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REACTIONS OF METAL-TO-METAL MULTIPLE BONDS. 5. ADDITION OF NITR--ETC(U)
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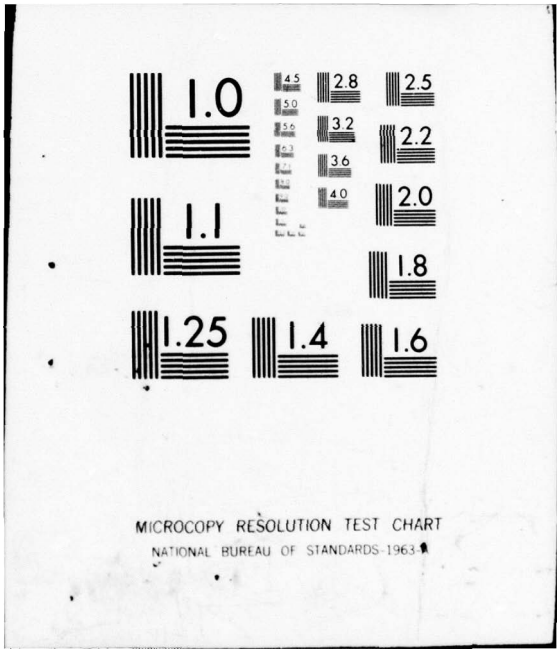
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OFFICE OF NAVAL RESEARCH
Contract N00014-76-C-0826
Task No. NR 056-625
TECHNICAL REPORT NO. 78-10

Reactions of Metal-to-Metal Multiple Bonds. 5. Addition of Nitric Oxide to Hexakis(tert-butoxy)-ditungsten. Preparation, Properties and Structural Characterization of Tris(tert-butoxy)(nitrosyl)(pyridine)tungsten

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Prepared for Publication
in
Inorganic Chemistry

20 April 1978

26 pp.

400 363

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Reactions of Metal-to-Metal Multiple Bonds. 5. Addition of Nitric Oxide to Hexakis(tert-butoxy)-ditungsten. Preparation, Properties and Structural Characterization of Tris (tert-butoxy)(nitrosyl)(pyridine)tungsten.		5. TYPE OF REPORT & PERIOD COVERED Technical Report, 1978 6. PERFORMING ORG. REPORT NUMBER TR-78-10
7. AUTHOR(s) M. H. Chisholm, F. A. Cotton, M. W. Extine and R. L. Kelly		8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-0826 NR 056-625
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Chemistry Princeton University Princeton, N. J. 08540		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Department of the Navy		12. REPORT DATE April 20, 1978 13. NUMBER OF PAGES 22
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Metal-to-Metal Multiple Bonds, Molybdenum, Nitrosyl, tert-butoxide.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The reaction between $W_2(OBu^t)_6$ and nitric oxide (2 equiv) in hydrocarbon solvents yields an insoluble pale-yellow product of empirical formula $W(OBu^t)_3NO$ (υ_{NO}=1560 cm^{-1}). Addition of the nitrogen donor ligands NH_3 and pyridine causes the above compound to dissolve with the formation of mononuclear compounds $W(OBu^t)_3(NO)(L)$. The yellow crystalline compound $W(OBu^t)_3(NO)(C_5H_5N)$ (υ_{NO}=1555 cm^{-1}) has been obtained directly by the reaction between $W_2(OBu^t)_6$ and NO(2 equiv) in pyridine as the solvent. The compound crystallizes in the

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S/N 0102-LF-014-6601

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

space group $P2_1/n$ with $Z=4$ and unit cell dimensions $a = 9.694(2)$, $b=15.686(3)$, $c=14.358(2)$Å, $\beta=97.40(1)^0$ and $V=2165.1(7)$Å.^{3} The coordination geometry of the WO_3N_2 moiety is a slightly distorted trigonal bipyramid with the axial positions occupied by the nitrogen atoms of the nitrosyl and pyridine ligands. The tungsten atom is displaced 0.34Å towards the nitrosyl ligand from the equatorial plane of the three alkoxy oxygen atoms. There is a linear W-N-O moiety with a short W-N bond distance, 1.732(8)Å, whereas the W-N bond distance to the coordinated pyridine is long, 2.323(7)Å.

Reactions of Metal-to-Metal Multiple Bonds. 5.[1] Addition of Nitric Oxide to Hexakis(tert-butoxy)-ditungsten. Preparation, Properties and Structural Characterization of Tris(tert-butoxy)(nitrosyl)(pyridine)tungsten.

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Contribution from the Departments of Chemistry, Princeton University, Princeton, New Jersey 08540 and Texas A and M University, College Station, Texas 77843.

Abstract

The reaction between $W_2(OBu^t)_6$ and nitric oxide (2 equiv) in hydrocarbon solvents yields an insoluble pale-yellow product of empirical formula $W(OBu^t)_3NO$ (ν_{NO} = 1560 cm^{-1}). Addition of the nitrogen donor ligands NH_3, NMe_3 and pyridine causes the above compound to dissolve with the formation of mononuclear compounds $W(OBu^t)_3(NO)(L)$. The yellow crystalline compound $W(OBu^t)_3(NO)(C_5H_5N)$ (ν_{NO} = 1555 cm^{-1}) has been obtained directly by the reaction between $W_2(OBu^t)_6$ and NO(2 equiv) in pyridine as the solvent. The compound crystallizes in the space group $P2_1/n$ with Z=4 and unit cell dimensions a = 9.694(2), b = 15.686(3), c = 14.358(2)Å, β = 97.40(1)^0 and V = 2165.1(7)Å.^{3} The coordination geometry of the WO_3N_2 moiety is a slightly distorted trigonal bipyramid with the axial positions occupied by the nitrogen atoms of the nitrosyl and pyridine ligands. The tungsten atom is displaced 0.34Å towards the nitrosyl ligand from the equatorial plane of the three alkoxy oxygen atoms. There is a linear W-N-O moiety with a short W-N bond distance, 1.732(8)Å, whereas the W-N bond distance to the coordinated pyridine is long, 2.323(7)Å.

Introduction

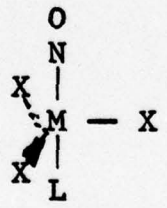
Previously we have shown that the molybdenum-to-molybdenum triple bond in the dinuclear alkoxides $Mo_2(OR)_6$[3] is cleaved in reaction 1.[4]

1 $(RO)_3Mo{\equiv}Mo(OR)_3 + 2NO \rightarrow [Mo(OR)_3(NO)]_2$

where R=Me_3C, Me_2CH and Me_3CCH_2

The structural characterization of $[Mo(OPr^i)_3NO]_2$ revealed two equivalent (inversion-related) distorted trigonal bipyramidal $Mo(OR)_4NO$ units fused along a common axial-to-equatorial edge through the agency of bridging iso-propoxy groups. With a Mo-to-Mo distance of 3.335(2)Å it can be safely assumed that no direct metal-to-metal bonding exists.[5] In a formal sense reaction 1 corresponds to the replacement of the metal-to-metal triple bond by two metal-to-ligand triple bonds followed by Lewis base association,[6]

We concluded[4] that "There would not seem to be any reason why discrete mononuclear complexes of type A, where X represents a univalent ligand, L a sigma donor, and M any atom or ion isoelectronic with Mo(III), should not exist as a general class."



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We report here our preparation and characterization of the first member of this class, namely $W(OBu^t)_3(NO)(C_5H_5N)$, formed in the reaction between $W_2(OBu^t)_6$ and NO(2 equiv) in pyridine.

Results and Discussion

Synthesis. Addition of nitric oxide (2 equiv) to hydrocarbon solutions of $W_2(OBu^t)_6$[7] leads to the formation of a fine yellow

precipitate of empirical formula $W(OBu^t)_3NO$ which shows a single sharp and very strong i.r. absorption at $1565cm^{-1}$ assignable to ν_{NO}. This compound is virtually insoluble in alkane and aromatic hydrocarbons which has hindered its further characterization. It is believed to be polymeric, $[W(OBu^t)_3NO]_n$, in contrast to the dimeric molybdenum analogue $[Mo(OBu^t)_3NO]_2$. $[W(OBu^t)_3NO]_n$ will dissolve in the presence of Me_3N and pyridine yielding $W(OBu^t)_3(NO)(L)$. The compound $W(OBu^t)_3(NO)(C_5H_5N)$ has also been made directly by the addition of NO (2 equiv) to a pyridine solution of $W_2(OBu^t)_6$ and is a yellow crystalline compound appreciably soluble in hydrocarbon solvents. For $W(OBu^t)_3(NO)(C_5H_5N)$ a strong sharp i.r. absorption at 1555 cm^{-1} is assignable to ν_{NO}; a sharp band of medium intensity at 1610 cm^{-1} is assigned to the stretching vibration of the coordinated pyridine. The nmr spectra in toluene-d_8 of $W(OBu^t)_3(NO)(C_5H_5N)$ show the presence of only one type of tert-butoxy ligand, even at -60^oC. This, together with the observation of a single nitrosyl stretching frequency, is consistent with the presence in solution of a structure akin to that found in the crystal.

