	130
6	16	-16	110	111	8	16	-4	259	253	12	16	-14	0*	5	16	16	-11	174	173	1	17	10	19*	25
6	16	-15	170	173	8	16	-3	596	600	12	16	-13	275	271	16	16	-10	58*	51	1	17	11	201	199
6	16	-14	167	178	8	16	-2	327	341	12	16	-12	27*	45	16	16	-9	195	197	1	17	12	86	84
6	16	-13	148	146	8	16	-1	273	263	12	16	-11	358	353	16	16	-8	105	103	1	17	13	163	165
6	16	-12	417	420	8	16	0	181	182	12	16	-10	85	84	16	16	-7	280	280	1	17	14	127	122
6	16	-11	180	185	8	16	1	211	211	12	16	-9	246	250	16	16	-6	181	178	1	17	15	105	107
6	16	-10	140	151	8	16	2	0*	13	12	16	-8	65	59	16	16	-5	287	288	1	17	16	154	153
6	16	-9	121	124	8	16	3	17*	28	12	16	-7	174	177	16	16	-4	51*	57	3	17	-17	35*	70
6	16	-8	236	227	8	16	4	47	56	12	16	-6	82	84	16	16	-3	158	156	3	17	-17	63	70
6	16	-7	201	206	8	16	5	157	164	12	16	-5	22*	38	16	16	-2	106	104	3	17	-16	112	111
6	16	-6	27*	5	8	16	6	80	68	12	16	-4	10*	2	16	16	-1	0*	19	3	17	-16	116	111
6	16	-5	133	132	8	16	7	199	202	12	16	-3	247	248	16	16	0	14*	4	3	17	-15	0*	1
6	16	-4	211	204	8	16	8	23*	27	12	16	-2	73	68	16	16	1	34*	1	3	17	-14	152	149
6	16	-3	228	234	8	16	9	123	130	12	16	-1	255	254	16	16	2	67	60	3	17	-13	90	94
6	16	-2	501	496	8	16	10	23*	23	12	16	0	0*	10	18	16	-8	112	110	3	17	-13	97	94
6	16	-1	429	431	8	16	11	138	134	12	16	1	317	315	18	16	-7	72	69	3	17	-12	180	179
6	16	0	421	408	8	16	12	81	79	12	16	2	84	75	18	16	-6	14*	32	3	17	-11	159	159
6	16	1	323	322	10	16	-17	9*	15	12	16	3	308	301	18	16	-5	21*	31	3	17	-10	129	126
6	16	2	480	469	10	16	-16	72	72	12	16	4	42	44	18	16	-4	15*	16	3	17	-9	208	209
6	16	3	282	274	10	16	-15	17*	7	12	16	5	199	198	1	17	-17	142	144	3	17	-8	29*	36
6	16	4	211	205	10	16	-14	10*	22	12	16	6	26*	14	1	17	-16	6*	11	3	17	-7	203	193
6	16	5	121	123	10	16	-13	215	220	12	16	7	45*	44	1	17	-15	136	141	3	17	-6	25*	21
6	16	6	153	158	10	16	-12	75	66	12	16	8	29*	38	1	17	-14	43*	58	3	17	-5	102	102
6	16	7	49*	55	10	16	-11	190	195	14	16	-15	205	201	1	17	-13	144	149	3	17	-4	38*	39
6	16	8	177	183	10	16	-10	137	134	14	16	-14	10*	9	1	17	-12	166	163	3	17	-3	18*	5

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
3	17	-2	19*	23	5	17	12	86	83	9	17	-4	1ØØ	99	13	17	-11	33*	42	Ø	18	Ø	271	247
3	17	-1	81	8Ø	5	17	13	148	148	9	17	-3	66	64	13	17	-1Ø	22*	26	Ø	18	1	231	229
3	17	Ø	153	161	5	17	14	33*	42	9	17	-2	16*	21	13	17	-9	75	75	Ø	18	2	45	38
3	17	1	55	47	7	17	-17	147	149	9	17	-1	9*	18	13	17	-8	26*	39	Ø	18	3	353	357
3	17	2	23*	14	7	17	-16	53	54	9	17	Ø	133	138	13	17	-7	35*	25	Ø	18	4	42	31
3	17	3	8*	16	7	17	-15	116	115	9	17	1	1Ø5	1ØØ	13	17	-6	24*	6	Ø	18	5	343	351
3	17	4	62	64	7	17	-14	113	117	9	17	2	21*	33	13	17	-5	57	55	Ø	18	6	73	69
3	17	5	187	186	7	17	-13	Ø*	17	9	17	3	51	52	13	17	-4	37*	38	Ø	18	7	492	49Ø
3	17	6	1Ø2	95	7	17	-12	99	98	9	17	4	45*	49	13	17	-3	53	53	Ø	18	8	3Ø*	31
3	17	7	11Ø	1Ø9	7	17	-11	Ø*	6	9	17	5	142	136	13	17	-2	94	93	Ø	18	9	284	289
3	17	8	77	85	7	17	-1Ø	119	116	9	17	6	126	124	13	17	-1	68	72	Ø	18	1Ø	66	74
3	17	9	138	144	7	17	-9	96	95	9	17	7	48	51	13	17	Ø	75	84	Ø	18	11	149	147
3	17	1Ø	2Ø3	191	7	17	-8	Ø*	8	9	17	8	128	127	13	17	1	53	51	Ø	18	12	Ø*	14
3	17	11	32*	33	7	17	-7	59	48	9	17	9	23*	19	13	17	2	152	152	Ø	18	13	133	139
3	17	12	171	171	7	17	-6	45	45	9	17	1Ø	174	174	13	17	3	136	133	Ø	18	14	134	137
3	17	13	Ø*	1	7	17	-5	124	126	9	17	11	75	7Ø	13	17	4	57	52	Ø	18	15	24*	3
3	17	14	152	148	7	17	-4	11*	18	11	17	-16	Ø*	7	13	17	5	111	116	Ø	18	16	1Ø9	116
3	17	15	81	8Ø	7	17	-3	19*	25	11	17	-15	133	138	13	17	6	35*	35	Ø	18	16	112	116
5	17	-17	1Ø7	1Ø7	7	17	-2	66	64	11	17	-14	29*	28	13	17	7	138	139	2	18	-17	35*	41
5	17	-16	8Ø	8Ø	7	17	-1	67	69	11	17	-13	162	159	15	17	-14	Ø*	6	2	18	-16	45*	56
5	17	-15	159	157	7	17	Ø	31*	37	11	17	-12	129	127	15	17	-13	38*	48	2	18	-15	83	82
5	17	-14	47	42	7	17	1	74	78	11	17	-11	69	71	15	17	-12	Ø*	14	2	18	-14	71	67
5	17	-13	2ØØ	2Ø1	7	17	2	216	218	11	17	-1Ø	59	59	15	17	-11	77	73	2	18	-13	192	191
5	17	-12	17*	13	7	17	3	45	48	11	17	-9	76	73	15	17	-1Ø	62	62	2	18	-12	1Ø1	1Ø9
5	17	-11	16Ø	157	7	17	4	119	123	11	17	-8	65*	65	15	17	-9	48	48	2	18	-11	329	329
5	17	-1Ø	21*	28	7	17	5	7Ø	7Ø	11	17	-7	11*	2Ø	15	17	-8	35*	26	2	18	-1Ø	2Ø*	14
5	17	-9	113	11Ø	7	17	6	172	174	11	17	-6	25*	37	15	17	-7	55*	58	2	18	-9	256	246
5	17	-8	99	95	7	17	7	185	187	11	17	-5	36*	59	15	17	-6	15*	24	2	18	-8	74	87
5	17	-7	2Ø*	4	7	17	8	Ø*	2	11	17	-4	19*	5	15	17	-5	Ø*	15	2	18	-7	225	226
5	17	-6	42	51	7	17	9	125	126	11	17	-3	1Ø*	7	15	17	-4	15*	41	2	18	-6	38	37
5	17	-5	41	4Ø	7	17	1Ø	15*	35	11	17	-2	61	55	15	17	-3	77	75	2	18	-5	61	61
5	17	-4	17*	18	7	17	11	132	135	11	17	-1	89	87	15	17	-2	9*	35	2	18	-4	27*	2Ø
5	17	-3	95	94	7	17	12	136	138	11	17	Ø	91	9Ø	15	17	-1	83	78	2	18	-3	346	345
5	17	-2	34	29	7	17	13	22*	13	11	17	1	Ø*	11	15	17	Ø	51	45	2	18	-2	22*	36
5	17	-1	13*	5	9	17	-17	Ø*	24	11	17	2	35*	44	15	17	1	154	148	2	18	-1	4Ø5	394
5	17	Ø	43	48	9	17	-16	126	13Ø	11	17	3	42*	55	15	17	2	22*	37	2	18	Ø	157	155
5	17	1	31*	4Ø	9	17	-15	1Ø3	1Ø2	11	17	4	146	143	15	17	3	97	95	2	18	1	4Ø1	411
5	17	2	58	59	9	17	-14	54	58	11	17	5	53*	55	17	17	-1Ø	9*	18	2	18	2	347	345
5	17	3	148	143	9	17	-13	145	15Ø	11	17	6	122	118	17	17	-9	24*	38	2	18	3	437	456
5	17	4	242	251	9	17	-12	5Ø	52	11	17	7	77	71	17	17	-8	33*	17	2	18	4	166	163
5	17	5	14*	26	9	17	-11	221	221	11	17	8	122	122	17	17	-7	43*	33	2	18	5	369	373
5	17	6	16Ø	158	9	17	-1Ø	54	59	11	17	9	139	137	17	17	-6	34*	35	2	18	6	8Ø	78
5	17	7	49	49	9	17	-9	1Ø5	11Ø	13	17	-15	63	7Ø	17	17	-5	7Ø	64	2	18	7	156	153
5	17	8	256	253	9	17	-8	Ø*	13	13	17	-15	8Ø	7Ø	17	17	-4	Ø*	17	2	18	8	15*	16
5	17	9	1Ø6	111	9	17	-7	116	118	13	17	-14	1ØØ	98	17	17	-3	47*	52	2	18	9	1Ø4	98
5	17	1Ø	129	129	9	17	-6	26*	34	13	17	-13	Ø*	12	17	17	-2	6*	5	2	18	1Ø	86	9Ø
5	17	11	8Ø	78	9	17	-5	7*	21	13	17	-12	4Ø*	45	17	17	-1	54	59	2	18	11	91	88

