

CHEMISTRY OF MATERIALS

Chem. Mater., 1996, 8(5), 1092-1105, DOI: [10.1021/cm950526w](https://doi.org/10.1021/cm950526w)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

Supplementary Material (41 pages)

**Self-Organization of 2,5-Di-*n*-Alkoxy-1,4-Benzoquinones in the Solid State:
Molecular Recognition involving Intermolecular Dipole-Dipole-,
Weak C-H...O=C Hydrogen Bond- and Van der Waals Interactions.**

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker and Leonardus W. Jenneskens.*

*Debye Institute, Department of Physical Organic Chemistry,
Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands.*

Arie Schouten, Huub Kooijman, Nora Veldman, and Anthony L. Spek
*Bijvoet Center for Biomolecular Research, Crystal and Structural Chemistry
Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands.*

Spectroscopic data (^1H , ^{13}C NMR, FT-IR) of compounds **1(n)** with $n=2, 4-8, 11$ and $13-19$.

2,5-diethoxy-1,4-benzoquinone (I(2)): Yield: 1.40 g (7.1 mmol, 20%). ^1H NMR δ 5.79 (s, 2H); 3.98 (q, 4H); 1.45 (t, 6H) ppm; ^{13}C NMR δ 181.84, 158.53, 105.70, 65.40, 13.72 ppm. DRIFT ν 3059.2, 2977.3, 1665, 1600.3, 1230.8, 1209.7 cm^{-1} .

2,5-di-*n*-butoxy-1,4-benzoquinone (I(4)): Yield: 1.40 g (13.6 mmol, 38%). ^1H NMR δ 5.81 (s, 2H); 3.91 (t, 4H); 1.81 (dt, 4H); 1.45 (m, 4H); 0.94 (t, 6H) ppm. ^{13}C NMR δ 181.97, 158.81, 105.78, 69.53, 30.13, 19.06, 13.65 ppm. DRIFT ν 2957.0, 2941.6, 2938.2, 2932.9, 2915.0, 1670.6, 1607.0, 1230.9, 1207.8 cm^{-1} .

2,5-di-*n*-pentoxy-1,4-benzoquinone (I(5)): Yield: 3.50 g (12.5 mmol, 35%). ^1H NMR δ 5.82 (s, 2H); 3.91 (t, 4H); 1.84 (dt, 4H); 1.38 (m, 8H); 0.91 (t, 6H) ppm. ^{13}C NMR δ 182.00, 158.83, 105.78, 69.85, 27.91, 27.88, 22.30, 13.90. DRIFT δ 2953.1, 2944.5, 2941.6, 2931.9, 1670.6, 1607.5, 1230.9, 1207.8 cm^{-1} .

2,5-di-*n*-hexoxy-1,4-benzoquinone (I(6)):⁴¹ Yield: 4.51 g (14.6 mmol, 41%). ^1H NMR δ 5.82 (s, 2H); 3.91 (t, 4H); 1.84 (dt, 4H); 1.37 (m, 12H); 0.87 (t, 6H) ppm. ^{13}C NMR δ

181.96, 158.78, 105.67, 69.65, 30.04, 28.07, 26.78, 22.29, 13.89 ppm. DRIFT v 2953.6, 2924.7, 2919.9, 2915.5, 1671.1, 1609.4, 1231.9, 1209.2 cm^{-1} .

2,5-di-n-heptoxy-1,4-benzoquinone (I(7)): Yield: 5.28 g (15.7 mmol, 44%). ^1H NMR δ 5.78 (s, 2H); 3.88 (t, 4H); 1.80 (dt, 4H); 1.30 (m, 16H); 0.84 (t, 6H) ppm. ^{13}C NMR δ 181.83, 158.67, 105.64, 69.71, 31.51, 28.74, 28.04, 25.62, 22.41, 13.91 ppm. DRIFT v 2928.1, 2919.9, 2915.1, 1669.7, 1608.4, 1230.4, 1209.7 cm^{-1} .

2,5-di-n-octoxy-1,4-benzoquinone (I(8)):⁴¹ Yield: 7.42 g (20.3 mmol, 57%). ^1H NMR δ 5.80 (s, 2H); 3.88 (t, 4H); 1.80 (dt, 4H); 1.30 (m, 20H); 0.84 (t, 6H) ppm. ^{13}C NMR δ 181.95, 158.77, 105.73, 69.80, 31.68, 29.11, 29.05, 28.11, 25.74, 22.56, 14.02 ppm. DRIFT v 2952.6, 2943.0, 2922.3, 2914.6, 1671.6, 1609.4, 1231.9, 1209.2 cm^{-1} .

2,5-di-n-undecyloxy-1,4-benzoquinone (I(11)): Yield: 6.25 g (13.9 mmol, 39%). ^1H NMR δ 5.82 (s, 2H); 3.90 (t, 4H); 1.83 (dt, 4H); 1.30 (m, 32H); 0.87 (t, 6H) ppm. ^{13}C NMR δ 181.96, 158.77, 105.74, 69.82, 31.84, 29.53, 29.49, 29.40, 29.27, 29.17, 28.12, 25.75, 22.64, 14.08 ppm. DRIFT v 2952.2, 2930.5, 2916.5, 28.49.5, 1670.2, 1605.5, 1471.5, 1226.6, 1206.8 cm^{-1} .

2,5-di-n-tridecyloxy-1,4-benzoquinone (I(13)): Yield: 5.95 g (11.7 mmol, 33%). ^1H NMR δ 5.82 (s, 2H); 3.91 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 40H); 0.88 (t, 6H) ppm. ^{13}C NMR δ 181.98, 158.84, 105.79, 69.85, 31.90, 29.61, 29.52, 29.44, 29.33, 29.20, 28.17, 25.79, 22.67, 14.09 ppm. DRIFT v 2931.7, 2917.1, 2849.8, 1672.8, 1607.1, 1473.9, 1230.5, 1207.0 cm^{-1} .

2,5-di-n-tetradecyloxy-1,4-benzoquinone (I(14)):⁴¹ Yield: 7.79 g (14.6 mmol, 41%). ^1H NMR δ 5.82 (s, 2H); 3.91 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 44H); 0.88 (t, 6H) ppm. ^{13}C NMR δ 181.97, 158.84, 105.80, 69.81, 31.87, 29.69, 29.57, 29.42, 29.33, 29.19, 28.20, 25.77, 22.66, 14.08 ppm. DRIFT v 2954.8, 2916.2, 2871.8, 2849.7, 1673.1, 1606.6, 1471.6, 1228.6, 1207.4 cm^{-1} .

2,5-di-n-pentadecyloxy-1,4-benzoquinone (I(15)): Yield: 4.80 g (8.6 mmol, 24%). ^1H NMR δ 5.82 (s, 2H); 3.92 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 48H); 0.88 (t, 6H) ppm. ^{13}C NMR δ 181.98, 158.84, 105.80, 69.85, 31.91, 29.64, 29.53, 29.44, 29.34, 29.20, 28.17, 25.79, 22.68,

14.10 ppm. DRIFT v 2961.5, 2951.9, 2916.2, 2869.9, 2849.7, 1673.1, 1607.6, 1471.6, 1227.6, 1207.4 cm^{-1} .

2,5-di-n-hexadecyloxy-1,4-benzoquinone (I(16)):⁴¹ Yield: 6.52 g (3.5 mmol, 31%). ^1H NMR δ 5.82 (s, 2H); 3.91 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 52H); 0.87 (t, 6H) ppm. ^{13}C NMR δ 181.97, 1548.84, 105.79, 69.83, 31.91, 29.63, 29.53, 29.45, 29.35, 29.22, 28.17, 25.80, 22.68, 14.08 ppm. DRIFT v 2953.6, 2916.0, 2849.5, 1673.0, 1607.0, 1472.0, 1228.8, 1207.3 cm^{-1} .

2,5-di-n-heptadecyloxy-1,4-benzoquinone (I(17)): Yield: 0.51 g (0.8 mmol, 21%; using 4 mmol of 2,5-dihydroxy-1,4-benzoquinone and 20 mmol of 1-heptadecanol). ^1H NMR δ 5.82 (s, 2H); 3.92 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 56H); 0.88 (t, 6H) ppm. ^{13}C NMR δ 181.97, 158.84, 105.80, 69.85, 31.91, 29.67, 29.65, 29.53, 29.44, 29.34, 29.20, 28.17, 25.80, 22.67, 14.09 ppm. DRIFT v 2952.1, 2916.4, 2849.7, 1673.2, 1606.8, 1473.5, 1229.1, 1207.5 cm^{-1} .

2,5-di-n-octadecyloxy-1,4-benzoquinone (I(18)): Yield: 2.24 g (3.5 mmol, 35%; performed at 10 mmol scale). ^1H NMR δ 5.83 (s, 2H); 3.92 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 60H); 0.88 (t, 6H) ppm. ^{13}C NMR δ 181.98, 158.84, 105.80, 69.85, 31.92, 29.68, 29.53, 29.44, 29.35, 29.21, 28.18, 25.80, 22.68, 14.10 ppm. DRIFT v 2953.6, 2915.1, 2849.5, 1674.5, 1607.0 1471.5, 1229.0, 1207.3 cm^{-1} .

2,5-di-n-nonadecyloxy-1,4-benzoquinone (I(19)): Yield: 0.16 g (0.2 mmol, 7%; using 3.5 mmol of 2,5-dihydroxy-1,4-benzoquinone and 7 mmol of 1-nonadecanol). ^1H NMR δ 5.83 (s, 2H); 3.92 (t, 4H); 1.84 (dt, 4H); 1.30 (m, 64H); 0.88 (t, 6H) ppm. DRIFT v 2954.0, 2915.5, 2850.1, 1673.9, 1606.9, 1472.5, 1228.8, 1207.2 cm^{-1} . Due to its low solubility no high resolution ^{13}C NMR spectrum could be obtained.

Minor solid-state phase transitions for 1(n) with n=odd (DSC)

In contrast to the second solid-solid phase transitions in the first DSC heating run, the new minor solid-solid phase transitions (**s2**, **s3**, **s4**; see Figure 3) observed in the second DSC heating run contribute only to a minor extent to the total sum of the enthalpy as well as entropy changes. These minor transitions are related to changes in *n*-alkoxy chain endgroup packing. Note:

- the small differences between the slope values of ΔH_{total} (7.18 KJ mol⁻¹) and $\Delta H_{(m+sI)}$ (6.42 KJ mol⁻¹), as well as ΔS_{total} (17.56 J K⁻¹ mol⁻¹) and $\Delta S_{(m+sI)}$ (16.19 J K⁻¹ mol⁻¹);
- the differences between ΔS^0_{total} (41.9 J K⁻¹ mol⁻¹) and $\Delta S^0_{(m+sI)}$ (29.6 J K⁻¹ mol⁻¹) of 12.3 J K⁻¹ mol⁻¹ in combination with the small difference between ΔH^0_{total} (12.6 KJ mol⁻¹) and $\Delta H^0_{(m+sI)}$ (11.5 KJ mol⁻¹) of 1.1 KJ mol⁻¹ suggests that the related phase transitions arise from a denser endgroup packing in going successively from the β - to the γ - and δ -phase.

Single crystal X-ray structure data of **1(3)**, **1(9)** and **1(10)** (37 pages).