Solid State Structure of $W(OBu^t)_3(NO)(C_5H_5N)$. The compound is composed of discrete mononuclear molecules in the solid state. Atomic positional and thermal parameters are given in Table I. The molecular structure is shown in Figure 1 along with the atom labelling scheme. Bond distances and angles are given in Table II. As can be seen from Figure 1, the coordination geometry is a slightly distorted trigonal bipyramid with the axial positions occupied by the nitrosyl and pyridine ligands.

The tungsten atom is displaced 0.34Å towards the nitrosyl ligand from the equatorial plane of the three alkoxy oxygen atoms.

The nitrosyl ligand is coordinated linearly and the W-N1 bond is quite short, 1.732(8)Å, indicative of some multiple bond character whereas the tungsten to pyridine bond is considerably longer, W-N2=2.323(7)Å. The W-O distances are in the expected range.

Bonding. The trigonal set of ligands splits the tungsten 5d orbitals into three sets: a (d_{z^2}), e ($d_{x^2-y^2}$, d_{xy}) and e (d_{xz}, d_{yz}). The second e set is but little involved in metal ligand σ-bonding and thus lies lowest in energy. In $W(OBu^t)_3(NO)(py)$ tungsten achieves only a fourteen valence shell electronic configuration. Ten electrons are involved in forming the five σ bonds and the remaining four occupy the lower e orbitals which have the appropriate symmetry to interact with the empty nitrosyl π* orbitals. The bonding is analogous to that in $[Mo(OPr^i)_3NO]_2$, where a bridging isopropoxide occupies the axial position trans to the nitrosyl ligand.

For a linear metal nitrosyl moiety, metal-to-nitrosyl π* bonding should be reflected in (i) the metal-to-nitrogen bond distance, (ii) the nitrogen-to-oxygen bond distance and (iii) the value of the N-O stretching frequency. A lengthening of the N-O bond and a lowering of ν(NO) should correlate with an increase in metal-to-nitrosyl π*-bonding. The shortness of the metal-to-nitrogen bond may also correlate with M-N multiple bond character but this distance will also be influenced by the nature of the metal σ-hybrid orbital used in forming the M-N bond. The latter is determined by the coordination number and geometry of the metal complex as well as by the nature of the other ligands bonded to the metal.

M-N and N-O bond distances and ν(NO) values for some compounds containing linear M-N-O moieties are given in Table 3 and are

illustrative of the above considerations. Certainly little can be inferred from the M-N distances alone. There does, however, seem to be the expected correlation between N-O bond length and ν(NO). This correlation is limited, however, by the relatively small changes and large experimental errors which occur in N-O distances. One can conclude that the generally accepted view that ν(NO) correlates with metal-to-nitrosyl π^* bonding finds structural support in N-O bond distances.

The trihaloruthenium complexes, which contain six coordinate metal atoms, all show very similar M-N-O parameters (see Table 3). Notably the values of ν(NO) are more than 200 cm^{-1} higher, and the N-O distances are significantly shorter than those of the five coordinate molybdenum and tungsten complexes. The metals here are all in the +2 oxidation state, if we assume the formalism $M^{-}\leftarrow(NO^{+})$ for the linear M-N-O moiety. Evidently the $(t_{2g})^6$-to-NOπ^* bonding is less effective in these Ru(2+) octahedral complexes than is the $(e)^4$-to-NOπ^* bonding in the Mo(2+) and W(2+) trigonal bipyramidal complexes, despite the presence of only 14-valence shell electrons in the latter. A plausible rationale for this observation may lie in the mixing of ligand-to-metal π-bonding (p$\rightarrow$d) and metal-to-NOπ^* bonding. Ligand (OR or NR_2)-to-metal-π bonding in the four-coordinate $Cr(NR_2)_3NO$ and five-coordinate $M(OR)_3(NO)L$ molecules will raise the energy of the filled metal d_{xz} and d_{yz} atomic orbitals from the level they would otherwise have had as a result of pure M-L σ-bonding. The energy separation between filled metal d_{xz} and d_{yz} orbitals and the vacant higher energy NOπ^* orbitals will be reduced and metal-to-nitrosyl π^* bonding enhanced. It is, of course, not possible to separate completely the σ and π-donor properties of a ligand. However, the values of ν(NO) do go down as the overall donor ($\sigma + \pi$) properties of the ligand increase: compare ν(NO)=1698 cm^{-1} for

$Cr(N(SiMe_3)_2)_3NO$ with $\nu(NO)=1640\ cm^{-1}$ for $Cr(NPr^i_2)_3NO$ and $\nu(NO)=1643$, 1640 and 1630 cm^{-1} for the compounds $[Mo(OR)_3NO]_2$ where R = CH_2CMe_3, $CHMe_2$ and CMe_3, respectively.

Experimental Section

General procedures have been described;[1] note the use of dry and oxygen free atmospheres and solvents.

$W_2(OBu^t)_6$ was prepared from the reaction between $W_2(NMe_2)_6$ and Bu^tOH (> 6 equiv) in benzene and was recrystallized from hexane solutions.[7]

$[W(OBu^t)_3NO]_n$: $W_2(OBu^t)_6$(0.63g, 0.78 mmol) was dissolved in hexane (10 mL) to give a red solution. Nitric oxide (1.56 mmol) was added with the use of a calibrated manifold to the above solution frozen at liquid nitrogen temperature which yielded upon warming to room temperature a green solution and a pale yellow precipitate. After 5h the pale yellow precipitate was collected by filtration, washed with hexane, and dried in vacuo (10^{-4} cm Hg, 25°C). Yield 0.56g (83% based on tungsten). Analysis found (calcd) for $W(OBu^t)_3NO$: C, 33.06 (33.27); H, 6.20 (6.28); N, 3.40 (3.23). I.r. data obtained from a nujol mull between CsI plates (2000-300 cm^{-1} range): 1565 vs, 1310 w, 1245 m, 1165 s (broad), 1090 s, 1030 w, 948 vs (broad), 928 vs, 912 s, 796 m (sharp), 784 m (sharp), 724 m (broad), 627 s (sharp), 595 m, 572 m, 485 w, 394 w, 381 w, 340 w.

$W(OBu^t)_3(NO)(C_5H_5N)$: $W_2(OBu^t)_6$(0.1844g, 0.23 mmol) was dissolved in pyridine (7 ml) to form a deep red solution. This was frozen at liquid nitrogen temperature and nitric oxide (0.46 mmol) was added using a calibrated vacuum manifold. The reaction mixture was allowed to warm to room temperature and left to stand for 12h. The pyridine was stripped and the residue extracted with

toluene (ca. 5 mL). The pale yellow solution was filtered to remove a small amount of a black insoluble material. The filtrate was collected and cooled to -10°C yielding pale yellow crystals (ca. 80 mg). Analysis found (calcd) for $W(OBu^t)_3(NO)(C_5H_5N)$: C, 39.65 (39.86); H, 6.25 (6.30); N, 5.40 (5.47). I.r. data obtained from a nujol mull using CsI plate in the range 2000-300 cm^{-1}: 1610 m (sharp), 1555 vs, 1305 w, 1240 m, 1222 m (sharp), 1170 m (broad), 1156 m (sharp), 1076 m (sharp), 1043 m (sharp), 1027 w, 1018 w, 1000 w, 965 m, 948 m, 937 vs (broad), 910 m, 900 w, 783 m, 762 m (sharp), 722 m (broad), 694 m (sharp), 621 s, 576 m, 485 w, 436 w, 380 w.

^{13}C nmr data obtained in toluene-d_8 at -50°C: $\delta(OC) = 80.8$, $\delta(\underline{CH_3}) = 32.9$. ($\delta$ in ppm rel. TMS).

X-Ray Crystallography.[8] A yellow crystal of $W(OBu^t)_3(NO)(C_5H_5N)$ measuring 0.23x0.28x0.58 mm was mounted, embedded in epoxy cement and sealed in a thin walled glass capillary, with its longest dimension nearly coincident with the phi axis. Omega scans of several intense low-angle reflections had peak widths at half height of ca. 0.2°. Cell constants and axial photographs indicated that the crystal belonged to the monoclinic system with a = 9.694(2), b = 15.686(3), c = 14.358(2)Å, β = 97.40(1)°, and V = 2165.1(7)Å^3. The observed volume was consistent with that expected for Z = 4. Systematic absences observed during data collection, on oko (k = 2n+1) and hol (h+l = 2n+1), uniquely determined the space group to be $P2_1/n$ (a non-standard setting of $P2_1/c$, No. 14).

The data were collected at 23±2°C with a Syntex $P\bar{1}$ autodiffractometer equipped with a graphite crystal monochromator and using MoKα (λ = 0.710730Å) radiation. Variable scan rates from 4.8 to 24.0°/min were used for symmetric $\theta/2\theta$ scans ranging from 1.0° below to 1.0° above the calculated MoKα_1,Kα_2 doublet. The

ratio of background to scan time was 0.5. A total of 2936 unique reflections having $0^0<2\theta_{MoK\alpha}<45^0$ were collected. The intensities of three standard reflections were monitored frequently throughout data collection and showed an approximately linear decrease of 12% over the period of data collection. The data were reduced to a set of relative $|Fo|^2$ values and then corrected for crystal decay. An empirical absorption correction based upon a series of psi scans was applied to the data (μ = 56.7 cm^{-1}); relative transmission factors ranged from 0.844 to 1.000 with an average of 0.949. The 2103 observations having $|F|>3\sigma(|F|)$ were retained as observed and used in subsequent structure solution and refinement.