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
2	18	12	96	104	6	18	-7	284	264	8	18	9	64	70	12	18	1	5*	13	1	19	-11	124	122
2	18	13	62	64	6	18	-6	368	375	8	18	10	13*	32	12	18	2	32*	41	1	19	-10	215	217
2	18	14	58	68	6	18	-5	432	437	8	18	11	114	117	12	18	3	96	93	1	19	-9	44	49
2	18	15	25*	45	6	18	-4	323	312	10	18	-16	162	157	12	18	4	136	143	1	19	-8	136	137
4	18	-17	94	106	6	18	-3	345	334	10	18	-15	6*	31	12	18	5	36*	28	1	19	-7	22*	15
4	18	-17	107	106	6	18	-2	287	293	10	18	-14	221	224	12	18	6	167	168	1	19	-6	72	74
4	18	-16	62	66	6	18	-1	143	138	10	18	-13	143	133	12	18	7	3*	18	1	19	-5	86	81
4	18	-15	215	220	6	18	0	134	141	10	18	-12	177	179	14	18	-14	112	108	1	19	-4	64	67
4	18	-14	16*	5	6	18	1	66	67	10	18	-11	54	61	14	18	-13	0*	0	1	19	-3	39*	52
4	18	-13	157	161	6	18	2	100	104	10	18	-10	210	210	14	18	-12	179	176	1	19	-2	85	82
4	18	-12	55	51	6	18	3	172	172	10	18	-9	26*	35	14	18	-11	33*	42	1	19	-1	78	88
4	18	-11	201	201	6	18	4	166	161	10	18	-8	42*	56	14	18	-10	308	302	1	19	0	80	87
4	18	-10	33*	17	6	18	5	194	189	10	18	-7	14*	14	14	18	-9	67	61	1	19	1	10*	5
4	18	-9	85	88	6	18	6	181	188	10	18	-6	208	204	14	18	-8	336	331	1	19	2	27*	37
4	18	-8	191	194	6	18	7	115	119	10	18	-5	124	125	14	18	-7	34*	13	1	19	3	18*	6
4	18	-7	249	256	6	18	8	244	242	10	18	-4	317	313	14	18	-6	225	226	1	19	4	92	90
4	18	-6	20*	15	6	18	9	221	220	10	18	-3	88	92	14	18	-5	73	69	1	19	5	130	133
4	18	-5	438	422	6	18	10	100	109	10	18	-2	376	372	14	18	-4	124	124	1	19	6	119	123
4	18	-4	168	169	6	18	11	123	129	10	18	-1	58	58	14	18	-3	54	57	1	19	7	96	93
4	18	-3	503	480	6	18	12	0*	1	10	18	0	428	436	14	18	-2	64	58	1	19	8	187	198
4	18	-2	368	365	6	18	13	56	64	10	18	1	156	153	14	18	-1	75	73	1	19	9	203	200
4	18	-1	685	676	8	18	-17	29*	32	10	18	2	253	256	14	18	0	143	142	1	19	10	65	58
4	18	0	241	228	8	18	-16	111	113	10	18	3	83	77	14	18	1	58	49	1	19	11	211	216
4	18	1	309	300	8	18	-15	76	73	10	18	4	113	119	14	18	2	187	181	1	19	12	11*	0
4	18	2	250	254	8	18	-14	108	116	10	18	5	6*	10	14	18	3	32*	37	1	19	13	160	155
4	18	3	183	192	8	18	-13	75	73	10	18	6	37*	22	14	18	4	156	156	1	19	14	94	98
4	18	4	139	139	8	18	-12	262	270	10	18	7	82	81	14	18	5	48	50	1	19	15	40*	49
4	18	5	167	172	8	18	-11	175	172	10	18	8	98	100	16	18	-12	209	205	3	19	-16	137	142
4	18	6	125	122	8	18	-10	353	361	10	18	9	29*	38	16	18	-11	50*	47	3	19	-15	20*	26
4	18	7	98	96	8	18	-9	301	301	10	18	10	82	76	16	18	-10	130	126	3	19	-14	160	159
4	18	8	156	158	8	18	-8	255	261	12	18	-16	104	105	16	18	-9	61	60	3	19	-13	0*	17
4	18	9	188	196	8	18	-7	150	156	12	18	-15	0*	28	16	18	-8	52*	74	3	19	-13	22*	17
4	18	10	146	151	8	18	-6	225	223	12	18	-14	115	114	16	18	-7	0*	8	3	19	-12	142	148
4	18	11	104	104	8	18	-5	87	85	12	18	-13	14*	30	16	18	-6	33*	11	3	19	-12	150	148
4	18	12	168	166	8	18	-4	64	66	12	18	-12	0*	10	16	18	-5	102	98	3	19	-11	67	65
4	18	13	143	146	8	18	-3	91	98	12	18	-11	20*	25	16	18	-4	177	178	3	19	-10	67	70
4	18	14	25*	41	8	18	-2	267	268	12	18	-10	204	197	16	18	-3	59	62	3	19	-9	105	102
6	18	-17	65	67	8	18	-1	175	175	12	18	-9	128	123	16	18	-2	195	197	3	19	-8	58	62
6	18	-16	9*	33	8	18	0	230	226	12	18	-8	282	283	16	18	-1	106	106	3	19	-7	101	108
6	18	-15	87	91	8	18	1	199	197	12	18	-7	49*	47	16	18	0	175	176	3	19	-6	132	132
6	18	-14	17*	27	8	18	2	315	325	12	18	-6	383	380	16	18	1	110	108	3	19	-5	119	113
6	18	-13	67	72	8	18	3	146	144	12	18	-5	0*	28	1	19	-16	21*	21	3	19	-4	133	140
6	18	-12	136	140	8	18	4	374	374	12	18	-4	464	460	1	19	-15	151	148	3	19	-3	69	70
6	18	-11	154	146	8	18	5	242	248	12	18	-3	68	70	1	19	-14	93	98	3	19	-2	74	70
6	18	-10	91	92	8	18	6	188	186	12	18	-2	253	252	1	19	-14	100	98	3	19	-1	52	51
6	18	-9	181	181	8	18	7	146	151	12	18	-1	25*	10	1	19	-13	162	161	3	19	0	0*	3
6	18	-8	201	190	8	18	8	44	50	12	18	0	165	163	1	19	-12	177	176	3	19	1	130	128