=====
S U P P L E M E N T A R Y M A T E R I A L
=====

B E L O N G I N G T O T H E P A P E R

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

b y

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Kooijman,
Nora Veldman and Anthony L. Spek

----- C O M P O U N D 1(3) -----

C o n t e n t s
=====

- Table S1 - Crystal Data and Details of the Structure Determination
for: S842A MOKA 60KV150MA LNT MON 160393
Table S2 - Final Coordinates and Equivalent Isotropic Thermal
Parameters of the non-Hydrogen atoms
for: S842A MOKA 60KV150MA LNT MON 160393
Table S3 - Hydrogen Atom Positions and Isotropic Thermal
Parameters
for: S842A MOKA 60KV150MA LNT MON 160393
Table S4 - (An)isotropic Thermal Parameters
for: S842A MOKA 60KV150MA LNT MON 160393
Table S5 - Bond Distances (Angstrom)
for: S842A MOKA 60KV150MA LNT MON 160393
Table S6 - Bond Angles (Degrees)
for: S842A MOKA 60KV150MA LNT MON 160393

Table S1 - Crystal Data and Details of the Structure Determination for: S842A MOKA 60KV150MA LNT MON 160393

Crystal Data			
Empirical Formula	C12 H16 O4		
Formula Weight	224.26		
Crystal System	Triclinic		
Space group	P-1	(No. 2)	
a, b, c [Angstrom]	4.2258(3)	5.1429(4)	13.3801(11)
alpha, beta, gamma [deg]	78.947(7)	86.409(6)	89.042(6)
V [Ang**3]	284.83(4)		
Z	1		
D(calc) [g/cm**3]	1.307		
F(000) [Electrons]	120		
Mu(MoKa) [/cm]	0.9		
Crystal Size [mm]	0.05 x 0.30 x 1.00		
Data Collection			
Temperature (K)	150		
Radiation [Angstrom]	MoKa (graphite monochromator) 0.71073		
Theta Min-Max [Deg]	1.6, 27.5		
Scan type	Omega / 2 Theta		
Scan, [Deg]	0.91 + 0.35 Tan(Theta)		
Hor. and vert. aperture [mm]	3.88	4.00	
Reference Reflection(s)	2 -1 -3, 1 -2 -5, 3 -2 -2		
Dataset	-4: 5 ; -6: 6 ; -17: 17		
Tot., Uniq. Data, R(int)	2403,	1316,	0.023
Observed data [I > 2.5 sigma(I)]	1053		
Refinement			
Npar	105		
R, wR, S	0.041, 0.051, 1.83		
w**2	sigma**2(F) + 0.000455 F**2		
Max. and Av. Shift/Error	0.121, 0.028		
Min. and Max. resd. dens. [e/Ang**3]	-0.24, 0.32		

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms for: S842A MOKA 60KV150MA LNT MON 160393

Atom	x	y	z	U(eq) [Ang**2]
----	---	---	---	-----
O(1)	0.6711(2)	0.2419(2)	0.13163(7)	0.0269(3)
O(2)	1.0134(2)	-0.16799(18)	0.20726(7)	0.0215(3)
C(1)	0.8102(3)	0.2280(3)	-0.03965(10)	0.0199(4)
C(2)	0.8202(3)	0.1344(3)	0.06968(10)	0.0193(4)
C(3)	1.0232(3)	-0.1046(3)	0.10583(10)	0.0181(4)
C(4)	1.2131(3)	-0.3853(3)	0.25194(11)	0.0228(4)
C(5)	1.1875(4)	-0.3976(3)	0.36555(11)	0.0249(5)
C(6)	1.2862(4)	-0.1421(3)	0.39495(12)	0.0318(5)

U(eq) = 1/3 of the trace of the orthogonalized U

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters
for: S842A MOKA 60KV150MA LNT MON 160393

Atom	x	y	z	U(iso) [Ang**2]
H(1)	0.686(4)	0.383(3)	-0.0620(11)	0.022(4)
H(41)	1.142(4)	-0.550(3)	0.2336(11)	0.023(4)
H(42)	1.441(4)	-0.350(3)	0.2226(12)	0.029(4)
H(51)	1.320(4)	-0.546(3)	0.3979(12)	0.037(5)
H(52)	0.963(4)	-0.440(3)	0.3934(13)	0.035(4)
H(61)	1.287(4)	-0.160(4)	0.4681(15)	0.038(5)
H(62)	1.141(5)	0.008(4)	0.3706(15)	0.048(5)
H(63)	1.494(5)	-0.084(4)	0.3646(15)	0.050(5)

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\pi^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$ for Isotropic Atoms

Table S4 - (An)isotropic Thermal Parameters
for: S842A MOKA 60KV150MA LNT MON 160393

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O(1)	0.0305(6)	0.0279(6)	0.0227(6)	-0.0075(4)	0.0010(4)	0.0076(4)
O(2)	0.0218(5)	0.0233(5)	0.0184(5)	-0.0021(4)	-0.0008(4)	0.0037(4)
C(1)	0.0196(7)	0.0174(7)	0.0223(7)	-0.0027(5)	-0.0021(5)	0.0001(6)
C(2)	0.0172(7)	0.0184(7)	0.0230(8)	-0.0058(6)	-0.0002(5)	-0.0035(5)
C(3)	0.0169(7)	0.0180(7)	0.0192(7)	-0.0026(5)	-0.0015(5)	-0.0038(5)
C(4)	0.0244(7)	0.0195(7)	0.0242(8)	-0.0030(6)	-0.0030(6)	0.0019(6)
C(5)	0.0297(8)	0.0224(8)	0.0218(8)	-0.0015(6)	-0.0035(6)	-0.0007(6)
C(6)	0.0401(10)	0.0301(9)	0.0273(9)	-0.0093(7)	-0.0057(7)	-0.0029(7)

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\pi^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$ for Isotropic Atoms
 $T = 2 * (\pi^{**2}) * \text{Sum}_{ij} (h(i) * h(j) * U(i,j) * \text{Astar}(i) * \text{Astar}(j))$, for
Anisotropic Atoms. $\text{Astar}(i)$ are Reciprocal Axial Lengths and
 $h(i)$ are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: S842A MOKA 60KV150MA LNT MON 160393

O(1)	-C(2)	1.2200(17)	C(1)	-H(1)	0.956(16)
O(2)	-C(3)	1.3318(16)	C(4)	-H(41)	0.983(16)
O(2)	-C(4)	1.4471(17)	C(4)	-H(42)	1.023(17)
C(1)	-C(2)	1.4528(19)	C(5)	-H(51)	0.986(16)
C(1)	-C(3)a	1.343(2)	C(5)	-H(52)	1.009(17)
C(2)	-C(3)	1.506(2)	C(6)	-H(61)	0.97(2)
C(4)	-C(5)	1.506(2)	C(6)	-H(62)	1.00(2)
C(5)	-C(6)	1.514(2)	C(6)	-H(63)	0.97(2)

Table S6 - Bond Angles (Degrees)
for: S842A MOKA 60KV150MA LNT MON 160393

C(3)	-O(2)	-C(4)	117.13(11)	C(5)	-C(4)	-H(41)	112.1(9)
C(2)	-C(1)	-C(3)a	120.83(13)	C(5)	-C(4)	-H(42)	111.4(9)
O(1)	-C(2)	-C(1)	122.35(13)	H(41)	-C(4)	-H(42)	108.2(13)
O(1)	-C(2)	-C(3)	119.93(12)	C(4)	-C(5)	-H(51)	108.4(9)
C(1)	-C(2)	-C(3)	117.73(12)	C(4)	-C(5)	-H(52)	110.1(10)
O(2)	-C(3)	-C(2)	111.63(11)	C(6)	-C(5)	-H(51)	110.2(9)
O(2)	-C(3)	-C(1)a	126.93(13)	C(6)	-C(5)	-H(52)	108.9(9)
C(1)a	-C(3)	-C(2)	121.44(12)	H(51)	-C(5)	-H(52)	106.3(13)
O(2)	-C(4)	-C(5)	106.87(12)	C(5)	-C(6)	-H(61)	111.3(12)
C(4)	-C(5)	-C(6)	112.75(13)	C(5)	-C(6)	-H(62)	112.4(12)
C(2)	-C(1)	-H(1)	117.3(9)	C(5)	-C(6)	-H(63)	112.0(12)
C(3)a	-C(1)	-H(1)	121.9(9)	H(61)	-C(6)	-H(62)	106.8(16)
O(2)	-C(4)	-H(41)	109.4(9)	H(61)	-C(6)	-H(63)	109.1(16)
O(2)	-C(4)	-H(42)	108.9(9)	H(62)	-C(6)	-H(63)	104.9(17)

=====
SUPPLEMENTARY MATERIAL
=====

BELONGING TO THE PAPER

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

by

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Kooijman,
Nora Veldman and Anthony L. Spek

COMPOUND 1(9)

+++++
+
+ NOTE: The atom numbering scheme in this supplementary +
+ material differs from that used in the original paper +
+
+
+++++

C o n t e n t s
=====

- Table S1 - Crystal Data and Details of the Structure Determination
for: S855A CUKA 45KV 25MA 22C NI 050493
Table S2 - Final Coordinates and Equivalent Isotropic Thermal
Parameters of the non-Hydrogen atoms
for: S855A CUKA 45KV 25MA 22C NI 050493
Table S3 - Hydrogen Atom Positions and Isotropic Thermal
Parameters
for: S855A CUKA 45KV 25MA 22C NI 050493
Table S4 - (An)isotropic Thermal Parameters
for: S855A CUKA 45KV 25MA 22C NI 050493
Table S5 - Bond Distances (Angstrom)
for: S855A CUKA 45KV 25MA 22C NI 050493

I-1105-9

Table S6 - Bond Angles (Degrees)
for: S855A CUKA 45KV 25MA 22C NI 050493

Table S1 - Crystal Data and Details of the Structure Determination
for: S855A CUKA 45KV 25MA 22C NI 050493

Crystal Data

Empirical Formula	C24 H40 O4		
Formula Weight	392.58		
Crystal System	Triclinic		
Space group	P-1	(No. 2)	
a, b, c [Angstrom]	4.1996(5)	5.3552(2)	26.044(2)
alpha, beta, gamma [deg]	87.489(5)	86.677(9)	86.980(7)
V [Ang**3]	583.44(9)		
Z	1		
D(calc) [g/cm**3]	1.117		
F(000) [Electrons]	216		
Mu(CuKa) [/cm]	5.8		
Crystal Size [mm]	0.1 x 0.4 x 0.6		

Data Collection

Temperature (K)	295		
Radiation [Angstrom]	CuKa (Ni filter)	1.54184	
Theta Min-Max [Deg]	1.7, 75.0		
Scan type	Omega / 2 Theta		
Scan, [Deg]	0.72 + 0.14 Tan(Theta)		
Hor. and vert. aperture [mm]	2.94	6.00	
Reference Reflection(s)	-2 0 5, 0 -2 8, 0 -2 2		
Dataset	-5: 4 ; -6: 6 ; -32: 32		
Tot., Uniq. Data, R(int)	4237,	2408,	0.058

Refinement

Npar	128		
wR2, R1, S	0.138, 0.050 [for 757 F > 4 sigma(F)], 0.75		
w	[sigma**2(F)+(0.0786P)**2]**-1, P=(Max(Fo**2,0)+2Fc**2)/3		
Max. and Av. Shift/Error	0.000, 0.000		
Min. and Max. resd. dens. [e/Ang^3]	-0.21, 0.16		

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms
for: S855A CUKA 45KV 25MA 22C NI 050493

Atom	x	y	z	U(eq) [Ang ²]
O(1)	0.1847(5)	1.7897(3)	0.06782(6)	0.0666(6)
O(2)	0.5304(4)	1.4074(3)	0.10465(6)	0.0509(5)
C(1)	0.3288(5)	1.6590(4)	0.03587(9)	0.0483(9)
C(2)	0.5295(5)	1.4358(4)	0.05376(9)	0.0430(9)
C(3)	0.3160(6)	1.7140(4)	-0.01897(9)	0.0492(9)
C(4)	0.7076(7)	1.1908(4)	0.12498(9)	0.0522(9)
C(5)	0.7058(6)	1.2047(4)	0.18213(10)	0.0543(9)
C(6)	0.8314(6)	0.9600(5)	0.20636(10)	0.0560(10)
C(7)	0.8848(6)	0.9645(5)	0.26343(9)	0.0588(11)
C(8)	0.9924(7)	0.7155(5)	0.28767(10)	0.0613(12)
C(9)	1.0610(7)	0.7234(5)	0.34386(9)	0.0640(12)
C(10)	1.1606(7)	0.4727(5)	0.36858(9)	0.0643(12)
C(11)	1.2365(8)	0.4795(5)	0.42444(10)	0.0753(12)
C(12)	1.3310(9)	0.2291(5)	0.44931(12)	0.0884(12)