The positions of the 24 unique non-hydrogen atoms were determined by standard heavy atom methods. The structure was refined to convergence using anisotropic thermal parameters for all 24 atoms. The final discrepancy indices were

$$R_1 = \Sigma||Fo|-|Fc||/|Fo| = 0.032$$

$$R_2 = [\Sigma w(|Fo|-|Fo|)^2/\Sigma w|Fo|^2]^{\frac{1}{2}} = 0.047$$

The estimated standard deviation of an observation of unit weight was 1.102. The top peaks in a final difference Fourier map were due to methyl group hydrogen atoms.

A table of observed and calculated structure factors (9 pages) is available as supplementary material. See any current masthead page for ordering information.

Acknowledgements

We thank the Office of Naval Research for support of this work at Princeton University and the National Science Foundation for support at Texas A & M University.

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8. All crystallographic computations were carried out using the Enraf Nonius Structure Determination Package and a PDP11/45 computer owned by Molecular Structure Corp., College Station, Texas.

TABLE I. POSITIONAL AND THERMAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS.

ATOM	X	Y	Z	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
W	0.05941(4)	0.23082(3)	0.08295(2)	2.90(1)	3.59(2)	2.80(1)	-0.09(1)	0.56(1)	0.45(1)
O1	-0.0626(6)	0.1482(4)	0.0250(4)	3.9(3)	4.4(3)	3.3(3)	-0.4(3)	-0.5(2)	0.4(3)
O2	0.2467(6)	0.1974(4)	0.1196(4)	3.2(3)	4.8(3)	3.5(3)	-0.0(2)	0.9(2)	0.7(2)
O3	-0.0194(6)	0.3097(4)	0.1602(4)	4.1(3)	3.6(3)	3.8(3)	0.0(3)	1.3(2)	0.7(2)
O4	0.0918(8)	0.3428(5)	-0.0806(5)	7.0(4)	5.7(4)	4.5(3)	0.6(3)	2.1(3)	2.6(3)
N1	0.0779(8)	0.2964(5)	-0.0117(5)	4.0(3)	4.5(4)	4.1(4)	0.4(3)	1.0(3)	1.1(3)
N2	0.0280(7)	0.1486(5)	0.2131(5)	2.8(3)	4.1(3)	3.1(3)	-0.3(3)	0.7(3)	0.1(3)
C1	-0.1302(11)	0.1312(7)	-0.0713(7)	5.4(5)	4.9(5)	3.0(4)	-0.1(4)	-0.8(4)	-0.6(4)
C2	-0.0146(13)	0.1150(9)	-0.1326(8)	8.0(7)	8.8(7)	3.3(5)	1.5(6)	-0.3(5)	-1.7(5)
C3	-0.2176(13)	0.2086(7)	-0.1062(9)	6.3(6)	4.9(6)	6.7(6)	0.8(5)	-0.7(5)	1.2(5)
C4	-0.2203(13)	0.0515(8)	-0.0594(9)	7.1(7)	6.0(6)	6.5(6)	-2.6(5)	-2.1(6)	0.2(5)
C5	0.3771(10)	0.2141(7)	0.0837(8)	3.2(4)	6.5(7)	5.4(5)	-0.3(4)	1.4(4)	0.3(5)
C6	0.4030(12)	0.3098(9)	0.0875(9)	6.2(6)	6.8(6)	8.5(7)	-2.7(5)	2.5(5)	-1.0(6)
C7	0.3682(11)	0.1819(9)	-0.0177(7)	5.2(5)	9.0(7)	4.1(5)	-0.2(6)	1.9(4)	-1.5(5)
C8	0.4869(11)	0.1626(10)	0.1500(9)	3.1(5)	12(1)	6.0(6)	1.0(6)	0.1(5)	1.0(7)
C9	-0.0600(10)	0.3984(6)	0.1535(7)	4.2(4)	3.4(4)	4.4(4)	-0.0(4)	1.2(4)	0.6(4)
C10	0.0691(11)	0.4526(7)	0.1492(8)	4.9(5)	4.2(5)	6.6(6)	-0.6(4)	0.4(5)	0.3(5)
C11	-0.1206(13)	0.4164(7)	0.2459(8)	10.7(7)	5.1(6)	4.9(5)	2.4(5)	3.7(5)	-0.1(4)
C12	-0.1686(11)	0.4125(7)	0.0670(8)	4.7(5)	5.9(6)	4.6(5)	1.2(4)	-0.4(4)	1.3(4)
C13	0.1261(9)	0.1046(6)	0.2641(6)	4.0(4)	3.9(4)	3.2(4)	1.1(4)	0.4(3)	0.3(4)
C14	0.1021(10)	0.0589(7)	0.3437(7)	3.9(5)	6.0(6)	4.3(5)	0.4(4)	0.2(4)	1.2(4)
C15	-0.0289(12)	0.0605(7)	0.3711(7)	6.5(6)	6.4(6)	3.4(4)	0.4(5)	1.0(4)	1.6(4)
C16	-0.1333(11)	0.1066(7)	0.3181(7)	5.6(5)	4.6(5)	4.9(5)	-0.4(4)	2.5(4)	1.0(4)
C17	-0.1003(10)	0.1497(7)	0.2390(7)	3.6(4)	4.5(5)	5.6(5)	-0.3(4)	0.9(4)	1.8(4)

The form of the anisotropic thermal parameter is:

$$\exp[-1/4(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*)]$$

Table II. Bond Distances (Å) and Angles (Deg) in $W(OBu^t)_3(NO)(C_5H_5N)$[a]

ATOMS		DISTANCE	ATOMS		DISTANCE
W	O1	1.876(6)	C1	C3	1.527(15)
W	O2	1.898(6)	C1	C4	1.547(15)
W	O3	1.887(6)	C5	C6	1.52(2)
W	N1	1.732(8)	C5	C7	1.533(15)
W	N2	2.323(7)	C5	C8	1.560(15)
O1	C1	1.476(11)	C9	C10	1.520(14)
O2	C5	1.449(11)	C9	C11	1.544(14)
O3	C9	1.446(11)	C9	C12	1.538(14)
O4	N1	1.250(10)	C13	C14	1.394(13)
N2	C13	1.318(11)	C14	C15	1.377(14)
N2	C17	1.343(11)	C15	C16	1.389(14)
C1	C2	1.53(2)	C16	C17	1.393(13)

ATOMS			ANGLE	ATOMS			ANGLE
O1	W	O2	117.3(3)	C2	C1	C3	111.(1)
O1	W	O3	115.7(3)	C2	C1	C4	113.(1)
O1	W	N1	100.7(3)	C3	C1	C4	112.(1)
O1	W	N2	80.4(3)	O2	C5	C6	108.3(9)
O2	W	O3	117.6(3)	O2	C5	C7	109.5(8)
O2	W	N1	100.9(3)	O2	C5	C8	104.3(8)
O2	W	N2	81.0(2)	C6	C5	C7	110.(1)
O3	W	N1	99.4(3)	C6	C5	C8	113.(1)
O3	W	N2	77.7(3)	C7	C5	C8	111.(1)
N1	W	N2	177.0(3)	O3	C9	C10	108.8(8)
W	O1	C1	135.9(6)	O3	C9	C11	104.4(8)
W	O2	C5	134.3(6)	O3	C9	C12	110.1(8)
W	O3	C9	136.0(5)	C10	C9	C11	110.(1)
W	N1	O4	179.2(8)	C10	C9	C12	111.6(9)
W	N2	C13	125.3(6)	C11	C9	C12	111.8(9)
W	N2	C17	116.0(6)	N2	C13	C14	122.7(9)
C13	N2	C17	118.7(8)	C13	C14	C15	118.8(9)
O1	C1	C2	107.4(8)	C14	C15	C16	119.1(9)
O1	C1	C3	108.9(8)	C15	C16	C17	118.(1)
O1	C1	C4	103.3(8)	N2	C17	C16	122.6(9)