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
3	19	2	55	56	7	19	-16	97	100	9	19	0	41*	44	13	19	-3	25*	29	2	20	-15	19*	7
3	19	3	189	195	7	19	-15	41*	56	9	19	1	41*	48	13	19	-2	41	46	2	20	-14	53	52
3	19	4	21*	36	7	19	-14	162	167	9	19	2	42	38	13	19	-1	64	64	2	20	-13	73	80
3	19	5	151	154	7	19	-14	167	167	9	19	3	203	210	13	19	0	135	140	2	20	-12	61	59
3	19	6	83	78	7	19	-13	34*	39	9	19	4	47	46	13	19	1	28*	21	2	20	-11	71	75
3	19	7	226	232	7	19	-12	233	231	9	19	5	178	176	13	19	2	65	61	2	20	-10	227	221
3	19	8	49*	53	7	19	-11	41*	31	9	19	6	83	85	13	19	3	27*	52	2	20	-9	104	107
3	19	9	94	99	7	19	-10	154	152	9	19	7	154	155	13	19	4	18*	34	2	20	-8	155	161
3	19	10	64	64	7	19	-9	8*	20	9	19	8	144	141	13	19	5	118	118	2	20	-7	19*	7
3	19	11	65	61	7	19	-8	121	127	9	19	9	21*	33	13	19	6	50*	39	2	20	-6	454	438
3	19	12	157	161	7	19	-7	29*	32	9	19	10	85	86	15	19	-12	14*	8	2	20	-5	233	244
3	19	13	64	67	7	19	-6	15*	14	11	19	-16	32*	50	15	19	-11	30*	41	2	20	-4	521	520
3	19	14	80	75	7	19	-5	42	40	11	19	-15	93	97	15	19	-10	14*	6	2	20	-3	44	38
5	19	-17	39*	54	7	19	-4	28*	12	11	19	-14	31*	40	15	19	-9	24*	7	2	20	-2	477	468
5	19	-16	91	92	7	19	-3	23*	44	11	19	-13	32*	42	15	19	-8	20*	0	2	20	-1	217	213
5	19	-15	112	109	7	19	-2	42	44	11	19	-12	61	62	15	19	-7	32*	34	2	20	0	156	148
5	19	-14	0*	13	7	19	-1	106	110	11	19	-11	26*	21	15	19	-6	21*	40	2	20	1	59	60
5	19	-13	105	102	7	19	0	22*	19	11	19	-10	135	132	15	19	-5	15*	32	2	20	2	188	197
5	19	-13	105	102	7	19	1	0*	21	11	19	-9	68	71	15	19	-4	21*	17	2	20	3	0*	9
5	19	-12	72	82	7	19	2	16*	35	11	19	-8	65	68	15	19	-3	59	55	2	20	4	331	331
5	19	-11	118	114	7	19	3	0*	12	11	19	-7	25*	5	15	19	-2	59*	59	2	20	5	120	121
5	19	-10	160	163	7	19	4	100	99	11	19	-6	102	98	15	19	-1	56	65	2	20	6	167	169
5	19	-9	71	71	7	19	5	163	170	11	19	-5	27*	14	15	19	0	20*	12	2	20	7	25*	37
5	19	-8	140	139	7	19	6	0*	26	11	19	-4	27*	16	15	19	1	87	84	2	20	8	257	262
5	19	-7	0*	43	7	19	7	219	221	11	19	-3	65*	61	15	19	2	59	52	2	20	9	242	239
5	19	-6	153	154	7	19	8	24*	6	11	19	-2	103	100	17	19	-7	0*	14	2	20	10	255	258
5	19	-5	0*	3	7	19	9	234	230	11	19	-1	59	65	17	19	-6	17*	9	2	20	11	29*	44
5	19	-4	55	52	7	19	10	89	89	11	19	0	42*	41	17	19	-5	26*	8	2	20	12	174	171
5	19	-3	70	71	7	19	11	121	121	11	19	1	161	163	17	19	-4	24*	8	2	20	13	6*	28
5	19	-2	34*	51	7	19	12	64	67	11	19	2	117	116	0	20	0	861	877	2	20	14	56	61
5	19	-1	75	78	9	19	-16	148	148	11	19	3	89	90	0	20	1	11*	32	4	20	-16	15*	18
5	19	0	27*	12	9	19	-15	19*	43	11	19	4	88	90	0	20	2	274	235	4	20	-15	115	115
5	19	1	175	182	9	19	-14	156	154	11	19	5	61	58	0	20	3	54	61	4	20	-14	87	88
5	19	2	15*	20	9	19	-13	128	131	11	19	6	107	105	0	20	4	231	232	4	20	-13	14*	16
5	19	3	111	116	9	19	-12	72	75	11	19	7	67	66	0	20	5	212	218	4	20	-12	199	198
5	19	4	15*	31	9	19	-11	73	71	11	19	8	28*	42	0	20	6	59	65	4	20	-11	203	210
5	19	5	100	104	9	19	-11	62	71	13	19	-14	76	77	0	20	7	157	167	4	20	-10	215	217
5	19	6	129	125	9	19	-10	53*	55	13	19	-13	32*	40	0	20	8	32*	36	4	20	-9	87	89
5	19	7	41*	32	9	19	-9	69	64	13	19	-12	101	96	0	20	9	17*	21	4	20	-8	480	471
5	19	8	88	80	9	19	-8	68	69	13	19	-11	94	94	0	20	10	195	193	4	20	-7	91	95
5	19	9	81	79	9	19	-7	24*	26	13	19	-10	61	59	0	20	11	90	91	4	20	-6	197	200
5	19	10	109	111	9	19	-6	21*	15	13	19	-9	21*	41	0	20	12	81	83	4	20	-5	128	123
5	19	11	187	186	9	19	-5	19*	32	13	19	-8	90	91	0	20	13	56	60	4	20	-4	178	170
5	19	12	0*	15	9	19	-4	74	75	13	19	-7	18*	32	0	20	13	57	60	4	20	-3	276	281
5	19	13	124	127	9	19	-3	30*	35	13	19	-6	34*	13	0	20	14	181	185	4	20	-2	30*	37
7	19	-17	117	121	9	19	-2	18*	8	13	19	-5	60	61	0	20	15	0*	0	4	20	-1	125	123
7	19	-17	121	121	9	19	-1	55	47	13	19	-4	58	60	2	20	-16	103	101	4	20	0	223	221

Reflections flagged with an asterisk were considered unobserved.

Fobs and Fcalc for Mn(CO)5 Yb (C5Me5)2 . 1/4(toluene) @ 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
4	2Ø	1	4Ø	41	8	2Ø	-12	1Ø9	113	1Ø	2Ø	7	195	199	16	2Ø	-5	268	268	3	21	-6	25*	28
4	2Ø	2	3Ø5	3Ø8	8	2Ø	-11	91	9Ø	1Ø	2Ø	8	67	69	16	2Ø	-4	41*	48	3	21	-5	76	78
4	2Ø	3	249	247	8	2Ø	-1Ø	33*	28	1Ø	2Ø	9	7Ø	73	16	2Ø	-3	57*	76	3	21	-4	56	53
4	2Ø	4	172	172	8	2Ø	-9	191	191	12	2Ø	-15	117	123	16	2Ø	-2	27*	34	3	21	-3	59	61
4	2Ø	5	238	236	8	2Ø	-8	147	143	12	2Ø	-14	31*	17	16	2Ø	-1	52	52	3	21	-2	62	56
4	2Ø	6	444	446	8	2Ø	-7	166	163	12	2Ø	-13	224	228	1	21	-15	124	123	3	21	-1	15*	4
4	2Ø	7	143	139	8	2Ø	-6	211	2Ø7	12	2Ø	-12	35*	32	1	21	-14	49	51	3	21	Ø	43	51
4	2Ø	8	177	182	8	2Ø	-5	372	372	12	2Ø	-11	283	285	1	21	-13	82	89	3	21	1	64	66
4	2Ø	9	33*	19	8	2Ø	-4	157	155	12	2Ø	-1Ø	93	9Ø	1	21	-12	124	123	3	21	2	12Ø	1Ø9
4	2Ø	1Ø	91	91	8	2Ø	-3	447	461	12	2Ø	-9	195	2Ø0	1	21	-11	1Ø*	26	3	21	3	11Ø	114
4	2Ø	11	66	67	8	2Ø	-2	348	348	12	2Ø	-8	24*	4Ø	1	21	-1Ø	162	163	3	21	4	34*	37
4	2Ø	12	51*	6Ø	8	2Ø	-1	246	243	12	2Ø	-7	153	156	1	21	-9	53	49	3	21	5	Ø*	22
4	2Ø	13	12Ø	123	8	2Ø	Ø	114	113	12	2Ø	-6	14*	33	1	21	-8	148	141	3	21	6	45	53
6	2Ø	-16	Ø*	35	8	2Ø	1	125	126	12	2Ø	-5	24*	24	1	21	-7	1Ø7	1Ø4	3	21	7	175	168
6	2Ø	-16	19*	35	8	2Ø	2	84	92	12	2Ø	-4	52	57	1	21	-6	1Ø9	117	3	21	8	161	171
6	2Ø	-15	72	78	8	2Ø	3	71	65	12	2Ø	-3	244	24Ø	1	21	-5	122	122	3	21	9	62	63
6	2Ø	-14	179	183	8	2Ø	4	38*	53	12	2Ø	-2	85	82	1	21	-4	84	87	3	21	1Ø	147	143
6	2Ø	-13	2Ø3	2Ø3	8	2Ø	5	158	159	12	2Ø	-1	254	252	1	21	-3	93	96	3	21	11	63	54
6	2Ø	-12	243	245	8	2Ø	6	63	62	12	2Ø	Ø	9*	2Ø	1	21	-2	5Ø	46	3	21	12	2Ø3	2Ø1
6	2Ø	-11	23*	19	8	2Ø	7	128	13Ø	12	2Ø	1	23Ø	233	1	21	-1	33*	4Ø	3	21	13	16*	32
6	2Ø	-1Ø	236	233	8	2Ø	8	57	51	12	2Ø	2	37*	22	1	21	Ø	91	92	3	21	13	24*	32
6	2Ø	-9	185	192	8	2Ø	9	84	88	12	2Ø	3	286	282	1	21	1	Ø*	7	3	21	14	94	94
6	2Ø	-8	1Ø8	111	8	2Ø	1Ø	24*	6	12	2Ø	4	23*	23	1	21	2	63	65	5	21	-16	83	81
6	2Ø	-7	36	36	8	2Ø	11	11Ø	111	12	2Ø	5	13Ø	133	1	21	3	68	68	5	21	-16	9Ø	81
6	2Ø	-6	94	95	1Ø	2Ø	-16	21*	33	12	2Ø	6	43*	49	1	21	4	127	128	5	21	-15	152	156
6	2Ø	-5	72	65	1Ø	2Ø	-15	37*	32	14	2Ø	-13	132	135	1	21	5	7*	4	5	21	-14	16*	21
6	2Ø	-4	313	3Ø4	1Ø	2Ø	-14	7Ø	76	14	2Ø	-12	41*	45	1	21	6	9Ø	96	5	21	-13	158	163
6	2Ø	-3	228	227	1Ø	2Ø	-13	13Ø	131	14	2Ø	-11	92	93	1	21	7	26*	33	5	21	-12	Ø*	1Ø
6	2Ø	-2	282	274	1Ø	2Ø	-12	128	118	14	2Ø	-1Ø	7*	4	1	21	8	118	121	5	21	-11	17Ø	17Ø
6	2Ø	-1	228	229	1Ø	2Ø	-11	192	197	14	2Ø	-9	11*	1Ø	1	21	9	126	12Ø	5	21	-1Ø	74	74
6	2Ø	Ø	329	321	1Ø	2Ø	-1Ø	9Ø	91	14	2Ø	-8	37*	35	1	21	1Ø	Ø*	7	5	21	-9	23*	3Ø
6	2Ø	1	4Ø1	4Ø2	1Ø	2Ø	-9	3Ø5	299	14	2Ø	-7	2Ø9	211	1	21	11	132	134	5	21	-8	36*	37
6	2Ø	2	3Ø5	314	1Ø	2Ø	-8	133	126	14	2Ø	-6	31*	11	1	21	12	67	65	5	21	-7	8*	17
6	2Ø	3	168	163	1Ø	2Ø	-7	444	438	14	2Ø	-5	221	223	1	21	13	133	137	5	21	-6	84	92
6	2Ø	4	237	243	1Ø	2Ø	-6	178	177	14	2Ø	-4	Ø*	13	1	21	14	142	14Ø	5	21	-5	79	73
6	2Ø	5	188	186	1Ø	2Ø	-5	265	264	14	2Ø	-3	269	276	1	21	15	65	6Ø	5	21	-4	39	43
6	2Ø	6	83	87	1Ø	2Ø	-4	69	72	14	2Ø	-2	97	89	3	21	-16	95	9Ø	5	21	-3	47	48
6	2Ø	7	52	46	1Ø	2Ø	-3	175	172	14	2Ø	-1	277	271	3	21	-15	16*	7	5	21	-2	3Ø*	46
6	2Ø	8	153	157	1Ø	2Ø	-2	28*	11	14	2Ø	Ø	2Ø*	35	3	21	-14	125	125	5	21	-1	79	8Ø
6	2Ø	9	1Ø1	1ØØ	1Ø	2Ø	-1	26*	46	14	2Ø	1	18Ø	178	3	21	-13	1Ø2	1Ø3	5	21	Ø	57	54
6	2Ø	1Ø	13*	23	1Ø	2Ø	Ø	75	73	14	2Ø	2	Ø*	3	3	21	-13	1Ø7	1Ø3	5	21	1	92	97
6	2Ø	11	116	117	1Ø	2Ø	1	21Ø	213	14	2Ø	3	4Ø	42	3	21	-12	151	156	5	21	2	118	114
6	2Ø	12	29*	34	1Ø	2Ø	2	6Ø	65	16	2Ø	-1Ø	19*	29	3	21	-11	15Ø	152	5	21	3	1Ø*	21
8	2Ø	-16	121	123	1Ø	2Ø	3	236	242	16	2Ø	-9	181	186	3	21	-1Ø	1Ø1	97	5	21	4	38*	52
8	2Ø	-15	46*	62	1Ø	2Ø	4	79	8Ø	16	2Ø	-8	125	118	3	21	-9	146	145	5	21	5	115	123
8	2Ø	-14	Ø*	12	1Ø	2Ø	5	213	217	16	2Ø	-7	196	2Ø0	3	21	-8	2Ø*	24	5	21	6	228	229
8	2Ø	-13	56	49	1Ø	2Ø	6	23*	7	16	2Ø	-6	122	118	3	21	-7	1Ø9	111	5	21	7	3Ø*	5Ø