U(eq) = 1/3 of the trace of the orthogonalized U

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters
for: S855A CUKA 45KV 25MA 22C NI 050493

Atom	x	y	z	U(iso) [Ang ²]
H(3)	0.1988(6)	1.8555(4)	-0.03048(9)	0.0590
H(4A)	0.9255(7)	1.1869(4)	0.11038(9)	0.0630
H(4B)	0.6104(7)	1.0394(4)	0.11602(9)	0.0630
H(5A)	0.4897(6)	1.2425(4)	0.19578(10)	0.0650
H(5B)	0.8374(6)	1.3385(4)	0.19083(10)	0.0650
H(6A)	1.0322(6)	0.9110(5)	0.18839(10)	0.0670
H(6B)	0.6820(6)	0.8326(5)	0.20121(10)	0.0670
H(7A)	1.0440(6)	1.0847(5)	0.26847(9)	0.0710
H(7B)	0.6874(6)	1.0225(5)	0.28127(9)	0.0710
H(8A)	1.1840(7)	0.6534(5)	0.26876(10)	0.0730
H(8B)	0.8283(7)	0.5975(5)	0.28422(10)	0.0730
H(9A)	0.8711(7)	0.7898(5)	0.36262(9)	0.0760
H(9B)	1.2292(7)	0.8381(5)	0.34720(9)	0.0760
H(10A)	0.9903(7)	0.3592(5)	0.36585(9)	0.0770
H(10B)	1.3474(7)	0.4047(5)	0.34929(9)	0.0770
H(11A)	1.4089(8)	0.5910(5)	0.42710(10)	0.0900
H(11B)	1.0507(8)	0.5499(5)	0.44364(10)	0.0900
H(12A)	1.382(6)	0.2511(8)	0.4842(3)	0.1320
H(12B)	1.514(4)	0.157(2)	0.4306(6)	0.1320
H(12C)	1.157(2)	0.1200(15)	0.4489(8)	0.1320

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8*(\text{Pi}^2)*U*(\text{Sin}(\text{Theta})/\text{Lambda})^2$ for Isotropic Atoms

Table S4 - (An)isotropic Thermal Parameters
for: S855A CUKA 45KV 25MA 22C NI 050493

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O(1)	0.0731(11)	0.0675(11)	0.0559(11)	-0.0083(8)	0.0050(10)	0.0243(9)
O(2)	0.0530(9)	0.0552(9)	0.0434(10)	-0.0025(7)	-0.0013(8)	0.0074(8)
C(1)	0.0405(10)	0.0493(14)	0.054(2)	-0.0068(12)	0.0067(12)	0.0005(11)
C(2)	0.0377(12)	0.0417(12)	0.049(2)	-0.0014(11)	-0.0005(11)	0.0020(10)
C(3)	0.0486(13)	0.0476(12)	0.050(2)	-0.0028(11)	0.0009(12)	0.0079(11)
C(4)	0.0536(13)	0.0515(14)	0.050(2)	0.0007(12)	-0.0049(12)	0.0107(12)
C(5)	0.0562(13)	0.0517(15)	0.054(2)	-0.0015(11)	-0.0028(13)	0.0063(12)
C(6)	0.0580(14)	0.060(2)	0.0506(15)	-0.0046(12)	-0.0056(13)	-0.0026(12)
C(7)	0.0596(14)	0.064(2)	0.052(2)	-0.0005(12)	-0.0024(14)	0.0009(13)
C(8)	0.066(2)	0.059(2)	0.058(2)	0.0030(12)	-0.0078(14)	0.0048(14)
C(9)	0.074(2)	0.062(2)	0.056(2)	0.0003(13)	-0.0096(15)	-0.0005(14)
C(10)	0.073(2)	0.068(2)	0.052(2)	0.0027(12)	-0.0111(14)	-0.0012(15)
C(11)	0.085(2)	0.076(2)	0.065(2)	0.0032(14)	-0.018(2)	0.005(2)
C(12)	0.106(2)	0.085(2)	0.074(2)	0.015(2)	-0.022(2)	0.002(2)

=====

The Temperature Factor has the Form of $\text{Exp}(-T)$ Where

$T = 8 * (\text{Pi}^2) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^2$ for Isotropic Atoms

$T = 2 * (\text{Pi}^2) * \text{Sum}_{ij} (h(i) * h(j) * U(i,j) * \text{Astar}(i) * \text{Astar}(j))$, for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: S855A CUKA 45KV 25MA 22C NI 050493

O(1)	-C(1)	1.223(3)	C(5)	-H(5A)	0.970(4)
O(2)	-C(2)	1.328(3)	C(5)	-H(5B)	0.970(3)
O(2)	-C(4)	1.442(3)	C(6)	-H(6A)	0.970(4)
C(1)	-C(2)	1.499(3)	C(6)	-H(6B)	0.970(4)
C(1)	-C(3)	1.449(3)	C(7)	-H(7A)	0.970(4)
C(2)	-C(3)a	1.351(3)	C(7)	-H(7B)	0.970(4)
C(4)	-C(5)	1.493(3)	C(8)	-H(8A)	0.970(4)
C(5)	-C(6)	1.512(3)	C(8)	-H(8B)	0.970(4)
C(6)	-C(7)	1.517(4)	C(9)	-H(9A)	0.970(4)
C(7)	-C(8)	1.509(4)	C(9)	-H(9B)	0.970(4)
C(8)	-C(9)	1.511(4)	C(10)	-H(10A)	0.970(4)
C(9)	-C(10)	1.513(4)	C(10)	-H(10B)	0.970(4)
C(10)	-C(11)	1.510(4)	C(11)	-H(11A)	0.970(4)
C(11)	-C(12)	1.508(4)	C(11)	-H(11B)	0.970(4)
C(3)	-H(3)	0.930(3)	C(12)	-H(12A)	0.959(11)
C(4)	-H(4A)	0.970(4)	C(12)	-H(12B)	0.959(16)
C(4)	-H(4B)	0.970(3)	C(12)	-H(12C)	0.960(9)

Table S6 - Bond Angles (Degrees)
for: S855A CUKA 45KV 25MA 22C NI 050493

C(2)	-O(2)	-C(4)	116.73(17)	C(5)	-C(6)	-H(6B)	108.5(3)
O(1)	-C(1)	-C(2)	119.2(2)	C(7)	-C(6)	-H(6A)	108.5(3)
O(1)	-C(1)	-C(3)	122.3(2)	C(7)	-C(6)	-H(6B)	108.5(3)
C(2)	-C(1)	-C(3)	118.5(2)	H(6A)	-C(6)	-H(6B)	107.5(3)
O(2)	-C(2)	-C(1)	113.32(19)	C(6)	-C(7)	-H(7A)	108.6(3)
O(2)	-C(2)	-C(3)a	126.7(2)	C(6)	-C(7)	-H(7B)	108.6(3)
C(1)	-C(2)	-C(3)a	120.0(2)	C(8)	-C(7)	-H(7A)	108.6(3)
C(1)	-C(3)	-C(2)a	121.5(2)	C(8)	-C(7)	-H(7B)	108.6(3)
O(2)	-C(4)	-C(5)	108.67(18)	H(7A)	-C(7)	-H(7B)	107.6(3)
C(4)	-C(5)	-C(6)	110.8(2)	C(7)	-C(8)	-H(8A)	108.6(3)
C(5)	-C(6)	-C(7)	115.2(2)	C(7)	-C(8)	-H(8B)	108.7(3)
C(6)	-C(7)	-C(8)	114.6(2)	C(9)	-C(8)	-H(8A)	108.6(3)
C(7)	-C(8)	-C(9)	114.4(2)	C(9)	-C(8)	-H(8B)	108.7(3)
C(8)	-C(9)	-C(10)	114.5(2)	H(8A)	-C(8)	-H(8B)	107.6(3)
C(9)	-C(10)	-C(11)	114.9(2)	C(8)	-C(9)	-H(9A)	108.6(3)
C(10)	-C(11)	-C(12)	114.9(2)	C(8)	-C(9)	-H(9B)	108.6(3)
C(1)	-C(3)	-H(3)	119.3(3)	C(10)	-C(9)	-H(9A)	108.6(3)
C(2)a	-C(3)	-H(3)	119.3(3)	C(10)	-C(9)	-H(9B)	108.6(3)
O(2)	-C(4)	-H(4A)	110.0(2)	H(9A)	-C(9)	-H(9B)	107.6(3)
O(2)	-C(4)	-H(4B)	109.9(3)	C(9)	-C(10)	-H(10A)	108.5(3)
C(5)	-C(4)	-H(4A)	110.0(3)	C(9)	-C(10)	-H(10B)	108.5(3)
C(5)	-C(4)	-H(4B)	110.0(2)	C(11)	-C(10)	-H(10A)	108.5(3)
H(4A)	-C(4)	-H(4B)	108.3(3)	C(11)	-C(10)	-H(10B)	108.6(3)
C(4)	-C(5)	-H(5A)	109.5(3)	H(10A)	-C(10)	-H(10B)	107.5(3)
C(4)	-C(5)	-H(5B)	109.5(3)	C(10)	-C(11)	-H(11A)	108.5(3)
C(6)	-C(5)	-H(5A)	109.5(3)	C(10)	-C(11)	-H(11B)	108.5(3)
C(6)	-C(5)	-H(5B)	109.5(3)	C(12)	-C(11)	-H(11A)	108.6(3)
H(5A)	-C(5)	-H(5B)	108.1(3)	C(12)	-C(11)	-H(11B)	108.5(3)
C(5)	-C(6)	-H(6A)	108.4(3)	H(11A)	-C(11)	-H(11B)	107.5(4)

Table S6 - Bond Angles (Degrees) (continued)
for: S855A CUKA 45KV 25MA 22C NI 050493

C(11)	-C(12)	-H(12A)	109.5(4)	H(12A)	-C(12)	-H(12B)	109.5(17)
C(11)	-C(12)	-H(12B)	109.4(8)	H(12A)	-C(12)	-H(12C)	109.5(17)
C(11)	-C(12)	-H(12C)	109.5(8)	H(12B)	-C(12)	-H(12C)	109.5(12)

L.I.S.T.I.N.G O.F
O.B.S.E.R.V.E.D A.N.D C.A.L.C.U.L.A.T.E.D
S.T.R.U.C.T.U.R.E. F.A.C.T.O.R.S
F.O.R

S855A - C(24) H(40) O(4)

BELONGING TO THE PAPER

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

b y

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Koolijman,
Nora Veldman and Anthony L. Spek

C O M P O U N D 1(9) -----

=====
S U P P L E M E N T A R Y M A T E R I A L
=====

B E L O N G I N G T O T H E P A P E R

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

b y

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Kooijman,
Nora Veldman and Anthony L. Spek

C O M P O U N D 1(10) -----

C o n t e n t s
=====

Table S1 - Crystal Data and Details of the Structure Determination
for: S641E MOKA 60KV150MA 22C MON 030492

Table S2 - Final Coordinates and Equivalent Isotropic Thermal
Parameters of the non-Hydrogen atoms
for: S641E MOKA 60KV150MA 22C MON 030492

Table S3 - Hydrogen Atom Positions and Isotropic Thermal
Parameters
for: S641E MOKA 60KV150MA 22C MON 030492

Table S4 - (An)isotropic Thermal Parameters
for: S641E MOKA 60KV150MA 22C MON 030492

Table S5 - Bond Distances (Angstrom)
for: S641E MOKA 60KV150MA 22C MON 030492

Table S6 - Bond Angles (Degrees)
for: S641E MOKA 60KV150MA 22C MON 030492

J-1105-15

Table S1 - Crystal Data and Details of the Structure Determination
for: S641E MOKA 60KV150MA 22C MON 030492