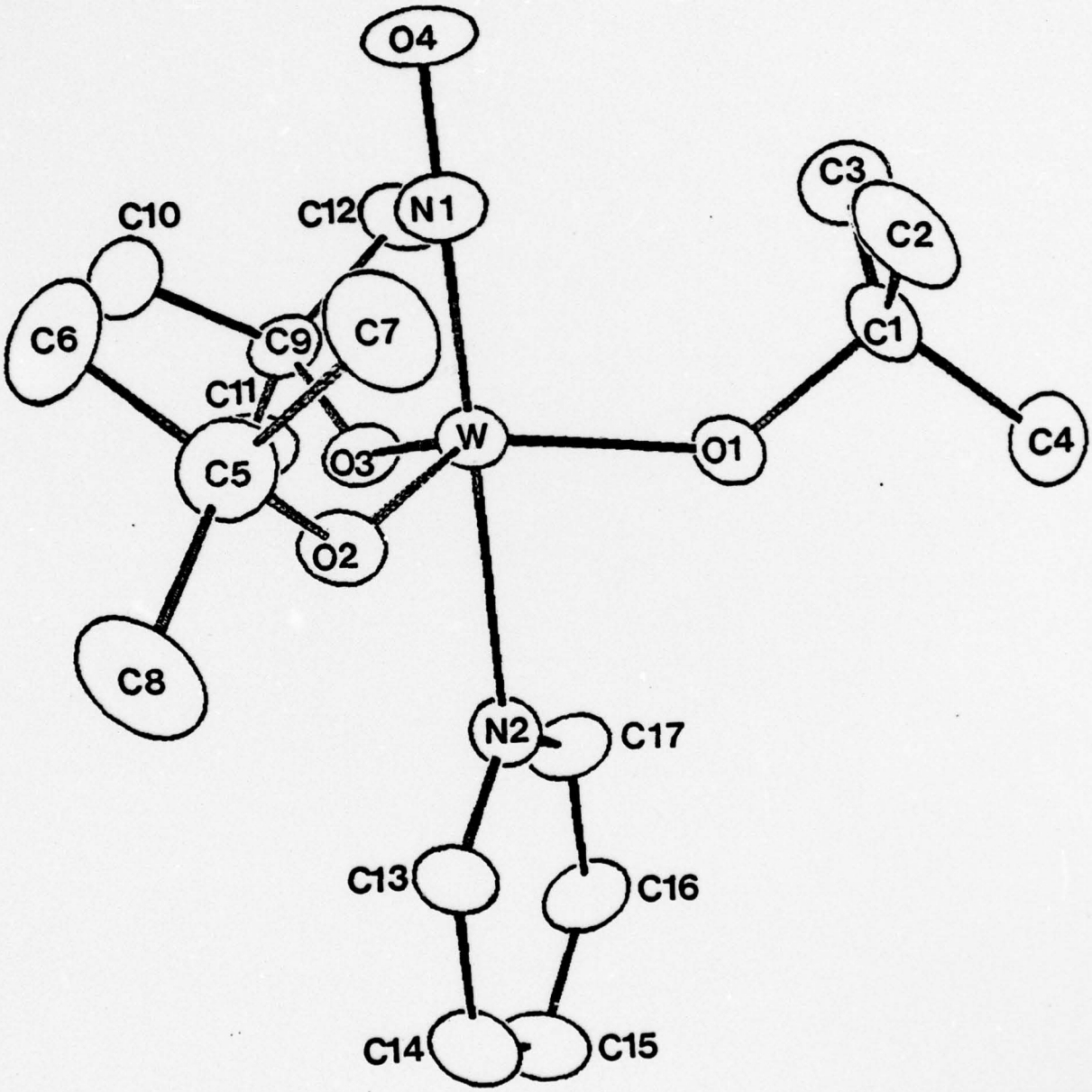
[a]Numbers in parentheses are estimated standard deviations in the least significant digits.

Table III

Compound	M-N Å	N-O Å	M-N-O angle°	ν(NO) cm^{-1}	ref.
$W(OBu^t)_3(NO)(pyridine)$	1.732(8)	1.25(1)	179.2(8)	1555	a
$[Mo(OPr^i)_3NO]_2$	1.754(7)	1.19(1)	178(1)	1640	b
$Cr(NSi_2Me_6)_3NO$	1.738(20)	1.191(28)	180[i]	1698[j]	c
$Ru(\eta^3\text{-allyl})(NO)(PPh_3)_2$	1.751(6)	1.188(8)	173.8(6)	1640	d
$RuCl_3(NO)(PPh_3)_2$	1.737(7)	1.142(8)	180[i]	1876	e
$RuCl_3(NO)(PPh_2Me)_2$	1.744(6)	1.132(6)	176.4(6)	1860[k]	f
$[RuBr_3(NO)(Et_2SO)]_2$	1.71(1)	1.16(1)	178(1)	1874	g
$[Mo(CN)_5NO]^{4-}$	1.95(3)	1.23(4)	175(3)	1455[l]	h

[a]this work; [b]ref. 4; [c]D. C. Bradley, M. B. Hursthouse, C. W. Newing and A. J. Welch, J.C.S. Chem. Commun, 567 (1972); [d] M. W. Schoonover and R. Eisenberg, J. Am. Chem. Soc. 99, 8371 (1977); [e]B. L. Haymore and J. A. Ibers, Inorg. Chem. 14, 3060 (1975); [f]A. J. Schultz, R. L. Henry and R. Eisenberg, Inorg. Chem. 13, 732 (1974); [g]J. E. Fergusson, C. T. Page and W. T. Robinson, Inorg. Chem., 15, 2270 (1976); [h]D. H. Svedung and N.-G. Vännerberg, Acta. Chem. Scand. 22, 1551 (1968); [i]crystallographically imposed linearity; [j]C. W. Newing, Ph.D. Thesis London University 1971; [k]J. Chatt and B. L. Shaw, J. Chem. Soc., A, 1811 (1966). [l]R.F. Riley and L. Ho, J. Inorg. Nucl. Chem. 24, 1121 (1962).

Figure 1. An ORTEP view of the $W(OBu^t)_3(NO)(C_5H_5N)$ molecule using 40% probability ellipsoids and showing the atom numbering scheme.


O4
C3
C2
C10
C12
N1
C1
C6
C9
C7
C11
C4
W
O1
O3
C5
O2
C8
N2
C17
C13
C16
C14
C15

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
0	0	2	1548	1556	0	4	7	529	475	0	8	3	1338	1369	0	13	7	649	649	1	1	10	297	311
0	0	4	1800	1792	0	4	8	692	673	0	8	4	192	197	0	14	0	197	156	1	1	13	680	713
0	0	6	2184	2205	0	4	9	687	639	0	8	5	597	603	0	14	1	511	507	1	1	15	754	716
0	0	8	644	676	0	4	10	718	708	0	8	6	938	975	0	14	2	207	150	1	2	-13	961	966
0	0	10	536	527	0	4	11	305	303	0	8	7	480	476	0	14	3	876	875	1	2	-11	808	824
0	0	12	1305	1328	0	4	12	904	898	0	8	8	443	452	0	14	5	456	429	1	2	-9	701	644
0	0	14	583	555	0	4	13	211	121	0	8	9	955	986	0	14	6	231	173	1	2	-8	722	712
0	1	1	200	185	0	4	14	293	333	0	8	10	356	353	0	14	7	330	323	1	2	-7	2006	2050
0	1	2	2452	2805	0	5	1	1380	1376	0	8	11	392	406	0	15	1	597	610	1	2	-6	870	734
0	1	3	771	727	0	5	2	1346	1442	0	8	12	453	431	0	15	5	580	530	1	2	-5	1215	1204
0	1	4	1676	1765	0	5	3	249	265	0	8	13	245	267	0	15	7	445	434	1	2	-4	1082	1090
0	1	5	158	214	0	5	4	1740	1807	0	9	1	1341	1307	0	16	1	305	306	1	2	-3	1124	1109
0	1	7	372	384	0	5	5	1034	1071	0	9	2	391	403	0	16	3	598	561	1	2	-2	221	140
0	1	8	1440	1433	0	5	6	155	130	0	9	4	488	433	0	16	5	275	269	1	2	-1	2568	2949
0	1	9	233	179	0	5	7	940	942	0	9	5	1395	1449	1	0	-15	267	281	1	2	0	128	129
0	1	10	1212	1190	0	5	8	1271	1277	0	9	6	167	123	1	0	-13	1011	1050	1	2	1	1428	1536
0	1	14	790	774	0	5	10	1132	1139	0	9	7	940	950	1	0	-11	791	764	1	2	2	645	546
0	2	1	625	741	0	5	11	464	450	0	9	8	466	453	1	0	-9	740	745	1	2	3	1208	1203
0	2	2	1832	1878	0	5	13	434	428	0	9	10	186	149	1	0	-7	2289	2322	1	2	4	1032	916
0	2	4	1139	1192	0	5	14	555	545	0	9	11	658	682	1	0	-5	1503	1400	1	2	5	1746	1736
0	2	5	414	495	0	6	0	1371	1342	0	9	13	559	562	1	0	-3	1717	1644	1	2	6	416	415
0	2	6	2006	2082	0	6	1	394	447	0	10	0	400	425	1	0	1	1956	2223	1	2	7	710	736
0	2	7	293	248	0	6	2	492	489	0	10	1	711	694	1	0	3	1520	1428	1	2	8	432	483
0	2	8	770	736	0	6	3	1591	1656	0	10	2	272	252	1	0	5	1648	1694	1	2	9	674	661
0	2	9	356	329	0	6	4	837	858	0	10	3	1225	1202	1	0	7	881	875	1	2	10	178	129
0	2	10	913	916	0	6	5	417	412	0	10	4	170	154	1	0	9	628	589	1	2	11	1126	1109
0	2	12	1130	1143	0	6	6	1326	1335	0	10	5	734	790	1	0	11	1189	1153	1	2	12	277	218
0	2	14	463	419	0	6	7	592	626	0	10	6	500	480	1	0	13	801	799	1	2	13	615	608
0	3	1	1355	1305	0	6	8	529	545	0	10	7	398	401	1	1	-15	673	670	1	3	-15	604	607
0	3	2	2464	2674	0	6	9	802	858	0	10	8	202	219	1	1	-11	1155	1133	1	3	-14	232	200
0	3	3	293	197	0	6	10	317	331	0	10	9	886	891	1	1	-9	1305	1335	1	3	-11	850	852
0	3	4	1751	1869	0	6	11	377	375	0	10	11	422	418	1	1	-8	224	221	1	3	-9	1483	1480
0	3	5	576	605	0	6	12	691	717	0	10	12	209	195	1	1	-6	286	288	1	3	-8	616	583
0	3	6	215	188	0	6	14	258	251	0	11	1	1267	1274	1	1	-5	1889	1797	1	3	-6	1280	1234
0	3	7	439	426	0	7	1	1025	955	0	11	2	207	177	1	1	-4	468	468	1	3	-5	1661	1662
0	3	8	1424	1470	0	7	2	842	846	0	11	5	886	916	1	1	-3	1509	1562	1	3	-4	281	336
0	3	9	209	206	0	7	3	163	158	0	11	7	1016	1024	1	1	-2	698	597	1	3	-3	1995	2022
0	3	10	1199	1230	0	7	4	1327	1344	0	11	8	210	237	1	1	-1	652	667	1	3	-2	909	978
0	3	13	236	227	0	7	5	1491	1516	0	11	11	582	597	1	1	0	570	616	1	3	-1	1171	1061
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0	4	3	1274	1304	0	7	13	444	464	0	12	7	340	347	1	1	5	314	221	1	3	4	188	204
0	4	4	1341	1280	0	8	0	527	520	0	12	9	694	699	1	1	6	411	374	1	3	6	670	668
0	4	5	1013	971	0	8	1	462	440	0	13	1	929	910	1	1	7	1072	1093	1	3	7	1405	1380
0	4	6	1597	1603	0	8	2	354	336	0	13	5	615	585	1	1	9	1119	1069	1	3	9	1375	1423