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
5	21	8	144	149	9	21	-3	Ø*	3	13	21	-3	55	5Ø	2	22	-4	1Ø3	93	4	22	9	131	126
5	21	9	18*	28	9	21	-2	141	14Ø	13	21	-2	2Ø*	37	2	22	-3	162	165	4	22	1Ø	84	83
5	21	1Ø	185	187	9	21	-1	124	125	13	21	-1	Ø*	18	2	22	-2	66	77	4	22	11	92	89
5	21	11	122	117	9	21	Ø	34*	21	13	21	Ø	145	145	2	22	-1	371	354	4	22	12	14Ø	143
5	21	12	Ø*	7	9	21	1	25*	11	13	21	1	1Ø7	1Ø4	2	22	Ø	111	1Ø8	4	22	13	98	97
7	21	-16	49	56	9	21	2	152	146	13	21	2	81	82	2	22	1	343	35Ø	6	22	-15	81	85
7	21	-16	56	56	9	21	3	138	144	13	21	3	76	75	2	22	2	173	172	6	22	-15	85	85
7	21	-15	82	84	9	21	4	52	52	13	21	4	93	88	2	22	3	56Ø	555	6	22	-14	22*	25
7	21	-14	52*	62	9	21	5	62	58	15	21	-11	28*	4Ø	2	22	4	11Ø	115	6	22	-14	26*	25
7	21	-13	45	54	9	21	6	6Ø	62	15	21	-1Ø	45	39	2	22	5	239	241	6	22	-13	27*	1Ø
7	21	-13	52	54	9	21	7	72	76	15	21	-9	56	56	2	22	6	39*	28	6	22	-12	144	145
7	21	-12	142	14Ø	9	21	8	161	156	15	21	-8	44	42	2	22	7	22Ø	223	6	22	-11	1Ø2	9Ø
7	21	-11	45*	52	9	21	9	51*	44	15	21	-7	35*	33	2	22	8	76	66	6	22	-1Ø	46	56
7	21	-1Ø	32*	49	11	21	-15	147	151	15	21	-6	Ø*	12	2	22	9	73	7Ø	6	22	-9	23Ø	232
7	21	-9	32*	43	11	21	-14	81	8Ø	15	21	-5	72	66	2	22	1Ø	1Ø9	111	6	22	-8	218	214
7	21	-8	77	87	11	21	-13	76	71	15	21	-4	Ø*	14	2	22	1Ø	1Ø7	111	6	22	-7	266	251
7	21	-7	144	137	11	21	-12	58	6Ø	15	21	-3	13*	27	2	22	11	4Ø*	38	6	22	-6	3Ø5	319
7	21	-6	49	54	11	21	-12	53	6Ø	15	21	-2	83	87	2	22	12	58	59	6	22	-5	437	448
7	21	-5	37*	5Ø	11	21	-11	112	1Ø5	15	21	-1	1Ø9	1Ø9	2	22	12	54	59	6	22	-4	249	254
7	21	-4	63	73	11	21	-1Ø	1Ø3	98	15	21	Ø	9*	13	2	22	13	76	78	6	22	-3	181	173
7	21	-3	131	127	11	21	-9	Ø*	12	Ø	22	Ø	87	71	2	22	14	68	76	6	22	-2	187	194
7	21	-2	Ø*	14	11	21	-8	17*	36	Ø	22	1	37Ø	364	4	22	-15	144	148	6	22	-1	143	136
7	21	-1	3Ø*	9	11	21	-7	56	48	Ø	22	2	41	43	4	22	-14	21*	4	6	22	Ø	159	162
7	21	Ø	173	174	11	21	-6	1*	16	Ø	22	3	332	334	4	22	-13	138	147	6	22	1	75	82
7	21	1	39*	55	11	21	-5	29*	37	Ø	22	4	154	158	4	22	-13	15Ø	147	6	22	2	178	19Ø
7	21	2	71	75	11	21	-4	133	139	Ø	22	5	4Ø7	4Ø2	4	22	-12	11Ø	1Ø5	6	22	3	75	81
7	21	3	56	56	11	21	-3	75	67	Ø	22	6	1Ø1	99	4	22	-11	115	1Ø9	6	22	4	136	138
7	21	4	212	2Ø4	11	21	-2	Ø*	25	Ø	22	7	331	328	4	22	-1Ø	38*	19	6	22	5	181	175
7	21	5	138	141	11	21	-1	26*	34	Ø	22	8	86	84	4	22	-9	149	165	6	22	6	177	179
7	21	6	71	8Ø	11	21	Ø	34*	37	Ø	22	9	298	298	4	22	-8	11Ø	115	6	22	7	1Ø5	1Ø1
7	21	7	82	8Ø	11	21	1	1Ø8	1Ø9	Ø	22	1Ø	Ø*	12	4	22	-7	282	277	6	22	8	2Ø4	2Ø2
7	21	8	52	57	11	21	2	124	124	Ø	22	11	1Ø5	1Ø2	4	22	-6	72	61	6	22	9	164	16Ø
7	21	9	143	142	11	21	3	19*	19	Ø	22	12	25*	1Ø	4	22	-5	292	282	6	22	1Ø	59	6Ø
7	21	1Ø	86	91	11	21	4	88	92	Ø	22	13	11Ø	1Ø7	4	22	-4	82	84	6	22	11	97	96
7	21	11	32*	41	11	21	5	13*	1Ø	Ø	22	14	91	94	4	22	-3	375	368	8	22	-15	71	65
9	21	-15	35*	33	11	21	6	164	161	2	22	-15	77	83	4	22	-2	34Ø	333	8	22	-14	9Ø	93
9	21	-14	76	76	11	21	7	1Ø9	1Ø7	2	22	-14	63	65	4	22	-1	458	459	8	22	-13	18*	13
9	21	-13	155	15Ø	13	21	-13	29*	23	2	22	-14	66	65	4	22	Ø	1Ø9	1Ø5	8	22	-12	15Ø	147
9	21	-12	2Ø*	15	13	21	-12	79	78	2	22	-13	144	14Ø	4	22	1	265	256	8	22	-11	166	159
9	21	-11	115	11Ø	13	21	-11	42*	49	2	22	-12	62	73	4	22	2	252	262	8	22	-1Ø	326	322
9	21	-1Ø	Ø*	36	13	21	-1Ø	17*	2	2	22	-11	341	344	4	22	3	121	129	8	22	-9	252	246
9	21	-9	165	159	13	21	-9	27*	6	2	22	-1Ø	13*	9	4	22	4	113	1Ø9	8	22	-8	184	192
9	21	-8	88	86	13	21	-8	Ø*	7	2	22	-9	176	17Ø	4	22	5	181	176	8	22	-7	169	169
9	21	-7	35*	52	13	21	-7	52	56	2	22	-8	2Ø*	5	4	22	6	87	88	8	22	-6	2Ø7	2ØØ
9	21	-6	52	56	13	21	-6	81	83	2	22	-7	259	272	4	22	7	128	128	8	22	-5	44*	38
9	21	-5	97	84	13	21	-5	Ø*	2	2	22	-6	85	81	4	22	8	129	13Ø	8	22	-4	89	97
9	21	-4	Ø*	2	13	21	-4	36*	17	2	22	-5	75	77	4	22	8	126	13Ø	8	22	-3	63	69