Crystal Data			
Empirical Formula	C26 H44 O4		
Formula Weight	420.63		
Crystal System	Triclinic		
Space group	P-1	(No. 2)	
a, b, c [Angstrom]	4.2118(3)	5.3337(5)	28.8117(19)
alpha, beta, gamma [deg]	91.826(6)	92.775(5)	92.992(7)
V [Ang**3]	645.22(9)		
Z	1		
D(calc) [g/cm**3]	1.082		
F(000) [Electrons]	232		
Mu(MoKa) [/cm]	0.7		
Crystal Size [mm]	0.05 x 0.09 x 0.78		
Data Collection			
Temperature (K)	298		
Radiation [Angstrom]	MoKa (graphite monochromator) 0.71073		
Theta Min-Max [Deg]	0.7, 27.5		
Scan type	Omega / 2 Theta		
Scan, [Deg]	0.80 + 0.35 Tan(Theta)		
Hor. and vert. aperture [mm]	3.00	4.00	
Reference Reflection(s)	-2 2 0, 0 2 7, -2 1 2		
Dataset	-5: 5 ; -6: 6 ; -37: 37		
Tot., Uniq. Data, R(int)	3508,	2938,	0.032
Observed data [I > 2.5 sigma(I)]	1294		
Refinement			
Npar	141		
R, wR, S	0.060, 0.062, 0.48		
w	sigma**-2(F)		
Max. and Av. Shift/Error	0.103, 0.023		
Min. and Max. resd. dens. [e/Ang^3]	-0.22, 0.20		

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms
for: S641E MOKA 60KV150MA 22C MON 030492

Atom	x	y	z	U(eq) [Ang^2]
----	---	---	---	-----
O(1)	1.7711(6)	1.7918(4)	0.43902(8)	0.0565(9)
O(2)	1.4013(5)	1.4114(4)	0.40565(7)	0.0438(8)
C(1)	1.6971(8)	1.7137(5)	0.51710(11)	0.0388(11)
C(2)	1.6483(8)	1.6605(5)	0.46770(11)	0.0376(11)
C(3)	1.4329(7)	1.4378(5)	0.45199(11)	0.0367(11)
C(4)	1.2105(8)	1.1943(6)	0.38707(10)	0.0445(11)
C(5)	1.1718(9)	1.2110(6)	0.33563(11)	0.0463(12)
C(6)	1.0278(9)	0.9646(6)	0.31392(11)	0.0500(12)
C(7)	0.9392(9)	0.9742(6)	0.26229(11)	0.0525(14)
C(8)	0.8142(9)	0.7240(6)	0.24073(11)	0.0538(14)
C(9)	0.7080(9)	0.7316(6)	0.18980(11)	0.0583(14)
C(10)	0.5941(9)	0.4799(6)	0.16768(12)	0.0607(14)
C(11)	0.4837(10)	0.4836(6)	0.11752(12)	0.0654(17)
C(12)	0.3749(11)	0.2286(8)	0.09653(14)	0.0827(19)
C(13)	0.2658(13)	0.2327(10)	0.04565(16)	0.122(3)

U(eq) = 1/3 of the trace of the orthogonalized U

E-1105-16

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters
for: S641E MOKA 60KV150MA 22C MON 030492

Atom	x	y	z	U(iso) [Ang^2]
H(11)	1.8319(8)	1.8608(5)	0.52819(11)	0.069(3)
H(41)	1.3174(8)	1.0411(6)	0.39478(10)	0.069(3)
H(42)	1.0010(8)	1.1904(6)	0.40051(10)	0.069(3)
H(51)	1.0303(9)	1.3457(6)	0.32811(11)	0.069(3)
H(52)	1.3802(9)	1.2481(6)	0.32295(11)	0.069(3)
H(61)	0.8361(9)	0.9170(6)	0.33024(11)	0.069(3)
H(62)	1.1841(9)	0.8364(6)	0.31812(11)	0.069(3)
H(71)	1.1280(9)	1.0309(6)	0.24611(11)	0.069(3)
H(72)	0.7737(9)	1.0952(6)	0.25818(11)	0.069(3)
H(81)	0.9835(9)	0.6054(6)	0.24379(11)	0.069(3)
H(82)	0.6315(9)	0.6643(6)	0.25792(11)	0.069(3)
H(91)	0.8884(9)	0.7972(6)	0.17275(11)	0.069(3)
H(92)	0.5332(9)	0.8453(6)	0.18686(11)	0.069(3)
H(101)	0.4161(9)	0.4135(6)	0.18513(12)	0.069(3)
H(102)	0.7702(9)	0.3673(6)	0.17029(12)	0.069(3)
H(111)	0.3061(10)	0.5947(6)	0.11474(12)	0.069(3)
H(112)	0.6607(10)	0.5503(6)	0.09990(12)	0.069(3)
H(121)	0.5519(11)	0.1170(8)	0.09938(14)	0.163(10)
H(122)	0.1970(11)	0.1620(8)	0.11397(14)	0.163(10)
H(131)	0.1969(13)	0.0627(10)	0.03418(16)	0.163(10)
H(132)	0.4421(13)	0.2967(10)	0.02761(16)	0.163(10)
H(133)	0.0877(13)	0.3430(10)	0.04230(16)	0.163(10)

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\text{Pi}^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$ for Isotropic Atoms

Table S4 - (An)isotropic Thermal Parameters
for: S641E MOKA 60KV150MA 22C MON 030492

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
O(1)	0.0730(18)	0.0523(15)	0.0412(15)	0.0054(11)	0.0031(13)	-0.0289(13)
O(2)	0.0520(15)	0.0427(13)	0.0344(14)	-0.0026(10)	-0.0004(12)	-0.0148(12)
C(1)	0.041(2)	0.0323(17)	0.041(2)	-0.0020(15)	-0.0040(17)	-0.0113(16)
C(2)	0.038(2)	0.0353(18)	0.039(2)	0.0041(16)	0.0002(17)	-0.0042(17)
C(3)	0.039(2)	0.0330(19)	0.037(2)	-0.0022(15)	-0.0009(18)	-0.0048(17)
C(4)	0.052(2)	0.0429(19)	0.036(2)	-0.0041(15)	-0.0034(17)	-0.0149(18)
C(5)	0.056(2)	0.042(2)	0.039(2)	-0.0012(15)	-0.0046(18)	-0.0064(18)
C(6)	0.056(2)	0.044(2)	0.048(2)	-0.0041(16)	-0.0052(19)	-0.0053(19)
C(7)	0.069(3)	0.050(2)	0.036(2)	-0.0050(16)	-0.007(2)	-0.007(2)
C(8)	0.065(3)	0.050(2)	0.044(2)	-0.0086(16)	-0.007(2)	-0.005(2)
C(9)	0.073(3)	0.055(2)	0.044(2)	-0.0109(18)	-0.010(2)	-0.004(2)
C(10)	0.067(3)	0.061(2)	0.051(2)	-0.0142(18)	-0.009(2)	-0.004(2)
C(11)	0.073(3)	0.075(3)	0.045(3)	-0.016(2)	-0.013(2)	0.000(2)
C(12)	0.093(4)	0.087(3)	0.062(3)	-0.031(2)	-0.018(3)	-0.012(3)
C(13)	0.122(5)	0.157(5)	0.078(4)	-0.053(4)	-0.027(4)	-0.003(4)

=====
The Temperature Factor has the Form of $\text{Exp}(-T)$ Where
 $T = 8 * (\text{Pi}^{**2}) * U * (\text{Sin}(\text{Theta}) / \text{Lambda})^{**2}$ for Isotropic Atoms
 $T = 2 * (\text{Pi}^{**2}) * \text{Sum}ij(h(i) * h(j) * U(i,j) * \text{Astar}(i) * \text{Astar}(j))$, for
Anisotropic Atoms. $\text{Astar}(i)$ are Reciprocal Axial Lengths and
 $h(i)$ are the Reflection Indices.

E-1105-17

Table S5 - Bond Distances (Angstrom)
for: S641E MOKA 60KV150MA 22C MON 030492

O(1)	-C(2)	1.217(4)	C(5)	-H(52)	0.980(5)
O(2)	-C(3)	1.338(4)	C(6)	-H(61)	0.980(5)
O(2)	-C(4)	1.447(4)	C(6)	-H(62)	0.980(5)
C(1)	-C(2)	1.445(4)	C(7)	-H(71)	0.980(5)
C(1)	-C(3)a	1.339(4)	C(7)	-H(72)	0.980(5)
C(2)	-C(3)	1.501(4)	C(8)	-H(81)	0.980(5)
C(4)	-C(5)	1.489(4)	C(8)	-H(82)	0.980(5)
C(5)	-C(6)	1.521(5)	C(9)	-H(91)	0.980(5)
C(6)	-C(7)	1.519(5)	C(9)	-H(92)	0.980(5)
C(7)	-C(8)	1.512(5)	C(10)	-H(101)	0.980(5)
C(8)	-C(9)	1.516(5)	C(10)	-H(102)	0.980(5)
C(9)	-C(10)	1.512(5)	C(11)	-H(111)	0.980(5)
C(10)	-C(11)	1.498(5)	C(11)	-H(112)	0.980(5)
C(11)	-C(12)	1.510(5)	C(12)	-H(121)	0.980(6)
C(12)	-C(13)	1.516(6)	C(12)	-H(122)	0.980(6)
C(1)	-H(11)	0.980(4)	C(13)	-H(131)	0.980(7)
C(4)	-H(41)	0.980(5)	C(13)	-H(132)	0.980(7)
C(4)	-H(42)	0.980(5)	C(13)	-H(133)	0.980(8)
C(5)	-H(51)	0.980(5)			

Table S6 - Bond Angles (Degrees)
for: S641E MOKA 60KV150MA 22C MON 030492

C(3)	-O(2)	-C(4)	116.5(2)	C(5)	-C(6)	-H(61)	108.4(3)
C(2)	-C(1)	-C(3)a	121.1(3)	C(5)	-C(6)	-H(62)	108.1(4)
O(1)	-C(2)	-C(1)	122.2(3)	C(7)	-C(6)	-H(61)	108.7(4)
O(1)	-C(2)	-C(3)	119.8(3)	C(7)	-C(6)	-H(62)	108.0(3)
C(1)	-C(2)	-C(3)	118.0(3)	H(61)	-C(6)	-H(62)	109.5(4)
O(2)	-C(3)	-C(2)	112.3(2)	C(6)	-C(7)	-H(71)	108.8(4)
O(2)	-C(3)	-C(1)a	126.8(3)	C(6)	-C(7)	-H(72)	108.1(3)
C(1)a	-C(3)	-C(2)	120.8(3)	C(8)	-C(7)	-H(71)	108.5(3)
O(2)	-C(4)	-C(5)	109.0(3)	C(8)	-C(7)	-H(72)	108.4(4)
C(4)	-C(5)	-C(6)	110.5(3)	H(71)	-C(7)	-H(72)	109.5(4)
C(5)	-C(6)	-C(7)	114.3(3)	C(7)	-C(8)	-H(81)	108.1(4)
C(6)	-C(7)	-C(8)	113.5(3)	C(7)	-C(8)	-H(82)	108.3(3)
C(7)	-C(8)	-C(9)	114.5(3)	C(9)	-C(8)	-H(81)	108.3(3)
C(8)	-C(9)	-C(10)	114.6(3)	C(9)	-C(8)	-H(82)	108.1(4)
C(9)	-C(10)	-C(11)	115.5(3)	H(81)	-C(8)	-H(82)	109.5(4)
C(10)	-C(11)	-C(12)	114.0(3)	C(8)	-C(9)	-H(91)	108.1(4)
C(11)	-C(12)	-C(13)	113.9(4)	C(8)	-C(9)	-H(92)	108.4(3)
C(2)	-C(1)	-H(11)	119.5(3)	C(10)	-C(9)	-H(91)	108.1(3)
C(3)a	-C(1)	-H(11)	119.4(4)	C(10)	-C(9)	-H(92)	108.1(4)
O(2)	-C(4)	-H(41)	109.5(3)	H(91)	-C(9)	-H(92)	109.5(4)
O(2)	-C(4)	-H(42)	109.7(3)	C(9)	-C(10)	-H(101)	107.9(4)
C(5)	-C(4)	-H(41)	109.6(3)	C(9)	-C(10)	-H(102)	107.9(4)
C(5)	-C(4)	-H(42)	109.6(3)	C(11)	-C(10)	-H(101)	107.9(4)
H(41)	-C(4)	-H(42)	109.5(4)	C(11)	-C(10)	-H(102)	108.1(4)
C(4)	-C(5)	-H(51)	109.3(3)	H(101)	-C(10)	-H(102)	109.5(4)
C(4)	-C(5)	-H(52)	109.4(4)	C(10)	-C(11)	-H(111)	108.4(4)
C(6)	-C(5)	-H(51)	109.0(4)	C(10)	-C(11)	-H(112)	108.2(4)
C(6)	-C(5)	-H(52)	109.3(3)	C(12)	-C(11)	-H(111)	108.5(4)
H(51)	-C(5)	-H(52)	109.5(4)	C(12)	-C(11)	-H(112)	108.2(4)