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	10	437	456	1	5	11	335	332	1	7	4	1461	1508	1	9	5	163	194	1	12	-2	827	816
1	3	11	251	220	1	5	12	448	439	1	7	5	401	411	1	9	6	1065	1072	1	12	0	255	268
1	3	13	663	688	1	5	13	407	488	1	7	6	1101	1119	1	9	7	499	556	1	12	1	206	183
1	4	-14	233	249	1	6	-14	234	248	1	7	7	857	879	1	9	8	335	303	1	12	2	1137	1138
1	4	-13	832	822	1	6	-13	660	661	1	7	8	236	256	1	9	9	468	495	1	12	4	531	525
1	4	-11	692	692	1	6	-12	218	248	1	7	9	913	931	1	9	10	627	598	1	12	8	824	818
1	4	-10	508	485	1	6	-11	507	514	1	7	10	479	483	1	9	12	609	631	1	12	10	372	375
1	4	-9	535	521	1	6	-10	785	812	1	7	12	551	564	1	10	-12	281	308	1	13	-8	586	579
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1	4	-5	1117	1031	1	6	-6	453	457	1	8	-11	272	311	1	10	-5	330	336	1	13	2	181	164
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1	4	11	1017	1052	1	6	8	940	984	1	8	4	852	832	1	10	10	453	484	1	15	-5	290	262
1	4	13	442	425	1	6	9	274	253	1	8	5	1046	1104	1	10	11	347	343	1	15	-2	529	527
1	4	14	389	391	1	6	10	527	527	1	8	6	715	753	1	10	12	216	166	1	15	0	682	637
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1	5	-12	511	499	1	6	13	299	308	1	8	8	833	866	1	11	-6	800	823	1	15	6	600	566
1	5	-11	861	891	1	6	14	419	426	1	8	9	322	317	1	11	-5	311	318	1	16	-4	571	568
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1	5	9	1024	1038	1	7	1	788	771	1	9	3	522	510	1	12	-5	239	230	2	0	4	1931	1881
1	5	10	349	347	1	7	3	1065	1083	1	9	4	1012	1039	1	12	-4	964	976	2	0	6	782	827

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	0	8	454	394	2	2	10	1115	1117	2	4	9	598	570	2	6	2	468	423	2	8	0	718	748
2	0	10	1148	1122	2	2	12	883	848	2	4	10	894	933	2	6	3	1101	1140	2	8	1	1251	1288
2	0	12	794	784	2	3	-15	331	305	2	4	12	752	736	2	6	4	1507	1524	2	8	2	269	274
2	1	-14	310	294	2	3	-13	321	303	2	4	13	406	392	2	6	5	289	303	2	8	3	938	915
2	1	-12	821	812	2	3	-12	749	720	2	4	14	222	203	2	6	6	816	837	2	8	4	833	799
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2	1	-8	416	391	2	3	-9	482	514	2	5	-12	585	590	2	6	8	358	364	2	8	6	638	673
2	1	-7	531	490	2	3	-8	490	465	2	5	-11	305	275	2	6	9	600	618	2	8	7	973	906
2	1	-6	1585	1551	2	3	-7	780	785	2	5	-10	1090	1061	2	6	10	802	804	2	8	8	206	251
2	1	-5	587	516	2	3	-6	1022	1036	2	5	-9	746	727	2	6	12	303	362	2	8	9	808	854
2	1	-4	1935	1874	2	3	-5	205	180	2	5	-8	579	577	2	6	13	481	456	2	8	10	688	685
2	1	-3	622	678	2	3	-4	1837	1843	2	5	-7	845	847	2	7	-13	703	666	2	9	-13	579	572
2	1	-2	1304	1196	2	3	-3	1094	1056	2	5	-6	555	559	2	7	-12	325	278	2	9	-10	264	309
2	1	-1	475	424	2	3	-2	764	659	2	5	-5	316	296	2	7	-11	258	270	2	9	-9	553	560
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2	1	10	433	411	2	3	9	378	392	2	5	6	766	769	2	7	-1	969	1026	2	9	1	406	416
2	1	11	305	268	2	3	10	437	426	2	5	7	533	543	2	7	0	671	694	2	9	2	635	680
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2	2	-14	813	823	2	4	-15	281	308	2	5	10	455	472	2	7	3	502	472	2	9	6	405	415
2	2	-12	865	869	2	4	-14	729	742	2	5	11	435	394	2	7	4	561	555	2	9	7	323	311
2	2	-11	205	229	2	4	-12	672	674	2	5	12	504	514	2	7	5	1224	1208	2	9	9	334	339
2	2	-10	301	329	2	4	-11	398	385	2	5	14	502	502	2	7	6	824	829	2	9	11	669	686
2	2	-9	221	218	2	4	-9	394	354	2	6	-14	495	519	2	7	7	550	580	2	9	12	259	305
2	2	-8	1784	1803	2	4	-8	1455	1430	2	6	-13	226	195	2	7	8	749	786	2	10	-11	721	725
2	2	-7	155	179	2	4	-7	247	232	2	6	-12	568	574	2	7	9	249	225	2	10	-9	678	656
2	2	-6	1386	1355	2	4	-6	1268	1229	2	6	-11	663	636	2	7	11	709	719	2	10	-8	306	301
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2	2	-4	829	734	2	4	-4	684	582	2	6	-9	619	620	2	8	-12	309	306	2	10	-5	1112	1066
2	2	-3	947	891	2	4	-3	972	914	2	6	-8	934	928	2	8	-11	787	766	2	10	-3	916	887
2	2	-2	2106	2168	2	4	-2	2079	2072	2	6	-7	470	451	2	8	-9	583	575	2	10	-2	507	489
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2	2	5	423	396	2	4	4	1662	1694	2	6	-2	1514	1492	2	8	-4	220	208	2	10	3	861	862
2	2	6	1258	1301	2	4	6	1179	1196	2	6	-1	310	320	2	8	-3	1049	1016	2	10	4	454	479
2	2	7	281	308	2	4	7	632	619	2	6	0	767	795	2	8	-2	1163	1151	2	10	6	299	309
2	2	9	403	401	2	4	8	204	172	2	6	1	1038	992	2	8	-1	820	832	2	10	8	251	230