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
8	22	-2	186	188	12	22	-4	39Ø	391	1	23	9	185	181	5	23	-5	42*	49	9	23	-12	63	63
8	22	-1	168	166	12	22	-3	79	84	1	23	1Ø	69	62	5	23	-4	7Ø	66	9	23	-11	48*	63
8	22	Ø	224	227	12	22	-2	199	2ØØ	1	23	11	192	2Ø1	5	23	-3	47*	53	9	23	-1Ø	14*	2Ø
8	22	1	8Ø	78	12	22	-1	15*	2Ø	1	23	12	16*	Ø	5	23	-2	11*	1	9	23	-9	22*	17
8	22	2	274	273	12	22	Ø	126	123	1	23	13	112	113	5	23	-1	91	89	9	23	-8	21*	26
8	22	3	115	118	12	22	1	Ø*	7	1	23	14	5Ø*	57	5	23	Ø	14*	7	9	23	-7	26*	16
8	22	4	349	35Ø	12	22	2	5Ø	44	3	23	-15	28*	44	5	23	1	15Ø	151	9	23	-6	51*	59
8	22	5	183	179	12	22	3	6Ø	62	3	23	-15	17*	44	5	23	2	Ø*	27	9	23	-5	65	73
8	22	6	138	138	12	22	4	111	113	3	23	-14	131	129	5	23	3	121	118	9	23	-4	44*	63
8	22	7	77	78	12	22	5	34*	4Ø	3	23	-13	2Ø*	4	5	23	4	23*	25	9	23	-3	14*	8
8	22	8	26*	36	14	22	-11	36*	44	3	23	-12	115	115	5	23	5	96	1Ø2	9	23	-2	17*	14
8	22	9	35*	37	14	22	-1Ø	239	243	3	23	-11	76	76	5	23	6	76	74	9	23	-1	27*	39
8	22	1Ø	23*	19	14	22	-9	6Ø	53	3	23	-1Ø	Ø*	26	5	23	7	Ø*	4	9	23	Ø	36*	4Ø
1Ø	22	-15	14*	24	14	22	-8	286	286	3	23	-9	62	57	5	23	8	9Ø	89	9	23	1	92	1Ø1
1Ø	22	-14	165	171	14	22	-7	8*	28	3	23	-8	6Ø	61	5	23	9	1Ø1	1ØØ	9	23	2	15*	11
1Ø	22	-13	122	123	14	22	-6	142	145	3	23	-7	73	72	5	23	1Ø	67	63	9	23	3	159	163
1Ø	22	-12	129	129	14	22	-5	4Ø*	39	3	23	-6	149	146	5	23	11	129	128	9	23	4	4Ø	42
1Ø	22	-11	11*	3Ø	14	22	-4	85	83	3	23	-5	59	49	5	23	12	2Ø*	24	9	23	5	152	148
1Ø	22	-1Ø	127	124	14	22	-3	61	57	3	23	-4	114	117	7	23	-15	48*	57	9	23	6	96	95
1Ø	22	-1Ø	119	124	14	22	-2	12*	11	3	23	-3	45	49	7	23	-14	132	133	9	23	7	95	1ØØ
1Ø	22	-9	25*	45	14	22	-1	79	75	3	23	-2	56	6Ø	7	23	-13	Ø*	24	9	23	8	94	93
1Ø	22	-8	29*	42	14	22	Ø	122	123	3	23	-1	32*	41	7	23	-12	16Ø	155	11	23	-13	19*	35
1Ø	22	-7	33*	22	14	22	1	23*	36	3	23	Ø	18*	11	7	23	-12	154	155	11	23	-12	53	5Ø
1Ø	22	-6	217	212	14	22	2	161	161	3	23	1	5Ø*	58	7	23	-11	2Ø*	4	11	23	-11	19*	7
1Ø	22	-5	1Ø1	1Ø1	1	23	-14	88	87	3	23	2	86	8Ø	7	23	-1Ø	17Ø	166	11	23	-1Ø	73	69
1Ø	22	-4	274	276	1	23	-13	134	137	3	23	3	151	159	7	23	-9	6*	19	11	23	-9	3Ø*	2Ø
1Ø	22	-3	1ØØ	98	1	23	-12	142	137	3	23	4	45	53	7	23	-8	124	131	11	23	-8	49*	6Ø
1Ø	22	-2	348	352	1	23	-11	112	11Ø	3	23	5	179	182	7	23	-7	Ø*	8	11	23	-7	31*	4Ø
1Ø	22	-1	5Ø	46	1	23	-1Ø	156	153	3	23	6	55	53	7	23	-6	18*	28	11	23	-6	43*	49
1Ø	22	Ø	395	394	1	23	-9	53	5Ø	3	23	7	18Ø	187	7	23	-5	8*	6	11	23	-5	11*	24
1Ø	22	1	125	125	1	23	-8	71	65	3	23	8	24*	23	7	23	-4	19*	1	11	23	-4	31*	27
1Ø	22	2	219	214	1	23	-7	13*	1Ø	3	23	9	11Ø	116	7	23	-3	59	63	11	23	-3	7*	21
1Ø	22	3	44	39	1	23	-6	Ø*	21	3	23	1Ø	81	87	7	23	-2	19*	2	11	23	-2	67	68
1Ø	22	4	1Ø1	98	1	23	-5	Ø*	12	3	23	1Ø	93	87	7	23	-1	39	41	11	23	-1	86	88
1Ø	22	5	25*	5	1	23	-4	Ø*	11	3	23	11	Ø*	9	7	23	Ø	Ø*	5	11	23	Ø	35*	47
1Ø	22	6	Ø*	26	1	23	-3	29*	33	3	23	12	96	97	7	23	1	36*	22	11	23	1	118	122
1Ø	22	7	55	54	1	23	-2	8Ø	84	3	23	13	45	37	7	23	2	3Ø*	13	11	23	2	97	1Ø2
1Ø	22	8	87	86	1	23	-1	17*	18	5	23	-15	69	78	7	23	3	22*	4	11	23	3	79	83
12	22	-13	24*	24	1	23	Ø	22*	18	5	23	-14	Ø*	4	7	23	4	34*	42	11	23	4	1Ø7	111
12	22	-12	26*	1	1	23	1	15*	16	5	23	-13	1Ø7	1Ø5	7	23	5	112	112	11	23	5	13*	18
12	22	-11	Ø*	Ø	1	23	2	21*	34	5	23	-12	75	74	7	23	6	Ø*	39	11	23	6	75	72
12	22	-1Ø	169	17Ø	1	23	3	71	72	5	23	-11	1Ø6	1Ø6	7	23	7	173	173	13	23	-12	9Ø	84
12	22	-9	8Ø	76	1	23	4	76	77	5	23	-1Ø	144	142	7	23	8	Ø*	8	13	23	-11	79	75
12	22	-8	199	2Ø4	1	23	5	13Ø	131	5	23	-9	73	75	7	23	9	144	148	13	23	-1Ø	42*	56
12	22	-7	Ø*	16	1	23	6	12Ø	121	5	23	-8	164	162	7	23	1Ø	45	52	13	23	-9	5Ø*	65
12	22	-6	3Ø6	3ØØ	1	23	7	174	177	5	23	-7	12*	5	9	23	-14	114	11Ø	13	23	-8	5Ø	52
12	22	-5	41	31	1	23	8	11Ø	1Ø6	5	23	-6	133	137	9	23	-13	83	82	13	23	-7	2Ø*	1

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
13	23	-6	35*	36	2	24	-1	24*	28	6	24	-10	127	124	10	24	-13	104	110	1	25	-13	80	79
13	23	-5	19*	27	2	24	0	274	265	6	24	-9	119	121	10	24	-12	72	60	1	25	-12	87	91
13	23	-4	26*	27	2	24	1	138	154	6	24	-8	123	127	10	24	-11	108	117	1	25	-11	0*	6
13	23	-3	43*	50	2	24	2	8*	9	6	24	-7	103	100	10	24	-11	116	117	1	25	-10	123	125
13	23	-2	44*	40	2	24	3	106	107	6	24	-6	22*	18	10	24	-10	85	90	1	25	-9	55	55
13	23	-1	74	74	2	24	4	149	152	6	24	-5	102	96	10	24	-9	222	216	1	25	-8	123	119
13	23	0	84	86	2	24	5	0*	11	6	24	-4	176	167	10	24	-8	84	82	1	25	-7	81	83
13	23	1	15*	16	2	24	6	258	262	6	24	-3	139	145	10	24	-7	288	281	1	25	-6	100	108
13	23	2	66	64	2	24	7	76	73	6	24	-2	251	245	10	24	-6	145	143	1	25	-5	112	110
13	23	3	45	52	2	24	8	170	173	6	24	-1	228	225	10	24	-5	226	227	1	25	-4	93	94
15	23	-8	0*	22	2	24	9	100	104	6	24	0	197	195	10	24	-4	37*	53	1	25	-3	81	88
15	23	-7	30*	8	2	24	10	232	241	6	24	1	260	254	10	24	-3	159	157	1	25	-2	74	74
15	23	-6	32*	39	2	24	11	50	53	6	24	2	265	270	10	24	-2	20*	15	1	25	-1	18*	17
15	23	-5	26*	23	2	24	11	53	53	6	24	3	196	195	10	24	-1	56	61	1	25	0	42*	44
15	23	-4	27*	17	2	24	12	95	95	6	24	4	140	140	10	24	0	14*	12	1	25	1	61	66
15	23	-3	9*	22	2	24	13	36*	23	6	24	5	98	101	10	24	1	120	121	1	25	2	98	102
15	23	-2	19*	16	4	24	-14	90	88	6	24	6	92	96	10	24	2	60	59	1	25	3	40*	51
0	24	0	586	570	4	24	-13	67	72	6	24	7	61	63	10	24	3	164	165	1	25	4	87	93
0	24	1	159	159	4	24	-12	118	113	6	24	7	65	63	10	24	4	45*	53	1	25	5	31*	41
0	24	2	423	410	4	24	-11	113	122	6	24	8	60	59	10	24	5	145	148	1	25	6	120	131
0	24	3	23*	23	4	24	-10	272	267	6	24	9	111	108	10	24	6	22*	16	1	25	7	54	53
0	24	4	128	127	4	24	-9	147	151	6	24	10	17*	0	12	24	-12	56	54	1	25	8	32*	43
0	24	5	37*	39	4	24	-8	344	332	8	24	-14	48	49	12	24	-11	225	225	1	25	9	61	57
0	24	6	140	145	4	24	-7	22*	41	8	24	-13	70	71	12	24	-10	56	52	1	25	10	21*	2
0	24	7	92	96	4	24	-6	263	269	8	24	-12	36*	39	12	24	-9	130	129	1	25	11	123	128
0	24	8	101	102	4	24	-5	123	117	8	24	-11	6*	15	12	24	-8	17*	11	1	25	12	86	87
0	24	9	83	83	4	24	-4	98	92	8	24	-10	22*	28	12	24	-7	106	102	1	25	13	88	89
0	24	10	123	120	4	24	-3	41*	55	8	24	-9	113	113	12	24	-6	0*	17	3	25	-14	99	104
0	24	11	9*	29	4	24	-2	129	132	8	24	-8	158	154	12	24	-5	19*	25	3	25	-13	78	85
0	24	12	137	146	4	24	-1	78	67	8	24	-7	183	183	12	24	-4	30*	17	3	25	-12	119	123
0	24	12	149	146	4	24	0	203	199	8	24	-6	183	176	12	24	-3	168	166	3	25	-11	139	138
0	24	13	72	72	4	24	1	115	117	8	24	-5	290	291	12	24	-2	61	59	3	25	-10	72	70
0	24	14	111	115	4	24	2	172	177	8	24	-4	214	204	12	24	-1	164	168	3	25	-9	135	132
2	24	-14	90	97	4	24	3	147	141	8	24	-3	410	412	12	24	0	32*	33	3	25	-8	0*	38
2	24	-14	101	97	4	24	4	286	288	8	24	-2	246	245	12	24	1	188	189	3	25	-7	98	98
2	24	-13	0*	9	4	24	5	267	266	8	24	-1	209	205	12	24	2	28*	42	3	25	-6	0*	3
2	24	-12	33*	35	4	24	6	292	296	8	24	0	121	119	12	24	3	191	186	3	25	-5	25*	5
2	24	-11	88	88	4	24	7	67	66	8	24	1	142	140	12	24	4	24*	21	3	25	-4	23*	33
2	24	-10	76	69	4	24	8	205	217	8	24	2	51	59	14	24	-9	15*	29	3	25	-3	29*	11
2	24	-9	29*	42	4	24	9	29*	44	8	24	3	56	53	14	24	-8	0*	1	3	25	-2	8*	16
2	24	-8	188	194	4	24	10	43*	51	8	24	4	42*	39	14	24	-7	146	151	3	25	-1	83	81
2	24	-7	124	119	4	24	11	19*	8	8	24	5	87	92	14	24	-6	11*	23	3	25	0	86	93
2	24	-6	266	259	4	24	12	64	67	8	24	6	58	64	14	24	-5	160	166	3	25	1	26*	32
2	24	-5	111	117	6	24	-14	85	85	8	24	7	121	119	14	24	-4	0*	18	3	25	2	44	44
2	24	-4	464	467	6	24	-13	124	129	8	24	8	48	46	14	24	-3	170	176	3	25	3	20*	18
2	24	-3	90	91	6	24	-12	196	197	8	24	9	67	73	14	24	-2	60	51	3	25	4	61	66
2	24	-2	279	278	6	24	-11	85	86	10	24	-13	118	110	14	24	-1	218	221	3	25	5	101	99