Table S6 - Bond Angles (Degrees) (continued)
for: S641E MOKA 60KV150MA 22C MON 030492

H(111) -C(11) -H(112)	109.5(4)	C(12) -C(13) -H(131)	109.9(5)
C(11) -C(12) -H(121)	108.6(5)	C(12) -C(13) -H(132)	109.4(5)
C(11) -C(12) -H(122)	108.3(4)	C(12) -C(13) -H(133)	109.1(5)
C(13) -C(12) -H(121)	108.2(5)	H(131) -C(13) -H(132)	109.5(6)
C(13) -C(12) -H(122)	108.3(5)	H(131) -C(13) -H(133)	109.5(7)
H(121) -C(12) -H(122)	109.5(5)	H(132) -C(13) -H(133)	109.5(7)

I-1105-19

L.I.S.T.I.N.G O.F

O.B.S.E.R.V.E.D A.N.D C.A.L.C.U.L.A.T.E.D

S.T.R.U.C.T.U.R.E. F.A.C.T.O.R.S

F.O.R

S842A MOKA 60KV150MA LNT MON 160393

BELONGING TO THE PAPER

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

by

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Kooijman,
Nora Veldman and Anthony L. Spek

----- COMPOUND 1(3) -----

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	0	0	262	267	-3	-4	1	16	15	0	2	1	137	143
2	0	0	118	116	-2	-4	1	46	46	1	2	1	49	48
3	0	0	37	38	-1	-4	1	75	74	2	2	1	300	292
4	0	0	63	62	0	-4	1	76	77	3	2	1	130	132
5	0	0	73	72	1	-4	1	78	76	4	2	1	14	9
-5	1	0	18	14	2	-4	1	54	54	5	2	1	20	21
-4	1	0	39	36	3	-4	1	12	11	-4	3	1	32	27
-3	1	0	117	112	4	-4	1	18	15	-3	3	1	12	6
-2	1	0	64	64	-4	-3	1	37	38	-2	3	1	53	51
-1	1	0	342	334	-3	-3	1	16	17	-1	3	1	44	43
0	1	0	109	115	-2	-3	1	44	43	0	3	1	69	74
1	1	0	513	516	-1	-3	1	117	114	1	3	1	156	152
2	1	0	122	117	0	-3	1	188	187	2	3	1	39	39
3	1	0	22	22	-4	-2	1	49	50	3	3	1	91	93
4	1	0	16	12	-3	-2	1	83	83	4	3	1	61	63
-4	2	0	47	43	-2	-2	1	19	18	-4	4	1	54	51
-3	2	0	71	68	-1	-2	1	44	41	-2	4	1	49	49
-2	2	0	38	38	0	-2	1	172	171	-1	4	1	143	143
-1	2	0	33	32	1	-2	1	200	189	0	4	1	14	13
0	2	0	162	167	2	-2	1	131	120	1	4	1	16	13
1	2	0	54	51	3	-2	1	103	99	2	4	1	77	76
2	2	0	47	43	5	-2	1	15	15	3	4	1	23	22
3	2	0	14	12	-4	-1	1	17	14	-3	5	1	47	44
4	2	0	38	38	-3	-1	1	19	17	-2	5	1	33	33
-3	3	0	35	36	-2	-1	1	48	47	-1	5	1	30	29
-2	3	0	97	95	-1	-1	1	16	17	0	5	1	75	75
-1	3	0	100	97	0	-1	1	75	78	1	5	1	39	40
0	3	0	149	150	1	-1	1	83	77	2	5	1	61	62
1	3	0	60	60	2	-1	1	34	31	3	5	1	30	29
2	3	0	34	34	3	-1	1	62	59	-2	6	1	28	24
3	3	0	55	56	4	-1	1	88	86	1	6	1	18	15
4	3	0	48	47	-5	0	1	71	72	2	6	1	20	16
-4	4	0	53	55	-4	0	1	19	17	-1	-6	2	23	24
-2	4	0	14	11	-2	0	1	129	126	0	-6	2	15	17
-1	4	0	15	15	-1	0	1	283	283	-3	-5	2	21	20
0	4	0	91	93	0	0	1	220	236	-2	-5	2	34	33
1	4	0	129	129	1	0	1	46	47	-1	-5	2	24	23
2	4	0	19	18	2	0	1	89	86	0	-5	2	36	36
3	4	0	31	31	3	0	1	37	36	1	-5	2	19	23
-3	5	0	27	30	4	0	1	28	27	2	-5	2	22	18
-1	5	0	19	18	-5	1	1	102	101	3	-5	2	38	40
0	5	0	43	44	-4	1	1	130	126	-4	-4	2	21	22
1	5	0	11	13	-3	1	1	13	13	-3	-4	2	36	37
2	5	0	60	62	-2	1	1	31	32	-2	-4	2	47	47
3	5	0	20	24	-1	1	1	78	75	-1	-4	2	44	43
-2	6	0	24	23	0	1	1	340	375	0	-4	2	12	10
0	6	0	28	27	1	1	1	530	528	2	-4	2	31	35
1	6	0	21	18	2	1	1	146	145	3	-4	2	14	10
2	6	0	27	26	3	1	1	34	35	4	-4	2	56	56
0	-6	1	38	39	5	1	1	44	44	-4	-3	2	29	27
2	-6	1	67	67	-5	2	1	27	26	-3	-3	2	31	32
-1	-5	1	47	48	-4	2	1	89	84	-2	-3	2	24	21
0	-5	1	42	41	-3	2	1	97	90	-1	-3	2	48	49
1	-5	1	72	73	-2	2	1	65	60	0	-3	2	27	25
3	-5	1	67	71	-1	2	1	87	89	1	-3	2	61	58

F-1105-20

Table with 10 columns: H, K, L, 10Fo, 10Fc. It contains 10 rows of data for each column, showing various numerical values and their relationships.

Table with 10 columns: H, K, L, 10Fo, 10Fc. It contains 10 rows of data for each column, showing various numerical values and their relationships.

J-1105-21

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	4	5	31	30	0	1	6	220	221	1	-2	7	93	98
-2	5	5	23	24	1	1	6	47	47	2	-2	7	99	101
-1	5	5	90	91	2	1	6	50	49	3	-2	7	36	38
0	5	5	91	93	3	1	6	54	52	-4	-1	7	13	15
2	5	5	19	14	-3	2	6	45	46	-3	-1	7	21	22
-2	6	5	16	16	-2	2	6	65	68	-2	-1	7	77	78
0	6	5	85	84	-1	2	6	62	58	-1	-1	7	14	11
1	6	5	59	62	0	2	6	19	18	0	-1	7	29	29
2	6	5	23	20	1	2	6	40	44	1	-1	7	40	38
-2	-5	6	74	71	2	2	6	26	23	2	-1	7	26	27
-1	-5	6	96	93	3	2	6	23	23	-4	0	7	27	31
0	-5	6	11	2	4	2	6	20	19	-3	0	7	57	59
1	-5	6	41	39	-4	3	6	22	21	-2	0	7	55	56
-1	-4	6	88	88	-3	3	6	42	43	-1	0	7	166	166
0	-4	6	134	135	-2	3	6	23	22	0	0	7	141	133
1	-4	6	22	27	-1	3	6	42	46	1	0	7	99	96
2	-4	6	12	10	0	3	6	49	46	2	0	7	20	21
3	-4	6	23	22	1	3	6	42	40	3	0	7	28	29
-3	-3	6	32	34	2	3	6	33	31	4	0	7	21	20
-1	-3	6	31	32	3	3	6	15	19	5	0	7	18	24
0	-3	6	89	89	4	3	6	17	19	-4	1	7	95	97
1	-3	6	76	80	-3	4	6	19	15	-3	1	7	25	28
2	-3	6	14	12	-2	4	6	50	52	-2	1	7	59	60
3	-3	6	11	10	1	4	6	62	55	-1	1	7	21	22
-4	-2	6	26	26	2	4	6	52	49	0	1	7	34	34
-3	-2	6	50	52	3	4	6	37	40	1	1	7	95	89
-2	-2	6	24	21	-1	5	6	12	9	2	1	7	136	136
-1	-2	6	101	97	0	5	6	39	35	4	1	7	41	40
0	-2	6	34	34	1	5	6	12	7	-4	2	7	17	19
1	-2	6	83	90	2	5	6	41	36	-3	2	7	42	43
2	-2	6	26	27	3	5	6	32	31	-2	2	7	32	30
3	-2	6	55	54	0	6	6	31	35	-1	2	7	12	10
-4	-1	6	14	17	1	6	6	74	73	0	2	7	31	29
-3	-1	6	26	25	2	6	6	23	22	1	2	7	126	128
-2	-1	6	26	27	0	-5	7	55	55	3	2	7	78	80
-1	-1	6	123	116	1	-5	7	33	36	5	2	7	22	27
0	-1	6	237	238	2	-5	7	25	28	-4	3	7	16	19
1	-1	6	24	28	-3	-4	7	18	15	-2	3	7	38	37
2	-1	6	75	77	-2	-4	7	38	36	-1	3	7	85	90
3	-1	6	61	63	-1	-4	7	113	114	0	3	7	82	84
4	-1	6	47	48	0	-4	7	85	86	1	3	7	46	44
-5	0	6	34	38	1	-4	7	48	48	2	3	7	89	90
-4	0	6	22	22	2	-4	7	28	29	4	3	7	30	30
-3	0	6	14	13	3	-4	7	36	36	-3	4	7	33	28
-1	0	6	122	122	-3	-3	7	16	16	-2	4	7	48	48
0	0	6	157	157	-2	-3	7	19	20	-1	4	7	63	67
1	0	6	252	250	-1	-3	7	21	19	0	4	7	65	72
2	0	6	59	60	0	-3	7	153	155	1	4	7	82	80
3	0	6	42	42	1	-3	7	139	147	2	4	7	36	39
4	0	6	31	29	4	-3	7	16	14	3	4	7	15	13
5	0	6	17	9	-4	-2	7	37	36	-2	5	7	47	47
-4	1	6	12	14	-3	-2	7	33	35	-1	5	7	60	60
-3	1	6	15	16	-2	-2	7	33	33	0	5	7	39	39
-2	1	6	44	43	-1	-2	7	15	15	1	5	7	13	14
-1	1	6	19	21	0	-2	7	27	28	2	5	7	44	43