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
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2	10	10	310	340	2	15	-1	782	758	3	2	-10	188	173	3	3	13	889	860	3	5	13	562	581
2	11	-11	219	191	2	15	1	253	274	3	2	-9	1580	1569	3	4	-14	209	154	3	6	-13	602	621
2	11	-9	663	647	2	15	3	461	468	3	2	-8	227	183	3	4	-13	780	809	3	6	-12	672	653
2	11	-7	859	849	2	15	5	636	648	3	2	-7	1534	1501	3	4	-12	340	349	3	6	-10	557	556
2	11	-5	261	270	2	16	-3	421	416	3	2	-6	745	770	3	4	-10	372	348	3	6	-9	830	816
2	11	-4	540	532	2	16	1	573	561	3	2	-5	420	401	3	4	-9	1211	1228	3	6	-8	304	313
2	11	-3	766	747	2	16	3	475	445	3	2	-4	563	551	3	4	-7	1221	1211	3	6	-7	980	913
2	11	-1	1079	1096	3	0	-15	570	664	3	2	-3	1960	1934	3	4	-6	517	495	3	6	-6	983	972
2	11	0	273	258	3	0	-13	697	742	3	2	-2	301	354	3	4	-4	1015	951	3	6	-4	1027	1035
2	11	1	549	515	3	0	-11	260	234	3	2	-1	1890	1932	3	4	-3	1854	1895	3	6	-3	1297	1252
2	11	2	271	285	3	0	-9	1661	1607	3	2	0	139	152	3	4	-1	1642	1708	3	6	-2	337	342
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2	11	5	908	891	3	0	-3	1550	1455	3	2	3	1589	1654	3	4	2	427	485	3	6	1	323	300
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2	12	-6	243	189	3	0	9	1434	1444	3	2	11	927	929	3	4	11	792	805	3	6	8	907	906
2	12	-5	882	835	3	0	11	1067	1053	3	2	12	221	214	3	4	12	321	346	3	6	9	651	679
2	12	-3	781	769	3	1	-15	275	326	3	3	-15	310	326	3	5	-14	499	504	3	6	11	502	525
2	12	1	1102	1125	3	1	-13	656	643	3	3	-14	370	369	3	5	-13	399	365	3	6	12	535	494
2	12	3	895	916	3	1	-11	1452	1466	3	3	-13	554	552	3	5	-11	829	840	3	7	-12	318	334
2	12	5	203	210	3	1	-9	843	821	3	3	-11	1237	1268	3	5	-10	408	417	3	7	-11	615	607
2	12	7	754	742	3	1	-7	1361	1308	3	3	-10	452	451	3	5	-9	430	409	3	7	-10	448	456
2	12	9	367	377	3	1	-6	290	247	3	3	-9	655	671	3	5	-8	929	855	3	7	-9	361	360
2	13	-9	552	541	3	1	-5	2098	2129	3	3	-8	546	550	3	5	-7	542	547	3	7	-8	858	831
2	13	-7	735	718	3	1	-4	253	211	3	3	-7	804	834	3	5	-6	199	206	3	7	-7	463	459
2	13	-5	244	236	3	1	-3	1013	979	3	3	-6	258	250	3	5	-5	1277	1286	3	7	-6	470	447
2	13	-3	574	567	3	1	-2	411	411	3	3	-5	1783	1797	3	5	-4	893	877	3	7	-5	1023	1026
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2	13	3	688	681	3	1	2	204	58	3	3	-2	1212	1193	3	5	-1	1183	1144	3	7	-2	1139	1101
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2	13	6	240	241	3	1	4	143	85	3	3	0	210	233	3	5	1	1820	1835	3	7	0	551	515
2	13	7	235	205	3	1	5	1149	1150	3	3	1	2511	2590	3	5	2	295	301	3	7	1	622	673
2	13	9	485	486	3	1	6	209	179	3	3	2	306	369	3	5	3	889	883	3	7	2	351	410
2	14	-8	194	142	3	1	7	1786	1759	3	3	3	937	928	3	5	4	835	803	3	7	3	468	429
2	14	-7	214	120	3	1	8	254	250	3	3	4	307	308	3	5	5	929	906	3	7	4	1164	1177
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2	14	-3	625	627	3	1	10	319	308	3	3	6	365	389	3	5	7	1131	1161	3	7	7	761	794
2	14	1	942	925	3	1	11	737	734	3	3	7	1487	1494	3	5	8	275	304	3	7	8	300	314
2	14	3	626	607	3	1	13	859	846	3	3	8	223	228	3	5	9	328	335	3	7	9	270	283
2	14	7	628	590	3	2	-15	587	658	3	3	9	507	508	3	5	10	649	672	3	7	10	568	583
2	15	-5	222	204	3	2	-13	756	755	3	3	10	731	708	3	5	11	414	373	3	7	11	332	374

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
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3	8	-13	340	316	3	10	-1	451	412	3	15	-2	766	774	4	2	0	327	294	4	4	4	1245	1249
3	8	-12	744	745	3	10	0	1019	1067	3	15	0	307	286	4	2	2	1582	1660	4	4	5	688	707
3	8	-10	595	626	3	10	1	175	230	3	15	2	417	385	4	2	4	1538	1654	4	4	6	203	279
3	8	-9	410	430	3	10	2	1095	1101	3	15	4	615	608	4	2	5	348	324	4	4	7	575	590
3	8	-7	804	782	3	10	3	310	284	3	16	0	531	563	4	2	7	396	408	4	4	8	740	757
3	8	-6	1207	1203	3	10	6	902	942	4	0	-14	602	617	4	2	8	1120	1130	4	4	10	745	741
3	8	-4	1026	1069	3	10	8	660	690	4	0	-12	335	298	4	2	10	954	914	4	4	11	373	384
3	8	-3	834	821	3	10	9	336	296	4	0	-10	1122	1094	4	2	11	238	239	4	5	-14	248	220
3	8	-1	820	835	3	11	-10	447	437	4	0	-8	1441	1424	4	3	-14	359	361	4	5	-12	771	777
3	8	0	1457	1466	3	11	-8	946	982	4	0	-6	194	175	4	3	-12	942	948	4	5	-11	345	320
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3	8	12	566	553	3	11	2	637	681	4	1	-14	371	409	4	3	-3	611	576	4	5	-3	1158	1201
3	9	-12	266	255	3	11	4	1134	1148	4	1	-12	1047	1088	4	3	-2	824	860	4	5	-2	1104	1096
3	9	-11	332	292	3	11	5	205	232	4	1	-10	831	823	4	3	-1	749	701	4	5	-1	549	526
3	9	-10	588	575	3	11	6	323	359	4	1	-9	245	246	4	3	0	1889	1888	4	5	0	1690	1761
3	9	-9	274	248	3	11	7	220	229	4	1	-8	962	937	4	3	1	387	376	4	5	1	434	409
3	9	-8	821	815	3	11	8	497	534	4	1	-7	155	177	4	3	2	1089	1076	4	5	2	609	637
3	9	-7	265	261	3	11	10	642	653	4	1	-6	1966	1995	4	3	3	986	914	4	5	3	922	940
3	9	-6	414	370	3	12	-10	634	634	4	1	-4	789	782	4	3	4	597	587	4	5	4	615	624
3	9	-5	933	935	3	12	-6	853	848	4	1	-3	228	164	4	3	5	338	348	4	5	5	839	854
3	9	-4	607	587	3	12	-4	846	876	4	1	-2	775	717	4	3	6	1411	1449	4	5	6	1088	1087
3	9	-3	589	577	3	12	0	884	865	4	1	-1	393	402	4	3	8	445	424	4	5	7	269	272
3	9	-2	1449	1438	3	12	2	892	897	4	1	0	2118	2146	4	3	9	649	642	4	5	8	411	441
3	9	-1	231	245	3	12	6	727	720	4	1	2	1559	1544	4	3	10	570	531	4	5	9	709	714
3	9	0	497	499	3	12	8	601	586	4	1	3	285	300	4	3	12	745	739	4	5	10	262	283
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3	9	5	234	212	3	13	-2	910	933	4	1	9	252	218	4	4	-10	985	976	4	6	-11	510	487
3	9	6	530	526	3	13	0	543	552	4	1	10	601	569	4	4	-8	1069	1076	4	6	-10	601	610
3	9	7	440	469	3	13	2	607	600	4	1	12	853	835	4	4	-7	743	717	4	6	-8	883	890
3	9	8	254	275	3	13	4	841	853	4	2	-14	602	638	4	4	-6	275	320	4	6	-7	772	752
3	9	10	708	679	3	13	6	301	297	4	2	-13	295	279	4	4	-5	687	711	4	6	-6	195	176
3	9	11	244	200	3	13	8	407	385	4	2	-10	1191	1191	4	4	-4	1506	1479	4	6	-5	1025	1001
3	10	-12	564	585	3	14	-6	636	619	4	2	-8	1352	1307	4	4	-3	388	364	4	6	-4	1251	1245
3	10	-10	722	710	3	14	-4	617	626	4	2	-7	267	307	4	4	-2	1587	1589	4	6	-2	1617	1637
3	10	-7	392	381	3	14	0	761	758	4	2	-5	532	514	4	4	-1	639	619	4	6	-1	1001	995
3	10	-6	1037	1093	3	14	2	688	664	4	2	-4	1279	1274	4	4	0	398	386	4	6	1	1139	1148
3	10	-5	298	307	3	14	6	571	561	4	2	-3	424	408	4	4	1	731	738	4	6	2	859	874
3	10	-4	1027	1013	3	15	-6	325	331	4	2	-2	1072	1138	4	4	2	1471	1467	4	6	4	1108	1168