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
3	25	6	72	71	7	25	Ø	73	73	11	25	4	129	133	2	26	7	136	142	6	26	-2	164	163
3	25	7	66	66	7	25	1	25*	17	13	25	-1Ø	28*	34	2	26	7	137	142	6	26	-1	97	98
3	25	8	1Ø1	1Ø2	7	25	2	15Ø	156	13	25	-9	41*	38	2	26	8	31*	38	6	26	Ø	15*	22
3	25	9	112	111	7	25	3	47*	53	13	25	-8	29*	37	2	26	9	85	92	6	26	1	55	6Ø
3	25	1Ø	178	181	7	25	4	98	91	13	25	-7	22*	11	2	26	1Ø	Ø*	36	6	26	2	77	83
3	25	1Ø	177	181	7	25	5	17*	25	13	25	-6	Ø*	12	2	26	1Ø	38*	36	6	26	3	1Ø4	1Ø2
3	25	11	Ø*	1Ø	7	25	6	115	12Ø	13	25	-5	41*	49	2	26	11	59	62	6	26	4	155	156
3	25	12	114	122	7	25	7	114	113	13	25	-4	49	55	2	26	11	38*	62	6	26	5	112	1Ø9
5	25	-14	36*	34	7	25	8	18*	11	13	25	-3	32*	27	2	26	12	86	95	6	26	6	148	151
5	25	-13	149	153	7	25	9	54	51	13	25	-2	Ø*	29	2	26	12	88	95	6	26	7	97	95
5	25	-12	13*	16	9	25	-13	78	76	13	25	-1	33*	45	4	26	-13	7Ø	87	6	26	8	169	166
5	25	-11	121	12Ø	9	25	-12	18*	31	13	25	Ø	18*	48	4	26	-13	86	87	6	26	9	119	121
5	25	-1Ø	28*	34	9	25	-11	133	134	13	25	1	26*	2Ø	4	26	-12	24*	31	8	26	-13	46*	6Ø
5	25	-9	74	8Ø	9	25	-1Ø	9*	19	Ø	26	Ø	84	71	4	26	-11	151	149	8	26	-12	165	166
5	25	-8	69	67	9	25	-9	69	63	Ø	26	1	133	128	4	26	-1Ø	35*	48	8	26	-11	56*	72
5	25	-7	37*	44	9	25	-8	2Ø*	17	Ø	26	2	73	67	4	26	-9	22*	14	8	26	-1Ø	169	171
5	25	-6	16*	2	9	25	-7	122	123	Ø	26	3	358	368	4	26	-9	Ø*	14	8	26	-9	184	178
5	25	-5	56	52	9	25	-6	22*	24	Ø	26	4	53	45	4	26	-8	1Ø6	113	8	26	-8	2Ø8	21Ø
5	25	-4	16*	24	9	25	-5	Ø*	13	Ø	26	5	279	287	4	26	-7	89	93	8	26	-7	86	89
5	25	-3	11Ø	1Ø8	9	25	-4	76	76	Ø	26	6	21*	23	4	26	-6	41*	44	8	26	-6	15Ø	149
5	25	-2	Ø*	22	9	25	-3	65	66	Ø	26	7	355	357	4	26	-5	259	256	8	26	-5	7Ø	61
5	25	-1	18*	9	9	25	-2	36*	42	Ø	26	8	25*	32	4	26	-4	184	187	8	26	-4	1Ø6	1Ø7
5	25	Ø	2Ø*	22	9	25	-1	18*	27	Ø	26	9	178	18Ø	4	26	-3	23Ø	229	8	26	-3	12*	31
5	25	1	34*	42	9	25	Ø	125	127	Ø	26	1Ø	41*	5Ø	4	26	-2	157	161	8	26	-2	14Ø	14Ø
5	25	2	Ø*	6	9	25	1	1Ø2	1Ø7	Ø	26	11	1Ø3	98	4	26	-1	359	364	8	26	-1	112	111
5	25	3	66	61	9	25	2	16*	16	Ø	26	11	95	98	4	26	Ø	133	13Ø	8	26	Ø	167	163
5	25	4	122	124	9	25	3	48	58	Ø	26	12	2Ø*	3	4	26	1	212	2Ø7	8	26	1	131	125
5	25	5	Ø*	28	9	25	4	4*	14	2	26	-13	155	155	4	26	2	87	91	8	26	2	227	227
5	25	6	117	118	9	25	5	97	1ØØ	2	26	-12	72	75	4	26	3	188	189	8	26	3	86	87
5	25	7	42*	49	9	25	6	92	97	2	26	-11	2Ø2	2Ø2	4	26	4	91	9Ø	8	26	4	216	217
5	25	8	185	185	9	25	7	Ø*	5	2	26	-1Ø	26*	32	4	26	5	43	45	8	26	5	1Ø6	114
5	25	9	7Ø	75	11	25	-12	8Ø	84	2	26	-9	269	259	4	26	6	1Ø3	1Ø2	8	26	6	134	135
5	25	1Ø	71	79	11	25	-11	17*	32	2	26	-8	39	42	4	26	7	4Ø*	34	8	26	7	7Ø	71
7	25	-14	76	77	11	25	-1Ø	27*	8	2	26	-7	165	17Ø	4	26	8	95	94	1Ø	26	-12	82	88
7	25	-13	Ø*	11	11	25	-9	24*	46	2	26	-6	1Ø1	1Ø2	4	26	9	12Ø	12Ø	1Ø	26	-11	54	61
7	25	-12	72	76	11	25	-8	24*	2Ø	2	26	-5	1ØØ	99	4	26	1Ø	9Ø	95	1Ø	26	-11	65	61
7	25	-11	6*	1Ø	11	25	-7	22*	41	2	26	-4	5Ø*	44	6	26	-13	49	5Ø	1Ø	26	-1Ø	1Ø9	11Ø
7	25	-1Ø	1ØØ	98	11	25	-6	73	68	2	26	-3	153	15Ø	6	26	-12	31*	43	1Ø	26	-9	26*	16
7	25	-9	1Ø8	111	11	25	-5	25*	3Ø	2	26	-2	97	87	6	26	-11	153	144	1Ø	26	-8	32*	6
7	25	-8	15*	18	11	25	-4	4Ø*	56	2	26	-1	221	2Ø7	6	26	-1Ø	115	119	1Ø	26	-7	19*	19
7	25	-7	97	91	11	25	-3	34*	37	2	26	Ø	3Ø*	34	6	26	-9	14Ø	141	1Ø	26	-6	93	95
7	25	-6	29*	32	11	25	-2	91	9Ø	2	26	1	427	428	6	26	-8	133	129	1Ø	26	-5	93	87
7	25	-5	14Ø	141	11	25	-1	71	69	2	26	2	194	187	6	26	-7	278	265	1Ø	26	-4	2Ø2	2Ø5
7	25	-4	Ø*	7	11	25	Ø	31*	39	2	26	3	412	398	6	26	-6	298	3Ø3	1Ø	26	-3	95	98
7	25	-3	35*	26	11	25	1	Ø*	25	2	26	4	59	53	6	26	-5	265	26Ø	1Ø	26	-2	248	248
7	25	-2	1Ø6	1Ø4	11	25	2	45	38	2	26	5	384	389	6	26	-4	23Ø	231	1Ø	26	-1	72	75
7	25	-1	83	81	11	25	3	38*	38	2	26	6	37*	49	6	26	-3	252	248	1Ø	26	Ø	285	286

Reflections flagged with an asterisk were considered unobserved.