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	6	7	25	22	1	2	8	50	49	-4	1	9	19	20
1	6	7	23	25	2	2	8	103	103	-3	1	9	85	86
-1	-5	8	25	23	3	2	8	76	76	-1	1	9	54	56
1	-5	8	35	34	4	2	8	27	28	0	1	9	10	6
-2	-4	8	24	22	-4	3	8	38	43	1	1	9	49	51
-1	-4	8	32	31	-3	3	8	24	22	2	1	9	21	19
0	-4	8	12	13	-2	3	8	65	67	3	1	9	49	50
1	-4	8	16	16	-1	3	8	28	31	4	1	9	40	42
2	-4	8	34	35	0	3	8	25	26	-4	2	9	15	17
-3	-3	8	33	29	1	3	8	50	53	-3	2	9	66	69
-2	-3	8	35	36	2	3	8	24	22	-2	2	9	57	59
-1	-3	8	52	51	3	3	8	60	62	-1	2	9	24	26
0	-3	8	68	69	4	3	8	43	47	0	2	9	94	95
1	-3	8	73	75	-3	4	8	41	43	1	2	9	104	102
2	-3	8	39	37	-2	4	8	48	48	2	2	9	25	26
3	-3	8	47	44	1	4	8	14	16	3	2	9	22	23
-4	-2	8	102	102	3	4	8	29	28	4	2	9	38	39
-3	-2	8	51	50	0	5	8	28	29	-3	3	9	41	44
-2	-2	8	15	13	1	5	8	37	34	-2	3	9	116	119
-1	-2	8	23	22	2	5	8	28	27	0	3	9	69	70
0	-2	8	19	19	3	5	8	37	36	1	3	9	90	90
1	-2	8	173	179	-1	6	8	22	24	2	3	9	79	77
2	-2	8	174	179	0	6	8	48	46	3	3	9	19	21
3	-2	8	20	17	-2	-4	9	58	57	4	3	9	27	30
4	-2	8	38	37	-1	-4	9	54	50	-3	4	9	47	48
-4	-1	8	21	21	2	-4	9	68	69	-2	4	9	22	24
-3	-1	8	65	67	-1	-3	9	23	24	-1	4	9	99	104
-2	-1	8	69	69	0	-3	9	50	50	0	4	9	11	9
-1	-1	8	90	88	1	-3	9	14	14	1	4	9	40	43
0	-1	8	32	30	2	-3	9	16	18	-2	5	9	53	56
1	-1	8	80	83	3	-3	9	30	30	0	5	9	23	24
2	-1	8	152	154	-3	-2	9	20	21	2	5	9	22	19
3	-1	8	142	144	-2	-2	9	33	30	0	6	9	18	15
-4	0	8	26	26	-1	-2	9	38	37	1	6	9	39	34
-2	0	8	48	50	0	-2	9	66	66	0	-4	10	24	24
-1	0	8	12	12	1	-2	9	42	45	1	-4	10	17	17
0	0	8	104	107	2	-2	9	15	6	2	-4	10	42	39
1	0	8	71	71	3	-2	9	35	34	-3	-3	10	41	42
2	0	8	68	68	-4	-1	9	57	56	-2	-3	10	61	59
3	0	8	68	68	-3	-1	9	153	155	-1	-3	10	38	39
4	0	8	38	39	-2	-1	9	66	65	0	-3	10	58	56
-4	1	8	60	62	-1	-1	9	37	39	2	-3	10	13	11
-3	1	8	18	18	0	-1	9	29	29	3	-3	10	76	74
-2	1	8	11	13	1	-1	9	103	105	-2	-2	10	34	34
-1	1	8	111	108	2	-1	9	143	144	0	-2	10	49	51
0	1	8	106	105	3	-1	9	84	85	1	-2	10	109	111
1	1	8	48	47	4	-1	9	16	14	3	-2	10	19	21
2	1	8	97	96	-4	0	9	58	58	4	-2	10	55	54
4	1	8	26	26	-3	0	9	36	36	-4	-1	10	35	33
5	1	8	22	19	-2	0	9	180	184	-3	-1	10	60	61
-4	2	8	33	35	-1	0	9	93	92	-2	-1	10	10	9
-3	2	8	94	99	1	0	9	16	13	-1	-1	10	17	20
-2	2	8	31	35	2	0	9	15	12	0	-1	10	81	81
-1	2	8	40	41	3	0	9	113	114	1	-1	10	12	10
0	2	8	13	10	4	0	9	107	108	2	-1	10	39	41

I-105-22

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	-1	10	25	26	-3	0	11	13	15	1	1	12	23	21
-3	0	10	92	94	-2	0	11	56	55	2	1	12	15	13
-2	0	10	145	147	-1	0	11	55	55	3	1	12	49	50
-1	0	10	24	22	0	0	11	41	42	4	1	12	25	28
1	0	10	81	80	3	0	11	37	37	-3	2	12	24	23
2	0	10	52	52	-4	1	11	27	29	-2	2	12	26	28
3	0	10	83	83	-2	1	11	53	52	-1	2	12	35	34
4	0	10	58	60	-1	1	11	157	160	0	2	12	83	80
-3	1	10	35	36	0	1	11	57	55	1	2	12	45	43
-2	1	10	81	81	1	1	11	35	38	2	2	12	24	25
-1	1	10	176	180	2	1	11	66	67	3	2	12	22	24
0	1	10	79	80	3	1	11	56	56	-3	3	12	17	14
1	1	10	23	23	-2	2	11	41	40	-2	3	12	25	25
2	1	10	12	13	-1	2	11	91	95	-1	3	12	17	19
3	1	10	23	24	0	2	11	208	211	0	3	12	62	62
4	1	10	115	114	1	2	11	32	30	1	3	12	109	107
-4	2	10	17	17	2	2	11	30	30	2	3	12	53	49
-3	2	10	16	17	3	2	11	37	36	0	4	12	40	39
-2	2	10	82	83	4	2	11	44	44	1	4	12	30	31
0	2	10	88	89	-3	3	11	41	40	2	4	12	100	100
1	2	10	95	94	-2	3	11	29	31	3	4	12	48	48
2	2	10	25	25	-1	3	11	95	98	-1	5	12	17	15
3	2	10	57	57	0	3	11	62	63	0	5	12	16	16
-2	3	10	28	30	1	3	11	140	137	1	5	12	75	75
-1	3	10	77	81	2	3	11	33	31	1	-3	13	19	19
0	3	10	52	54	-3	4	11	18	13	-2	-2	13	23	22
1	3	10	21	21	-2	4	11	21	21	-2	-1	13	16	9
2	3	10	20	18	-1	4	11	52	54	-1	-1	13	23	20
4	3	10	30	35	0	4	11	85	86	0	-1	13	27	28
-3	4	10	47	45	-2	5	11	25	27	2	-1	13	14	15
-2	4	10	25	28	-1	5	11	20	20	3	-1	13	25	20
-1	4	10	52	55	0	5	11	49	52	-3	0	13	30	30
0	4	10	35	37	1	5	11	18	21	-2	0	13	45	44
2	4	10	32	32	2	5	11	19	10	-1	0	13	24	19
3	4	10	39	37	-2	-3	12	17	9	0	0	13	20	24
-1	5	10	14	15	-1	-3	12	27	27	1	0	13	68	74
0	5	10	76	77	1	-3	12	46	44	-2	1	13	58	56
1	5	10	18	21	-2	-2	12	28	29	-1	1	13	24	20
2	5	10	40	37	-1	-2	12	26	30	0	1	13	29	31
0	6	10	17	15	0	-2	12	43	42	1	1	13	72	73
1	6	10	56	55	1	-2	12	12	2	2	1	13	87	90
0	-4	11	29	27	2	-2	12	55	53	3	1	13	14	13
-2	-3	11	35	34	-1	-1	12	75	78	-2	2	13	13	14
1	-3	11	19	19	0	-1	12	59	65	-1	2	13	51	52
2	-3	11	25	28	2	-1	12	30	29	0	2	13	48	48
-2	-2	11	46	44	3	-1	12	25	24	1	2	13	53	53
-1	-2	11	90	93	-3	0	12	30	29	2	2	13	59	57
0	-2	11	42	44	-2	0	12	13	13	3	2	13	43	44
1	-2	11	12	9	0	0	12	84	84	-2	3	13	33	36
3	-2	11	29	32	1	0	12	56	61	1	3	13	97	92
-2	-1	11	41	43	2	0	12	50	53	2	3	13	43	43
-1	-1	11	47	47	3	0	12	45	45	-2	4	13	41	37
0	-1	11	80	85	-2	1	12	12	11	-1	4	13	32	31
1	-1	11	60	64	-1	1	12	45	44	0	4	13	14	11
2	-1	11	47	48	0	1	12	20	23	1	4	13	49	48

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	4	13	90	90	-2	3	14	30	27	0	3	15	66	61
-1	5	13	31	30	0	3	14	15	15	1	3	15	27	27
1	5	13	18	22	3	3	14	25	18	2	3	15	26	27
2	-2	14	48	44	0	4	14	17	15	1	4	15	38	38
1	-1	14	37	36	2	4	14	29	31	1	-1	16	36	36
2	-1	14	21	24	0	-2	15	29	28	-1	0	16	47	41
3	-1	14	32	30	1	-2	15	44	40	0	0	16	23	20
-1	0	14	23	20	-1	-1	15	21	21	1	0	16	19	16
1	0	14	18	19	0	-1	15	46	40	-1	1	16	30	25
2	0	14	28	26	2	-1	15	29	23	0	1	16	54	45
-2	1	14	25	23	-2	0	15	27	25	2	1	16	29	26
-1	1	14	23	21	-1	0	15	53	44	-1	2	16	54	46
0	1	14	11	7	0	0	15	27	27	1	2	16	30	25
1	1	14	21	22	1	0	15	22	17	2	2	16	18	10
2	1	14	24	23	-2	1	15	33	30	-1	3	16	30	26
-2	2	14	16	13	-1	1	15	15	17	0	3	16	19	18
-1	2	14	30	28	1	1	15	21	23	0	0	17	17	16
0	2	14	35	32	2	1	15	23	26	0	1	17	57	51
1	2	14	16	13	-1	2	15	27	26	1	1	17	29	27
2	2	14	32	35	0	2	15	29	30	0	2	17	64	57
3	2	14	37	35	1	2	15	43	40	1	2	17	54	50

I-1105-23

*** H, 0, 0 ***	*** H, -6, 1 ***	0	922	856	27
1 10 10 7	-2 1 1 10	1	331	345	13
2 76 68 3	-1 1 1 10	2	36	36	1
3 3 3 7	0 0 1 7	3	1	1	7
4 5 6 1	1 0 0 10	4	4	7	1
5 9 9 1	2 1 0 10	5	5	4	1
*** H, 1, 0 ***	*** H, -5, 1 ***	*** H, 1, 1 ***			
-5 0 1 10	-3 2 2 10	-5 31 20 1			
-4 38 36 11	-2 0 1 10	-4 20 24 6			
-3 20 18 2	-1 32 32 2	-3 14 14 2			
-2 26 24 1	0 12 12 1	-2 35 36 1			
-1 125 148 4	1 1 2 7	-1 166 171 7			
0 333 348 5	2 0 0 10	0 21 25 0			
1 2645 2873 58	3 8 5 10	1 12733 11250 457			
2 180 187 31	*** H, -4, 1 ***	2 49 50 7			
3 0 1 7	-4 1 0 10	3 12 14 1			
4 0 0 1	-3 0 0 10	4 0 0 7			
5 1 0 10	-2 9 9 1	5 1 1 10			
*** H, 2, 0 ***	-1 18 18 1	*** H, 2, 1 ***			
-4 2 2 10	0 277 293 7	-4 4 6 1			
-3 40 45 6	1 26 27 2	-3 107 100 13			
-2 7 7 7	2 0 0 7	-2 41 41 1			
-1 4 2 7	3 0 0 10	-1 74 82 6			
0 214 230 3	4 8 2 10	0 62 69 2			
1 18 22 2	*** H, -3, 1 ***	1 92 94 9			
2 91 92 18	-4 0 0 10	2 845 849 59			
3 302 300 4	-3 7 5 7	3 27 29 2			
4 0 1 10	-2 2 2 7	4 0 0 10			
5 0 0 10	-1 114 105 9	5 0 0 10			
*** H, 3, 0 ***	0 64 74 1	*** H, 3, 1 ***			
-4 0 0 10	1 38 34 1	-4 3 4 10			
-3 0 0 7	2 118 125 12	-3 3 2 7			
-2 216 217 15	3 3 3 7	-2 248 256 16			
-1 203 196 3	4 0 0 10	-1 0 1 7			
0 8 7 5	*** H, -2, 1 ***	0 1 0 5			
1 59 60 1	-5 0 0 10	1 30 31 2			
2 5 3 7	-4 10 10 1	2 9 8 7			
3 24 22 1	-3 4 9 2	3 40 36 1			
4 13 10 1	-2 146 136 9	4 43 33 1			
*** H, 4, 0 ***	-1 30 30 4	*** H, 4, 1 ***			
-4 7 4 1	0 298 309 3	-4 7 3 10			
-3 0 0 10	1 0 1 7	-3 1 1 10			
-2 3 2 7	2 156 153 4	-2 2 2 7			
-1 100 101 3	3 148 141 15	-1 42 43 2			
0 86 96 3	4 1 2 10	0 56 62 3			
1 12 12 1	*** H, -1, 1 ***	1 2 3 7			
2 19 19 1	-5 1 0 10	2 7 7 7			
3 0 0 10	-4 1 1 7	3 1 0 10			
4 2 2 10	-3 1 3 7	4 6 4 10			
*** H, 5, 0 ***	-2 1270 1280 238	*** H, 5, 1 ***			
-3 11 10 10	-1 174 194 3	-3 9 11 10			
-2 0 0 10	0 3 2 5	-2 1 1 10			
-1 1 0 7	1 424 467 7	-1 1 0 7			
0 11 12 1	2 1 0 7	0 38 44 3			
1 51 52 5	3 11 11 7	1 52 58 5			
2 3 3 10	4 1 2 7	2 2 2 10			
3 1 1 10	5 1 0 10	3 2 2 10			
*** H, 6, 0 ***	*** H, 0, 1 ***	*** H, 6, 1 ***			
-2 7 3 10	-5 9 10 1	-2 8 4 10			
-1 0 0 10	-4 3 2 7	-1 1 1 10			
0 0 0 7	-3 7 6 7	0 0 0 7			
1 3 3 10	-2 3 4 7	1 2 3 10			
2 9 8 10	-1 1743 1680 22	2 2 2 10			