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
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4	6	7	915	918	4	9	-9	660	648	4	12	-5	728	736	5	2	-13	197	115	5	4	-12	340	330
4	6	8	640	684	4	9	-7	358	348	4	12	-1	647	650	5	2	-11	691	669	5	4	-11	671	664
4	6	10	620	632	4	9	-6	654	649	4	12	1	857	850	5	2	-9	1148	1145	5	4	-9	1014	1009
4	6	11	450	464	4	9	-5	546	554	4	12	5	715	720	5	2	-8	354	322	5	4	-8	301	302
4	7	-13	343	333	4	9	-4	667	668	4	12	7	669	657	5	2	-7	456	450	5	4	-7	336	358
4	7	-12	577	553	4	9	-3	1182	1161	4	13	-7	479	439	5	2	-6	371	322	5	4	-6	780	786
4	7	-11	393	362	4	9	-1	661	699	4	13	-5	414	395	5	2	-5	990	998	5	4	-5	897	898
4	7	-10	470	475	4	9	0	634	606	4	13	-3	821	818	5	2	-3	1477	1502	5	4	-4	518	487
4	7	-9	682	670	4	9	1	588	582	4	13	-1	466	452	5	2	-2	187	262	5	4	-3	1610	1611
4	7	-8	239	250	4	9	2	194	161	4	13	1	344	344	5	2	-1	449	439	5	4	-2	639	623
4	7	-7	375	361	4	9	3	1126	1124	4	13	3	751	759	5	2	0	359	317	5	4	-1	493	456
4	7	-6	1100	1106	4	9	4	262	278	4	13	5	408	371	5	2	1	1272	1266	5	4	0	959	951
4	7	-5	527	482	4	9	5	458	463	4	13	7	271	281	5	2	2	397	379	5	4	1	932	967
4	7	-4	596	599	4	9	6	376	432	4	14	-7	534	523	5	2	3	1624	1682	5	4	2	267	294
4	7	-3	1177	1165	4	9	7	356	331	4	14	-5	573	531	5	2	4	652	683	5	4	3	1326	1375
4	7	-2	580	585	4	9	8	357	350	4	14	-1	556	551	5	2	5	357	347	5	4	4	573	590
4	7	-1	749	665	4	9	9	674	653	4	14	1	620	635	5	2	6	207	214	5	4	5	412	426
4	7	0	939	966	4	10	-11	674	648	4	14	5	494	499	5	2	7	995	995	5	4	6	592	628
4	7	1	398	416	4	10	-8	333	357	4	15	-3	609	600	5	2	8	222	244	5	4	7	714	728
4	7	2	485	442	4	10	-7	895	917	4	15	-1	347	379	5	2	9	1015	971	5	4	9	742	702
4	7	3	965	968	4	10	-6	227	221	4	15	1	277	267	5	2	11	215	152	5	4	11	233	190
4	7	4	324	340	4	10	-5	951	930	4	15	3	607	625	5	3	-14	219	217	5	4	12	248	268
4	7	5	689	658	4	10	-4	354	339	5	0	-11	723	730	5	3	-13	629	651	5	5	-13	614	585
4	7	6	758	761	4	10	-2	474	464	5	0	-9	1373	1373	5	3	-12	214	200	5	5	-11	486	472
4	7	7	234	230	4	10	-1	976	1013	5	0	-7	537	507	5	3	-11	791	783	5	5	-10	511	490
4	7	8	451	494	4	10	1	951	926	5	0	-5	1160	1188	5	3	-10	189	149	5	5	-9	434	434
4	7	9	566	585	4	10	2	442	438	5	0	-3	1399	1472	5	3	-9	480	485	5	5	-8	426	406
4	7	11	334	321	4	10	5	809	826	5	0	-1	649	669	5	3	-8	323	302	5	5	-7	847	836
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4	8	-10	361	381	4	10	8	226	225	5	0	3	1834	1823	5	3	-5	908	911	5	5	-5	813	777
4	8	-8	622	613	4	11	-10	218	185	5	0	5	295	323	5	3	-4	403	419	5	5	-4	1042	1077
4	8	-7	727	708	4	11	-9	887	880	5	0	7	974	935	5	3	-3	551	565	5	5	-3	517	518
4	8	-5	1101	1121	4	11	-7	408	408	5	0	9	1096	1072	5	3	-2	858	789	5	5	-2	898	954
4	8	-4	776	788	4	11	-6	267	255	5	1	-14	193	93	5	3	-1	1320	1349	5	5	-1	1486	1503
4	8	-2	884	892	4	11	-5	591	610	5	1	-13	857	868	5	3	0	263	249	5	5	0	185	197
4	8	-1	1187	1212	4	11	-4	377	340	5	1	-11	676	693	5	3	1	1354	1391	5	5	1	870	915
4	8	1	1028	1060	4	11	-3	985	982	5	1	-7	1615	1645	5	3	2	644	636	5	5	2	821	869
4	8	2	664	643	4	11	-1	465	501	5	1	-5	1353	1326	5	3	3	443	467	5	5	3	353	372
4	8	4	525	526	4	11	0	284	263	5	1	-2	439	358	5	3	4	166	107	5	5	4	505	507
4	8	5	796	773	4	11	1	377	387	5	1	-1	1815	1833	5	3	5	1252	1266	5	5	5	999	978
4	8	7	741	756	4	11	3	928	930	5	1	1	1250	1206	5	3	6	216	206	5	5	7	481	480
4	8	8	490	523	4	11	4	209	183	5	1	2	242	221	5	3	7	644	650	5	5	8	543	534
4	8	10	465	445	4	11	5	456	471	5	1	3	366	351	5	3	8	407	406	5	5	9	330	308
4	8	11	423	408	4	11	6	250	251	5	1	5	1515	1519	5	3	9	350	351	5	5	10	381	419
4	9	-12	369	363	4	11	7	368	389	5	1	7	949	951	5	3	10	331	303	5	5	11	614	635
4	9	-11	413	390	4	11	9	665	657	5	1	9	227	226	5	3	11	662	697	5	6	-12	486	502

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	6	-11	555	539	5	8	0	971	1033	5	11	-2	544	551	6	2	-10	1206	1199	6	4	0	841	883
5	6	-9	881	873	5	8	1	583	601	5	11	-1	250	232	6	2	-8	707	706	6	4	1	210	154
5	6	-8	523	544	5	8	2	312	333	5	11	0	186	206	6	2	-7	396	417	6	4	2	1303	1334
5	6	-7	238	216	5	8	3	508	549	5	11	2	828	812	6	2	-6	1029	1008	6	4	3	470	452
5	6	-6	806	788	5	8	4	676	713	5	11	4	612	626	6	2	-4	1543	1527	6	4	4	464	438
5	6	-5	812	791	5	8	6	643	624	5	11	5	237	216	6	2	-3	277	298	6	4	5	495	471
5	6	-3	1189	1193	5	8	7	386	405	5	11	6	205	156	6	2	-2	335	359	6	4	6	609	607
5	6	-2	788	798	5	8	8	212	188	5	11	8	583	615	6	2	-1	528	516	6	4	7	252	282
5	6	-1	312	339	5	8	9	486	523	5	12	-8	531	558	6	2	0	1061	1072	6	4	8	753	742
5	6	0	804	820	5	8	10	357	348	5	12	-6	786	795	6	2	2	1547	1574	6	4	10	337	288
5	6	1	672	672	5	9	-11	309	286	5	12	-2	559	567	6	2	3	464	469	6	5	-12	526	540
5	6	3	1050	1022	5	9	-10	686	678	5	12	0	744	733	6	2	4	573	571	6	5	-11	468	467
5	6	4	588	618	5	9	-8	444	416	5	12	4	465	482	6	2	5	392	401	6	5	-9	353	399
5	6	5	337	320	5	9	-7	452	456	5	12	6	722	740	6	2	6	831	811	6	5	-8	908	880
5	6	6	769	807	5	9	-6	361	360	5	13	-6	216	198	6	2	8	1048	1017	6	5	-6	851	840
5	6	7	479	480	5	9	-5	418	412	5	13	-4	677	664	6	2	10	247	259	6	5	-5	878	894
5	6	9	609	628	5	9	-4	921	920	5	13	-2	434	427	6	3	-12	615	618	6	5	-3	837	844
5	6	10	394	328	5	9	-2	661	678	5	13	2	727	714	6	3	-11	278	278	6	5	-2	1191	1201
5	7	-11	425	419	5	9	-1	510	524	5	13	4	471	441	6	3	-10	225	238	6	5	0	823	831
5	7	-10	627	628	5	9	0	280	287	5	14	-2	505	477	6	3	-9	307	277	6	5	1	769	816
5	7	-9	206	214	5	9	1	318	305	5	14	0	649	615	6	3	-8	1118	1127	6	5	3	410	392
5	7	-8	245	277	5	9	2	920	950	6	0	-12	735	707	6	3	-6	1003	987	6	5	4	831	844
5	7	-7	887	938	5	9	3	291	323	6	0	-10	1063	1051	6	3	-5	298	281	6	5	6	561	574
5	7	-6	257	229	5	9	4	649	670	6	0	-8	909	907	6	3	-4	237	278	6	5	7	455	528
5	7	-5	654	620	5	9	5	366	390	6	0	-6	965	937	6	3	-3	395	411	6	5	8	215	176
5	7	-4	1174	1175	5	9	6	306	307	6	0	-4	1622	1589	6	3	-2	1428	1461	6	5	9	398	378
5	7	-3	416	415	5	9	7	297	309	6	0	-2	531	537	6	3	0	1216	1246	6	5	10	578	579
5	7	-2	880	885	5	9	8	681	647	6	0	0	1343	1287	6	3	1	635	653	6	6	-12	310	336
5	7	-1	985	1013	5	10	-9	287	276	6	0	2	1780	1800	6	3	3	278	227	6	6	-11	278	248
5	7	0	211	204	5	10	-8	613	634	6	0	4	598	563	6	3	4	1222	1274	6	6	-10	574	596
5	7	1	492	489	5	10	-6	876	904	6	0	6	858	813	6	3	6	829	860	6	6	-9	472	481
5	7	2	995	1014	5	10	-5	297	300	6	0	8	1124	1098	6	3	7	307	318	6	6	-8	232	219
5	7	4	633	647	5	10	-3	345	344	6	0	10	237	263	6	3	8	224	249	6	6	-7	573	554
5	7	5	611	684	5	10	-2	705	688	6	1	-12	741	726	6	3	9	285	300	6	6	-6	333	358
5	7	6	192	205	5	10	0	981	996	6	1	-9	252	215	6	3	10	672	683	6	6	-5	394	369
5	7	7	494	482	5	10	1	386	427	6	1	-8	1285	1281	6	4	-13	446	420	6	6	-4	1046	1052
5	7	8	613	646	5	10	2	272	322	6	1	-6	1380	1362	6	4	-12	358	371	6	6	-3	528	511
5	7	10	370	337	5	10	3	184	163	6	1	-4	444	435	6	4	-10	1043	1016	6	6	-2	572	576
5	8	-12	565	571	5	10	4	598	581	6	1	-2	1547	1523	6	4	-9	253	290	6	6	-1	908	944
5	8	-11	355	328	5	10	6	787	763	6	1	0	1283	1271	6	4	-8	282	291	6	6	0	544	524
5	8	-9	405	480	5	10	7	206	235	6	1	2	220	250	6	4	-7	644	662	6	6	1	305	288
5	8	-8	611	627	5	10	9	262	220	6	1	3	181	230	6	4	-6	652	659	6	6	2	842	852
5	8	-6	783	769	5	11	-10	684	670	6	1	4	1195	1197	6	4	-5	183	192	6	6	3	488	470
5	8	-5	452	434	5	11	-8	607	618	6	1	6	984	982	6	4	-4	1398	1464	6	6	4	317	333
5	8	-4	343	338	5	11	-6	305	311	6	1	10	749	743	6	4	-3	554	540	6	6	5	565	591
5	8	-3	629	635	5	11	-5	221	208	6	2	-13	311	341	6	4	-2	642	644	6	6	6	368	372
5	8	-2	780	826	5	11	-4	838	823	6	2	-12	477	483	6	4	-1	841	878	6	6	7	205	175