Fobs and Fclc for Mn(CO)5 Yb (C5Me5)2 . 1/4(toluene) @ 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
10	26	1	55	63	3	27	-7	17*	35	7	27	-6	54	50	0	28	1	22*	24	4	28	-3	31*	44
10	26	2	181	179	3	27	-6	106	105	7	27	-5	23*	3	0	28	2	339	336	4	28	-2	56	60
10	26	3	48	42	3	27	-5	27*	26	7	27	-4	0*	7	0	28	3	0*	15	4	28	-1	37*	50
10	26	4	72	74	3	27	-4	106	106	7	27	-3	40*	50	0	28	4	205	205	4	28	0	114	109
10	26	5	13*	16	3	27	-3	22*	34	7	27	-2	25*	8	0	28	5	0*	25	4	28	1	82	83
12	26	-10	117	118	3	27	-2	75	75	7	27	-1	21*	19	0	28	6	128	128	4	28	2	176	179
12	26	-9	38*	47	3	27	-1	18*	17	7	27	0	20*	31	0	28	7	17*	30	4	28	3	134	136
12	26	-8	144	151	3	27	0	19*	24	7	27	1	36*	41	0	28	8	70	66	4	28	4	223	228
12	26	-7	30*	20	3	27	1	98	100	7	27	2	27*	37	0	28	9	53	60	4	28	5	188	186
12	26	-6	195	197	3	27	2	32*	40	7	27	3	50	48	0	28	10	118	114	4	28	6	222	225
12	26	-5	19*	13	3	27	3	102	109	7	27	4	21*	3	0	28	10	116	114	4	28	7	100	100
12	26	-4	236	243	3	27	4	99	109	7	27	5	56	57	0	28	11	31*	24	4	28	8	151	156
12	26	-3	0*	27	3	27	5	180	184	7	27	6	23*	35	2	28	-12	0*	35	4	28	9	12*	15
12	26	-2	155	158	3	27	6	11*	8	7	27	7	135	133	2	28	-12	44	35	6	28	-12	162	164
12	26	-1	0*	17	3	27	7	112	117	9	27	-11	44*	58	2	28	-11	46	43	6	28	-11	96	97
12	26	0	105	107	3	27	8	26*	12	9	27	-10	22*	0	2	28	-10	0*	41	6	28	-10	79	84
12	26	1	24*	18	3	27	9	96	96	9	27	-9	26*	3	2	28	-9	0*	11	6	28	-9	94	92
12	26	2	20*	11	3	27	10	75	75	9	27	-8	19*	3	2	28	-9	33*	11	6	28	-8	76	83
1	27	-12	120	125	5	27	-13	81	76	9	27	-7	0*	2	2	28	-8	170	173	6	28	-7	84	79
1	27	-11	69	68	5	27	-12	60	60	9	27	-6	67	65	2	28	-7	87	90	6	28	-6	0*	13
1	27	-10	103	104	5	27	-11	79	85	9	27	-5	63	64	2	28	-6	256	261	6	28	-5	38*	36
1	27	-9	50	57	5	27	-10	116	115	9	27	-4	16*	21	2	28	-5	50	56	6	28	-4	102	101
1	27	-8	82	77	5	27	-9	65	64	9	27	-3	22*	16	2	28	-4	321	328	6	28	-3	133	132
1	27	-7	22*	13	5	27	-8	142	144	9	27	-2	9*	31	2	28	-3	34*	49	6	28	-2	196	195
1	27	-6	0*	21	5	27	-7	0*	7	9	27	-1	0*	14	2	28	-2	262	268	6	28	-1	190	185
1	27	-5	33*	7	5	27	-6	117	121	9	27	0	0*	10	2	28	-1	54	55	6	28	0	188	193
1	27	-4	35*	41	5	27	-5	14*	21	9	27	1	122	121	2	28	0	183	182	6	28	1	173	172
1	27	-3	0*	9	5	27	-4	73	70	9	27	2	56	54	2	28	1	61	67	6	28	2	195	189
1	27	-2	58	55	5	27	-3	22*	37	9	27	3	96	100	2	28	2	58	58	6	28	3	158	159
1	27	-1	19*	21	5	27	-2	6*	5	9	27	4	33*	35	2	28	3	20*	28	6	28	4	109	111
1	27	0	44	51	5	27	-1	82	85	9	27	5	125	124	2	28	4	57	67	6	28	5	90	93
1	27	1	17*	25	5	27	0	25*	14	11	27	-10	36*	45	2	28	5	55	51	6	28	6	52	55
1	27	2	21*	25	5	27	1	85	92	11	27	-9	14*	9	2	28	6	187	197	6	28	7	30*	20
1	27	3	86	90	5	27	2	69	74	11	27	-8	69	62	2	28	7	81	77	6	28	8	66	68
1	27	4	57	63	5	27	3	130	126	11	27	-7	55	50	2	28	8	144	150	8	28	-11	0*	3
1	27	5	94	97	5	27	4	29*	26	11	27	-6	15*	18	2	28	9	69	68	8	28	-10	5*	15
1	27	6	108	110	5	27	5	23*	34	11	27	-5	0*	3	2	28	10	152	154	8	28	-9	70	65
1	27	7	148	152	5	27	6	0*	22	11	27	-4	39*	39	4	28	-12	101	91	8	28	-8	102	96
1	27	8	73	70	5	27	7	35*	19	11	27	-3	27*	7	4	28	-12	94	91	8	28	-7	137	134
1	27	9	127	128	5	27	8	86	91	11	27	-2	15*	7	4	28	-11	71	75	8	28	-6	130	126
1	27	10	54	50	5	27	9	83	86	11	27	-1	114	111	4	28	-10	234	233	8	28	-5	221	218
1	27	11	134	138	7	27	-12	116	112	11	27	0	79	82	4	28	-9	121	114	8	28	-4	161	159
3	27	-12	82	85	7	27	-11	0*	13	11	27	1	53*	69	4	28	-8	249	241	8	28	-3	293	285
3	27	-11	40*	44	7	27	-10	152	149	11	27	2	64	67	4	28	-7	51	56	8	28	-2	171	170
3	27	-10	25*	34	7	27	-9	31*	23	13	27	-5	34*	3	4	28	-6	214	214	8	28	-1	173	169
3	27	-9	51	57	7	27	-8	85	89	13	27	-4	0*	5	4	28	-5	90	92	8	28	0	96	94
3	27	-8	56	61	7	27	-7	0*	14	0	28	0	441	436	4	28	-4	116	112	8	28	1	115	118