*** H, -6, 2 ***	0	126	146	4
-2 0 0 10	1 1 2 7			
-1 0 0 10	2 174 168 5			
0 0 0 7	3 4 5 7			
1 0 0 10	4 2 2 7			
2 12 4 10	5 0 0 10			
*** H, -5, 2 ***	*** H, 1, 2 ***	*** H, -5, 3 ***		
-3 1 1 10	-5 29 21 1	-3 6 5 10		
-2 96 103 2	-4 31 35 10	-2 7 7 10		
-1 0 0 1	-3 3 2 7	-1 0 0 7		
0 0 0 5	-2 30 27 2	0 1 0 5		
1 0 1 7	-1 13 13 7	1 2 1 7		
2 0 0 10	0 3395 3280 38	2 0 0 10		
3 4 2 10	1 67 104 13	3 8 6 10		
*** H, -4, 2 ***	2 105 111 10	*** H, -4, 3 ***		
-4 0 0 10	3 5 6 7	-4 0 0 10		
-3 0 0 10	4 0 0 7	-3 0 1 10		
-2 16 15 1	5 1 1 10	-2 5 5 7		
-1 31 31 1	*** H, 2, 2 ***	-1 424 411 5		
0 28 27 0	-4 147 183 4	0 0 0 5		
1 17 15 1	-3 29 30 4	1 1 2 7		
2 3 3 7	-2 12 11 7	2 0 1 7		
3 0 0 10	-1 74 81 6	3 0 0 10		
4 7 1 10	0 4 6 5	4 5 1 10		
*** H, -3, 2 ***	1 31 35 2	*** H, -3, 3 ***		
-4 1 0 10	2 1253 1233 38	-4 2 1 10		
-3 1 0 7	3 15 14 1	-3 0 0 7		
-2 0 0 7	4 2 1 10	-2 0 1 7		
-1 69 64 5	5 0 0 10	-1 73 63 6		
0 57 54 0	*** H, 3, 2 ***	0 468 477 4		
1 790 805 24	-4 2 3 10	1 1 1 7		
2 34 35 4	-3 33 34 2	2 3 2 7		
3 0 0 7	-2 103 106 2	3 2 3 7		
4 1 0 10	-1 47 49 6	4 0 0 10		
*** H, -2, 2 ***	0 53 57 2	*** H, -2, 3 ***		
-5 0 0 10	1 2 4 7	-5 2 1 10		
-4 25 26 1	2 15 15 1	-4 23 20 1		
-3 26 28 1	3 163 147 6	-3 5 4 7		
-2 10 8 7	4 8 9 1	-2 2 1 7		
-1 6 8 7	*** H, 4, 2 ***	-1 12 10 7		
0 341 357 3	-4 7 1 10	0 174 167 1		
1 111 116 3	-3 5 6 10	1 12 15 7		
2 17 19 1	-2 0 0 7	2 455 466 29		
3 58 55 3	-1 263 270 12	3 21 21 1		
4 1 2 10	0 1 1 5	4 0 0 10		
*** H, -1, 2 ***	1 0 0 7	*** H, -1, 3 ***		
-5 0 0 10	2 2 4 7	-5 0 0 10		
-4 0 0 1	3 3 2 10	-4 1 3 1		
-3 64 73 11	4 15 11 1	-3 52 57 11		
-2 112 117 36	*** H, 5, 2 ***	-2 140 133 31		
-1 429 423 7	-3 10 11 10	-1 1 0 7		
0 203 198 2	-2 3 2 10	0 16 18 5		
1 296 331 36	-1 2 3 7	1 344 368 55		
2 18 21 1	0 1 1 5	2 108 113 3		
3 6 7 7	1 11 12 1	3 32 34 4		
4 43 42 11	2 0 0 10	4 16 21 4		
5 0 1 10	3 1 1 10	5 0 0 10		
*** H, 0, 2 ***	*** H, 6, 2 ***	*** H, 0, 3 ***		
-5 9 8 1	-2 7 4 10	-5 7 7 1		
-4 1 0 7	-1 2 1 10	-4 0 1 7		
-3 0 0 7	0 0 0 7	-3 1 1 7		
-2 3 8 7	1 4 5 10	-2 432 421 14		
-1 5842 5271 248	2 9 9 10	-1 3059 3012 112		

7-1105-24

0	298	345	10	*** H, -6, 4 ***	2	186	191	3
1	341	328	52	-2 0 0 10	3	72	79	6
2	102	103	1	-1 0 0 10	4	14	15	2
3	23	25	2	0 1 0 7	5	4	2	10
4	2	3	7	1 9 6 10	*** H, 1, 4 ***			
5	7	5	10	*** H, -5, 4 ***	-5	9	5	1
*** H, 1, 3 ***				-3 19 16 1	-4	21	26	1
-5	9	6	1	-2 0 0 10	-3	7	6	7
-4	27	35	1	-1 3 4 7	-2	0	0	7
-3	0	0	7	0 4 3 5	-1	1171	1143	38
-2	1	2	7	1 4 2 10	0	3968	3814	34
-1	10	8	7	2 1 0 10	1	5	10	7
0	2317	2225	20	3 0 0 10	2	63	65	1
1	220	263	52	*** H, -4, 4 ***	3	16	14	1
2	33	36	1	-4 0 0 10	4	6	5	1
3	27	26	1	-3 1 1 10	5	5	4	10
4	4	5	1	-2 50 46 2	*** H, 2, 4 ***			
5	0	0	10	-1 1 1 7	-4	16	19	1
*** H, 2, 3 ***				0 4 4 5	-3	57	49	7
-4	60	72	2	1 5 4 7	-2	1	1	7
-3	79	73	8	2 8 5 7	-1	2	2	7
-2	7	6	7	3 2 0 10	0	26	26	0
-1	56	57	2	4 1 0 10	1	21	23	1
0	18	19	1	*** H, -3, 4 ***	2	30	28	1
1	629	702	45	-4 1 0 10	3	8	9	1
2	2	14	5	-3 2 1 7	4	1	1	10
3	15	15	1	-2 1 1 7	5	1	1	10
4	0	0	10	-1 8 6 7	*** H, 3, 4 ***			
5	0	0	10	0 1213 1195 10	-4	8	9	10
*** H, 3, 3 ***				1 0 0 7	-3	45	42	6
-4	4	6	10	2 8 11 7	-2	138	136	2
-3	357	336	41	3 0 1 7	-1	13	12	1
-2	30	33	1	4 0 0 10	0	29	30	1
-1	3	2	7	*** H, -2, 4 ***	1	12	12	7
0	22	24	1	-4 15 13 1	2	80	81	1
1	1	1	7	-3 16 17 2	3	2	2	7
2	22	21	1	-2 13 7 7	4	2	1	10
3	109	95	6	-1 8 9 7	*** H, 4, 4 ***			
4	3	2	10	0 100 100 1	-3	6	7	10
*** H, 4, 3 ***				1 1716 1675 96	-2	310	335	14
-4	5	1	10	2 0 0 7	-1	56	53	7
-3	3	3	10	3 0 0 7	0	1	1	5
-2	92	99	7	4 0 0 10	1	2	2	7
-1	46	47	5	*** H, -1, 4 ***	2	0	0	7
0	18	20	1	-5 0 0 10	3	8	7	10
1	9	10	1	-4 11 12 2	4	10	8	10
2	0	0	7	-3 172 186 25	*** H, 5, 4 ***			
3	5	6	10	-2 67 48 12	-3	4	4	10
4	15	11	1	-1 1 1 7	-2	2	2	10
*** H, 5, 3 ***				0 230 223 2	-1	83	91	11
-3	7	6	10	1 162 146 31	0	21	25	2
-2	4	4	10	2 191 195 10	1	5	5	7
-1	2	2	7	3 75 81 7	2	1	1	10
0	133	166	14	4 4 6 1	3	0	0	10
1	1	1	7	5 0 0 10	*** H, 6, 4 ***			
2	0	0	10	*** H, 0, 4 ***	-2	4	1	10
3	0	0	10	-5 5 4 10	-1	1	1	10
*** H, 6, 3 ***				-4 1 1 7	0	3	4	7
-2	6	4	10	-3 2 4 7	1	31	38	1
-1	3	2	10	-2 37 33 1	2	1	1	10
0	1	1	7	-1 296 294 5	*** H, -6, 5 ***			
1	7	8	10	0 34 35 1	-2	0	0	10
2	2	2	10	1 13 12 7	-1	0	0	10