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
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6	6	9	255	253	6	9	2	195	164	7	1	-3	1214	1230	7	4	-3	564	581	7	7	-8	262	219
6	7	-12	400	397	6	9	3	690	722	7	1	-1	935	931	7	4	-2	596	588	7	7	-7	555	548
6	7	-11	591	578	6	9	4	464	466	7	1	2	303	337	7	4	-1	663	676	7	7	-6	759	779
6	7	-10	196	103	6	9	5	220	230	7	1	3	1104	1109	7	4	0	438	419	7	7	-4	821	816
6	7	-9	582	547	6	9	6	353	341	7	1	5	872	831	7	4	1	967	993	7	7	-3	708	726
6	7	-8	659	644	6	9	7	589	582	7	1	9	677	638	7	4	2	563	543	7	7	-1	644	661
6	7	-7	293	304	6	10	-9	452	434	7	2	-11	901	919	7	4	3	570	560	7	7	0	728	732
6	7	-6	574	577	6	10	-7	885	864	7	2	-10	221	152	7	4	4	502	502	7	7	2	616	643
6	7	-5	981	1011	6	10	-5	274	316	7	2	-9	541	577	7	4	5	502	511	7	7	3	588	607
6	7	-3	1026	1065	6	10	-3	560	580	7	2	-8	427	437	7	4	7	770	770	7	7	5	487	495
6	7	-2	815	831	6	10	-2	262	239	7	2	-7	613	628	7	4	9	319	290	7	7	6	623	623
6	7	-1	216	237	6	10	-1	849	844	7	2	-5	1278	1315	7	5	-10	443	426	7	7	8	469	441
6	7	0	641	661	6	10	0	231	229	7	2	-4	200	265	7	5	-9	785	766	7	8	-10	309	348
6	7	1	828	830	6	10	1	373	321	7	2	-3	419	454	7	5	-7	669	661	7	8	-8	786	739
6	7	3	743	751	6	10	2	348	385	7	2	-2	385	425	7	5	-6	623	618	7	8	-5	416	388
6	7	4	614	639	6	10	3	487	468	7	2	-1	764	760	7	5	-4	623	661	7	8	-4	361	365
6	7	5	199	168	6	10	5	794	771	7	2	0	270	239	7	5	-3	808	801	7	8	-3	445	442
6	7	6	469	462	6	10	7	359	314	7	2	1	1342	1341	7	5	-1	918	961	7	8	-2	929	930
6	7	7	635	606	6	11	-5	825	846	7	2	2	321	306	7	5	0	775	793	7	8	0	272	299
6	7	9	484	476	6	11	-3	530	510	7	2	3	623	659	7	5	2	399	404	7	8	1	583	600
6	8	-10	381	368	6	11	1	741	738	7	2	4	324	311	7	5	3	728	714	7	8	2	306	289
6	8	-9	486	514	6	11	3	625	601	7	2	5	481	483	7	5	5	630	654	7	8	3	287	270
6	8	-7	753	725	6	12	-7	676	710	7	2	6	238	221	7	5	6	407	372	7	8	4	679	697
6	8	-6	341	341	6	12	-5	240	225	7	2	7	892	848	7	5	7	225	116	7	8	5	258	282
6	8	-5	397	390	6	12	-3	416	425	7	2	9	272	307	7	5	8	345	361	7	8	6	256	261
6	8	-4	517	503	6	12	-1	734	731	7	3	-12	280	313	7	5	9	495	507	7	8	7	415	414
6	8	-3	643	666	6	12	1	297	274	7	3	-9	986	974	7	6	-11	517	529	7	9	-9	224	189
6	8	-2	213	206	6	12	3	455	464	7	3	-7	1010	1005	7	6	-10	355	338	7	9	-7	336	334
6	8	-1	948	988	6	12	5	659	694	7	3	-6	383	397	7	6	-9	345	309	7	9	-6	719	742
6	8	0	304	295	6	13	-5	651	643	7	3	-4	240	276	7	6	-8	637	628	7	9	-4	756	771
6	8	1	369	354	6	13	-3	423	419	7	3	-3	1086	1081	7	6	-7	404	384	7	9	-3	295	311
6	8	2	465	498	6	13	1	606	625	7	3	-1	975	991	7	6	-6	293	291	7	9	-1	541	551
6	8	3	516	519	6	13	3	513	510	7	3	0	488	481	7	6	-5	721	748	7	9	0	598	598
6	8	4	230	191	7	0	-11	881	867	7	3	2	385	390	7	6	-4	458	438	7	9	2	606	601
6	8	5	738	735	7	0	-9	614	618	7	3	3	791	787	7	6	-3	583	583	7	9	3	468	438
6	8	6	278	277	7	0	-7	547	528	7	3	4	209	144	7	6	-2	780	738	7	9	5	292	339
6	8	7	233	223	7	0	-5	1355	1409	7	3	5	939	935	7	6	-1	427	452	7	9	6	515	564
6	8	8	439	453	7	0	-3	379	343	7	3	6	207	168	7	6	0	201	241	7	10	-8	638	629
6	8	9	286	286	7	0	-1	1059	1054	7	3	9	650	609	7	6	1	677	702	7	10	-6	299	285
6	9	-9	538	490	7	0	1	1537	1516	7	4	-11	728	763	7	6	2	262	262	7	10	-5	372	344
6	9	-8	263	285	7	0	3	457	437	7	4	-10	393	354	7	6	3	293	292	7	10	-4	446	449
6	9	-7	244	236	7	0	5	443	355	7	4	-9	398	439	7	6	4	563	544	7	10	-2	732	760
6	9	-6	330	321	7	0	7	876	843	7	4	-8	384	367	7	6	5	372	383	7	10	0	371	372
6	9	-5	753	738	7	0	9	393	392	7	4	-7	564	585	7	6	6	270	237	7	10	1	427	412
6	9	-3	911	918	7	1	-9	849	843	7	4	-6	244	230	7	6	7	600	605	7	10	2	366	371
6	9	-2	347	321	7	1	-7	1111	1125	7	4	-5	1162	1179	7	7	-10	540	568	7	10	3	214	146

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
7	10	4	658	677	8	3	-4	719	690	8	6	6	561	573	9	2	-7	796	782	9	6	-1	616	645
7	11	-6	589	584	8	3	-1	199	154	8	7	-8	492	468	9	2	-5	639	638	9	6	1	374	386
7	11	-4	538	532	8	3	0	232	220	8	7	-7	578	577	9	2	-4	275	283	9	6	2	419	431
7	11	-1	248	260	8	3	1	356	370	8	7	-5	523	566	9	2	-3	235	239	9	7	-6	491	452
7	11	0	610	611	8	3	2	573	545	8	7	-4	370	374	9	2	-1	808	814	9	7	-5	312	294
7	11	2	573	569	8	3	4	917	919	8	7	-2	682	682	9	2	1	757	710	9	7	-3	464	501
7	12	-4	399	460	8	3	5	218	161	8	7	-1	507	542	9	2	2	303	243	9	7	-2	301	298
7	12	-2	621	614	8	4	-10	457	444	8	7	1	405	442	9	2	5	684	679	9	7	-1	239	160
7	12	0	357	333	8	4	-9	321	305	8	7	2	523	540	9	3	-9	616	666	9	7	0	489	481
7	12	2	330	332	8	4	-8	369	346	8	7	4	441	459	9	3	-8	210	211	9	7	1	360	340
8	0	-10	401	465	8	4	-6	825	873	8	7	5	470	432	9	3	-7	312	324	9	8	-4	528	533
8	0	-8	310	310	8	4	-5	293	265	8	8	-7	295	300	9	3	-6	250	229	9	8	-2	436	444
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8	3	-7	338	333	8	6	4	361	348	9	1	5	237	233	9	6	-4	389	427					
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