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
8	28	2	24*	17	1	29	1Ø	18*	22	7	29	-1Ø	49	48	2	3Ø	-1Ø	Ø*	3	6	3Ø	-2	87	87
8	28	3	2Ø*	19	3	29	-11	1Ø7	1Ø6	7	29	-9	54*	65	2	3Ø	-9	134	132	6	3Ø	-1	93	98
8	28	4	23*	9	3	29	-1Ø	66	68	7	29	-8	22*	29	2	3Ø	-8	28*	3	6	3Ø	Ø	42*	47
8	28	5	73	77	3	29	-1Ø	64	68	7	29	-7	96	99	2	3Ø	-7	144	14Ø	6	3Ø	1	11*	5
8	28	6	23*	29	3	29	-9	118	121	7	29	-6	1Ø*	11	2	3Ø	-6	22*	15	6	3Ø	2	69	74
1Ø	28	-1Ø	54	47	3	29	-8	25*	44	7	29	-5	6Ø*	75	2	3Ø	-5	26*	5	6	3Ø	3	81	79
1Ø	28	-9	177	18Ø	3	29	-7	83	82	7	29	-4	13*	16	2	3Ø	-4	82	77	6	3Ø	4	9Ø	93
1Ø	28	-8	7Ø	66	3	29	-6	21*	24	7	29	-3	56	5Ø	2	3Ø	-3	89	85	6	3Ø	5	1Ø8	11Ø
1Ø	28	-7	2Ø2	2Ø4	3	29	-5	6*	22	7	29	-2	27*	36	2	3Ø	-2	Ø*	5	6	3Ø	6	121	126
1Ø	28	-6	81	77	3	29	-4	17*	23	7	29	-1	12*	2Ø	2	3Ø	-1	226	219	6	3Ø	6	127	126
1Ø	28	-5	181	18Ø	3	29	-3	2Ø*	18	7	29	Ø	84	88	2	3Ø	Ø	9Ø	92	8	3Ø	-9	1Ø6	1Ø2
1Ø	28	-4	31*	19	3	29	-2	22*	23	7	29	1	24*	2	2	3Ø	1	219	221	8	3Ø	-8	118	124
1Ø	28	-3	128	123	3	29	-1	28*	47	7	29	2	1Ø8	115	2	3Ø	2	94	89	8	3Ø	-7	87	89
1Ø	28	-2	24*	21	3	29	Ø	48*	58	7	29	3	23*	24	2	3Ø	3	318	325	8	3Ø	-6	146	143
1Ø	28	-1	41*	51	3	29	1	53	52	7	29	4	91	98	2	3Ø	4	88	91	8	3Ø	-5	3Ø*	11
1Ø	28	Ø	35*	24	3	29	2	31*	42	7	29	5	44*	48	2	3Ø	5	196	2Ø5	8	3Ø	-4	4Ø*	48
1Ø	28	1	92	93	3	29	3	28*	11	7	29	6	56	65	2	3Ø	6	26*	28	8	3Ø	-3	Ø*	18
1Ø	28	2	36*	29	3	29	4	Ø*	18	9	29	-9	1Ø6	1Ø4	2	3Ø	7	1Ø9	115	8	3Ø	-2	85	78
1Ø	28	3	143	145	3	29	5	41*	51	9	29	-8	26*	19	2	3Ø	8	33*	34	8	3Ø	-1	1Ø7	1Ø5
12	28	-6	25*	21	3	29	6	42*	35	9	29	-7	54	53	2	3Ø	9	31*	33	8	3Ø	Ø	133	132
12	28	-5	25*	16	3	29	7	77	79	9	29	-6	Ø*	1Ø	4	3Ø	-1Ø	Ø*	8	8	3Ø	1	94	9Ø
12	28	-4	Ø*	9	3	29	8	1ØØ	1Ø4	9	29	-5	Ø*	35	4	3Ø	-1Ø	29*	8	8	3Ø	2	164	166
12	28	-3	1ØØ	1Ø2	3	29	8	1ØØ	1Ø4	9	29	-4	14*	22	4	3Ø	-9	32*	36	8	3Ø	3	82	86
12	28	-2	32*	42	3	29	9	47	56	9	29	-3	Ø*	5	4	3Ø	-8	24*	37	1Ø	3Ø	-6	96	94
1	29	-11	33*	21	5	29	-11	1Ø3	1ØØ	9	29	-2	65	69	4	3Ø	-7	135	135	1Ø	3Ø	-5	55	55
1	29	-11	29*	21	5	29	-11	1ØØ	1ØØ	9	29	-1	Ø*	32	4	3Ø	-6	69	68	1Ø	3Ø	-4	134	133
1	29	-1Ø	84	85	5	29	-1Ø	22*	22	9	29	Ø	81	81	4	3Ø	-5	144	143	1Ø	3Ø	-3	81	86
1	29	-9	19*	41	5	29	-9	41	38	9	29	1	46*	56	4	3Ø	-4	66	68	1Ø	3Ø	-2	197	193
1	29	-9	48	41	5	29	-9	35*	38	9	29	2	55	52	4	3Ø	-3	226	227	1Ø	3Ø	-1	52	59
1	29	-8	9Ø	88	5	29	-8	32*	27	9	29	3	39*	54	4	3Ø	-2	18Ø	176	1	31	-9	42	39
1	29	-7	73	74	5	29	-7	15*	2Ø	11	29	-6	21*	18	4	3Ø	-1	239	239	1	31	-9	41	39
1	29	-6	96	97	5	29	-6	5*	16	11	29	-5	34*	25	4	3Ø	Ø	66	6Ø	1	31	-8	68	72
1	29	-5	96	97	5	29	-5	4Ø*	58	11	29	-4	42	5Ø	4	3Ø	1	187	187	1	31	-8	72	72
1	29	-4	74	77	5	29	-4	24*	16	11	29	-3	21*	14	4	3Ø	2	127	129	1	31	-7	14*	6
1	29	-3	14*	46	5	29	-3	38*	52	11	29	-2	2Ø*	32	4	3Ø	3	89	97	1	31	-6	Ø*	3Ø
1	29	-2	8Ø	81	5	29	-2	Ø*	1	11	29	-1	16*	24	4	3Ø	4	52	55	1	31	-5	16*	2Ø
1	29	-1	6*	1	5	29	-1	38*	4Ø	Ø	3Ø	Ø	35*	39	4	3Ø	5	78	71	1	31	-4	22*	33
1	29	Ø	53	53	5	29	Ø	22*	9	Ø	3Ø	1	162	157	4	3Ø	6	53	45	1	31	-3	6*	22
1	29	1	5Ø	54	5	29	1	9*	7	Ø	3Ø	2	27*	31	4	3Ø	7	22*	52	1	31	-2	77	78
1	29	2	86	86	5	29	2	35*	45	Ø	3Ø	3	158	161	6	3Ø	-1Ø	34*	49	1	31	-1	33*	18
1	29	3	71	77	5	29	3	24*	32	Ø	3Ø	4	23*	31	6	3Ø	-9	129	134	1	31	Ø	31*	4Ø
1	29	4	111	11Ø	5	29	4	1Ø1	1Ø4	Ø	3Ø	5	211	216	6	3Ø	-8	15Ø	147	1	31	1	15*	29
1	29	5	27*	31	5	29	5	Ø*	28	Ø	3Ø	6	67	6Ø	6	3Ø	-7	137	135	1	31	2	18*	3Ø
1	29	6	55*	73	5	29	6	126	127	Ø	3Ø	7	2Ø8	2ØØ	6	3Ø	-6	162	162	1	31	3	24*	19
1	29	7	36	21	5	29	7	25*	2	Ø	3Ø	8	Ø*	4	6	3Ø	-5	233	225	1	31	4	48	45
1	29	8	37*	42	5	29	8	112	1Ø7	Ø	3Ø	9	158	161	6	3Ø	-4	179	18Ø	1	31	5	55*	67
1	29	9	86	86	7	29	-1Ø	27*	48	2	3Ø	-1Ø	Ø*	3	6	3Ø	-3	129	129	1	31	6	67*	7Ø

Reflections flagged with an asterisk were considered unobserved.

Fobs and Fcalc for Mn(CO)5 Yb (C5Me5)2 . 1/4(toluene) @ 25 C

H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc	H	K	L	Fobs	Fcalc
1	31	7	72	75	9	31	-5	12*	10	6	32	-2	104	107	0	34	4	0*	29					
1	31	8	79	81	9	31	-4	65	62	6	32	-1	96	96	2	34	-4	0*	20					
3	31	-9	34*	44	9	31	-3	39*	38	6	32	0	136	138	2	34	-3	109	107					
3	31	-8	32*	34	9	31	-2	14*	11	6	32	1	205	201	2	34	-2	12*	9					
3	31	-7	28*	30	9	31	-1	56	50	6	32	2	146	141	2	34	-1	123	121					
3	31	-6	70	68	0	32	0	391	386	6	32	3	102	101	2	34	0	12*	13					
3	31	-5	36*	50	0	32	1	11*	10	8	32	-4	85	83	2	34	1	177	178					
3	31	-4	88	93	0	32	2	163	165	8	32	-3	203	200	2	34	2	97	95					
3	31	-3	14*	17	0	32	3	31*	29	8	32	-2	154	156	2	34	3	214	212					
3	31	-2	31*	25	0	32	4	164	162	8	32	-1	139	136	4	34	-4	65	60					
3	31	-1	28*	47	0	32	5	97	94	1	33	-6	69	62	4	34	-3	126	126					
3	31	0	23*	23	0	32	6	29*	50	1	33	-5	45*	54	4	34	-2	112	109					
3	31	1	31*	53	0	32	7	27*	35	1	33	-4	65	67	4	34	-1	216	212					
3	31	2	60	62	2	32	-8	85	86	1	33	-3	34*	44	4	34	0	72	70					
3	31	3	115	117	2	32	-7	21*	11	1	33	-2	50	54	4	34	1	96	100					
3	31	4	13*	22	2	32	-6	220	216	1	33	-1	33*	26	1	35	0	35*	43					
3	31	5	86	88	2	32	-5	97	95	1	33	0	57	56										
3	31	6	45	39	2	32	-4	224	218	1	33	1	31*	28										
3	31	7	123	129	2	32	-3	23*	23	1	33	2	70	67										
5	31	-9	7*	29	2	32	-2	221	214	1	33	3	18*	39										
5	31	-8	87	87	2	32	-1	97	95	1	33	4	77	81										
5	31	-7	29*	25	2	32	0	90	87	1	33	5	0*	24										
5	31	-6	95	98	2	32	1	20*	37	1	33	6	51	58										
5	31	-5	18*	13	2	32	2	113	105	3	33	-6	40	36										
5	31	-4	38	43	2	32	3	24*	23	3	33	-5	22*	26										
5	31	-3	55	57	2	32	4	112	106	3	33	-4	14*	6										
5	31	-2	32*	31	2	32	5	39*	35	3	33	-3	25*	31										
5	31	-1	25*	36	2	32	6	79	81	3	33	-2	33*	31										
5	31	0	53	48	4	32	-8	241	235	3	33	-1	6*	21										
5	31	1	111	112	4	32	-7	39*	57	3	33	0	32*	33										
5	31	2	0*	9	4	32	-6	91	98	3	33	1	26*	51										
5	31	3	46*	53	4	32	-5	31*	34	3	33	2	45	52										
5	31	4	0*	15	4	32	-4	92	91	3	33	3	26*	11										
5	31	5	64	62	4	32	-3	107	102	3	33	4	10*	5										
7	31	-8	87	90	4	32	-2	24*	13	5	33	-6	0*	9										
7	31	-7	33*	30	4	32	-1	71	63	5	33	-5	50	48										
7	31	-6	7*	1	4	32	0	86	81	5	33	-4	28*	19										
7	31	-5	26*	42	4	32	1	19*	14	5	33	-3	33*	43										
7	31	-4	28*	23	4	32	2	146	145	5	33	-2	25*	10										
7	31	-3	25*	12	4	32	3	114	112	5	33	-1	12*	38										
7	31	-2	40	37	4	32	4	108	115	5	33	0	18*	16										
7	31	-1	81	80	4	32	5	130	130	5	33	1	0*	10										
7	31	0	25*	8	6	32	-7	24*	24	5	33	2	59	57										
7	31	1	12*	3	6	32	-6	20*	36	0	34	0	79	71										
7	31	2	0*	4	6	32	-5	25*	25	0	34	1	99	95										
7	31	3	29*	5	6	32	-4	139	134	0	34	2	38*	49										
9	31	-6	3*	4	6	32	-3	87	87	0	34	3	146	143										

Reflections flagged with an asterisk were considered unobserved.

TECHNICAL INFORMATION DEPARTMENT
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UNIVERSITY OF CALIFORNIA
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