0	4	3	7	*** H, 1, 5 ***	-1	0	1	10
1	0	1	10	-5 4 2 10	0	1	1	5
*** H, -5, 5 ***				-4 13 16 1	1	8	6	10
-3	2	2	10	-3 7 6 7	2	0	1	10
-2	0	0	10	-2 24 23 1	3	8	3	10
-1	1	0	7	-1 26 23 1	*** H, -4, 6 ***			
0	1	2	5	0 78 85 2	-4	0	0	10
1	5	3	10	1 9 7 7	-3	20	19	1
2	5	3	10	2 6 9 7	-2	38	35	2
3	13	9	10	3 35 32 1	-1	0	0	7
*** H, -4, 5 ***				4 32 34 2	0	4	2	5
-4	0	0	10	5 2 1 10	1	2	7	7
-3	2	1	10	*** H, 2, 5 ***	2	15	10	7
-2	39	39	2	-4 20 21 1	3	0	0	10
-1	3	2	7	-3 55 48 7	*** H, -3, 6 ***			
0	14	13	1	-2 13 14 1	-4	1	0	10
1	21	21	2	-1 24 26 1	-3	0	0	7
2	6	2	7	0 74 74 1	-2	6	5	1
3	1	0	10	1 622 747 45	-1	9	10	1
*** H, -3, 5 ***				2 2 1 7	0	20	18	0
-4	1	0	10	3 9 8 7	1	20	18	2
-3	1	0	7	4 1 0 10	2	27	28	5
-2	3	3	7	5 2 1 10	3	5	2	7
-1	204	188	17	*** H, 3, 5 ***	4	0	0	10
0	10	10	5	-4 13 14 1	*** H, -2, 6 ***			
1	42	42	4	-3 20 19 2	-4	2	3	10
2	16	18	3	-2 85 77 3	-3	2	2	7
3	10	7	7	-1 2 4 7	-2	14	7	7
4	4	2	10	0 1 1 5	-1	17	18	2
*** H, -2, 5 ***				1 14 14 1	0	827	894	8
-4	1	0	10	2 4 4 7	1	24	26	4
-3	4	2	7	3 2 1 7	2	47	42	6
-2	11	6	7	4 2 2 10	3	17	15	1
-1	18	16	2	*** H, 4, 5 ***	4	3	3	10
0	19	24	0	-3 14 13 1	*** H, -1, 6 ***			
1	1275	1227	109	-2 13 12 1	-5	2	2	10
2	0	0	7	-1 103 106 15	-4	78	112	3
3	6	7	7	0 6 5 5	-3	4	4	7
4	0	1	10	1 4 4 7	-2	6	3	7
*** H, -1, 5 ***				2 2 3 7	-1	30	29	5
-5	0	0	10	3 1 1 10	0	113	126	1
-4	10	12	1	4 2 2 10	1	23	26	6
-3	18	16	2	*** H, 5, 5 ***	2	264	252	36
-2	75	63	12	-3 1 1 10	3	0	0	7
-1	117	79	19	-2 2 3 10	4	2	3	10
0	41	43	0	-1 109 114 15	5	0	0	10
1	98	78	19	0 36 43 3	*** H, 0, 6 ***			
2	576	584	55	1 1 2 7	-5	1	1	10
3	4	4	7	2 1 0 10	-4	0	0	10
4	1	0	7	3 0 0 10	-3	131	129	14
5	0	0	10	*** H, 6, 5 ***	-2	2	1	7
*** H, 0, 5 ***				-1 1 1 10	-1	89	87	1
-5	2	2	10	0 30 31 6	0	309	355	9
-4	1	1	7	1 8 10 10	1	0	0	7
-3	17	17	2	2 1 1 10	2	70	75	9
-2	754	719	20	*** H, -6, 6 ***	3	64	71	1
-1	292	300	4	-2 0 0 10	4	5	5	1
0	0	1	5	-1 0 0 10	5	0	0	10
1	282	210	87	0 10 11 7	*** H, 1, 6 ***			
2	59	58	4	1 3 3 10	-5	1	0	10
3	111	129	7	*** H, -5, 6 ***	-4	5	5	10
4	18	20	3	-3 1 0 10	-3	4	5	7
5	0	0	10	-2 0 0 10	-2	8	6	7

K-1105-25

-1	1048	1010	39	*** H,	-4,	7	***	5	3	2	10
0	475	499	12	-4	1	0	10	*** H,	2,	7	***
1	39	45	12	-3	1	0	10	-4	0	0	10
2	25	26	3	-2	2	1	7	-3	12	11	7
3	7	6	1	-1	0	0	1	-2	18	16	1
4	27	27	2	0	1	1	5	-1	89	81	1
5	5	3	10	1	5	7	7	0	132	121	5
*** H,	2,	6	***	2	2	2	7	1	124	136	9
-4	4	3	10	3	2	1	10	2	12	13	1
-3	25	22	4	*** H,	-3,	7	***	3	1	2	7
-2	21	22	1	-4	0	1	10	4	1	0	10
-1	119	115	1	-3	0	0	7	5	2	0	10
0	46	46	2	-2	36	31	1	*** H,	3,	7	***
1	79	95	7	-1	172	156	18	-4	2	3	10
2	2	2	7	0	15	15	1	-3	1	0	7
3	2	3	7	1	7	6	7	-2	28	26	2
4	4	3	10	2	2	5	7	-1	26	28	2
5	10	6	10	3	15	14	1	0	112	107	5
*** H,	3,	6	***	4	0	0	10	1	25	35	1
-4	11	13	1	*** H,	-2,	7	***	2	20	19	1
-3	24	18	3	-4	0	1	10	3	0	0	7
-2	92	85	7	-3	0	0	7	4	1	1	10
-1	3	5	7	-2	4	3	7	*** H,	4,	7	***
0	17	18	0	-1	8	6	7	-3	24	29	1
1	0	0	7	0	47	48	0	-2	10	8	7
2	82	83	1	1	17	21	3	-1	55	53	6
3	1	0	7	2	5	4	7	0	0	0	5
4	4	1	10	3	10	11	1	1	5	6	7
*** H,	4,	6	***	4	2	2	10	2	9	9	1
-3	3	3	10	*** H,	-1,	7	***	3	3	3	10
-2	24	24	1	-5	3	1	10	4	0	0	10
-1	66	66	9	-4	1	2	10	*** H,	5,	7	***
0	0	1	5	-3	2	3	7	-3	0	0	10
1	3	2	7	-2	0	0	7	-2	0	1	10
2	0	0	7	-1	90	100	22	-1	13	10	10
3	0	0	10	0	2	3	5	0	27	32	2
4	0	0	10	1	64	59	20	1	1	0	7
*** H,	5,	6	***	2	10	10	7	2	1	1	10
-3	0	0	10	3	6	7	7	3	3	3	10
-2	7	5	10	4	5	6	1	*** H,	6,	7	***
-1	5	4	10	5	1	0	10	-1	1	0	10
0	36	44	3	*** H,	0,	7	***	0	2	2	7
1	4	4	7	-5	1	0	10	1	9	12	10
2	0	0	10	-4	5	7	1	2	2	1	10
3	0	0	10	-3	226	210	19	*** H,	-6,	8	***
*** H,	6,	6	***	-2	16	17	1	-1	2	3	10
-1	0	0	10	-1	5	2	7	0	0	0	7
0	21	21	4	0	23	28	1	1	1	0	10
1	12	13	10	1	111	78	39	*** H,	-5,	8	***
2	1	2	10	2	0	0	7	-3	0	0	10
*** H,	-6,	7	***	3	47	53	1	-2	0	0	10
-2	0	0	10	4	0	0	7	-1	0	0	10
-1	1	2	10	5	0	0	10	0	1	1	7
0	0	1	7	*** H,	1,	7	***	1	0	0	10
1	1	0	10	-4	4	5	10	2	2	2	10
*** H,	-5,	7	***	-3	1	0	7	3	0	0	10
-3	0	0	10	-2	608	534	36	*** H,	-4,	8	***
-2	0	0	10	-1	37	38	3	-4	8	6	10
-1	1	0	10	0	12	9	5	-3	4	4	10
0	0	0	5	1	93	103	23	-2	5	5	1
1	8	7	10	2	0	0	7	-1	1	0	7
2	0	0	10	3	21	24	2	0	6	4	5
3	4	2	10	4	1	0	1	1	1	1	7

2	3	2	7	2	7	8	7	3	7	7	7
3	1	0	10	3	0	0	7	4	0	0	10
*** H,	-3,	8	***	4	7	7	1	*** H,	-2,	9	***
-4	0	0	10	5	0	0	10	-4	0	0	10
-3	4	2	7	*** H,	3,	8	***	-3	5	4	7
-2	0	1	7	-4	1	1	10	-2	6	4	7
-1	6	5	7	-3	1	1	7	-1	0	0	7
0	0	0	5	-2	17	16	2	0	25	22	0
1	2	1	7	-1	7	8	7	1	0	0	7
2	5	6	7	0	129	117	10	2	14	8	7
3	3	3	7	1	49	55	1	3	1	2	7
4	9	7	10	2	14	14	1	4	4	5	10
*** H,	-2,	8	***	3	1	2	7	*** H,	-1,	9	***
-4	1	1	10	4	0	0	10	-4	1	2	10
-3	3	2	7	*** H,	4,	8	***	-3	0	0	7
-2	5	1	7	-3	1	2	10	-2	35	30	3
-1	74	73	15	-2	0	0	7	-1	21	23	3
0	456	465	4	-1	15	16	1	0	28	30	0
1	57	58	12	0	7	6	5	1	153	121	35
2	5	3	7	1	47	54	3	2	20	23	5
3	2	5	7	2	0	0	7	3	1	0	7
4	4	4	10	3	7	7	10	4	0	1	10
*** H,	-1,	8	***	4	0	0	10	5	0	0	10
-4	1	3	10	*** H,	5,	8	***	*** H,	0,	9	***
-3	0	0	7	-3	2	2	10	-4	0	0	10
-2	31	30	2	-2	12	13	10	-3	14	15	1
-1	5	5	7	-1	1	0	10	-2	1	1	7
0	10	11	5	0	17	19	1	-1	126	149	9
1	78	59	20	1	0	0	7	0	11	11	5
2	0	0	7	2	1	1	10	1	171	132	46
3	0	0	7	3	2	2	10	2	0	0	7
4	1	0	10	*** H,	6,	8	***	3	1	0	7
5	1	0	10	-1	1	1	10	4	0	0	10
*** H,	0,	8	***	0	3	2	7	5	0	0	10
-5	2	1	10	1	7	8	10	*** H,	1,	9	***
-4	13	17	1	2	1	1	10	-4	5	7	10
-3	0	0	7	*** H,	-6,	9	***	-3	19	18	2
-2	0	0	7	-1	0	0	10	-2	0	0	7
-1	12	15	7	0	2	2	7	-1	0	0	7
0	276	314	7	1	2	1	10	0	74	83	2
1	82	52	22	*** H,	-5,	9	***	1	59	56	12
2	75	67	17	-3	0	0	10	2	28	28	6
3	7	7	1	-2	1	1	10	3	28	28	4
4	0	0	7	-1	1	2	10	4	2	2	10
5	0	0	10	0	4	4	7	5	0	0	10
*** H,	1,	8	***	1	1	1	10	*** H,	2,	9	***
-4	3	4	10	2	3	2	10	-4	5	6	10
-3	7	6	7	*** H,	-4,	9	***	-3	4	4	7
-2	306	270	18	-3	6	6	10	-2	14	11	7
-1	78	74	3	-2	0	0	1	-1	109	107	5
0	9	9	5	-1	1	2	7	0	56	52	1
1	32	36	8	0	2	2	5	1	1	0	7
2	14	11	7	1	1	0	7	2	9	9	7
3	7	8	1	2	11	6	7	3	0	0	7
4	16	18	3	3	2	2	10	4	11	9	1
5	0	0	10	*** H,	-3,	9	***	*** H,	3,	9	***
*** H,	2,	8	***	-4	0	0	10	-4	2	3	10
-4	3	3	10	-3	20	15	2	-3	12	12	1
-3	7	6	7	-2	0	0	1	-2	2	1	7
-2	0	0	7	-1	31	32	5	-1	2	1	7
-1	327	334	4	0	10	9	5	0	19	27	2
0	20	18	1	1	22	16	7	1	29	29	1
1	0	0	7	2	3	2	7	2	0	0	7

J-1105-26

3	0	0	7	-4	0	0	10	0	0	1	7
4	0	0	10	-3	0	0	7	1	0	0	10
*** H,	4,	9	***	-2	47	43	3	2	0	0	10
-3	1	4	10	-1	2	1	7	3	5	5	10
-2	4	5	7	0	265	303	3	*** H,	6,	10	***
-1	7	8	7	1	72	55	16	-1	0	0	10
0	0	0	5	2	5	5	7	0	0	0	7
1	20	25	2	3	7	5	7	1	1	1	10
2	14	14	1	4	0	0	10	2	0	0	10
3	2	1	10	*** H,	0,	10	***	*** H,	-6,	11	***
4	0	0	10	-4	13	16	1	-1	0	0	10
*** H,	5,	9	***	-3	2	1	7	0	0	0	7
-2	1	1	10	-2	0	0	7	1	0	0	10
-1	0	1	10	-1	132	148	10	*** H,	-5,	11	***
0	4	6	5	0	58	64	0	-2	2	2	10
1	1	1	10	1	0	0	7	-1	2	2	10
2	17	19	1	2	31	28	9	0	1	2	6
3	1	1	10	3	4	4	7	1	0	0	10
*** H,	6,	9	***	4	0	0	10	2	0	0	10
-1	2	1	10	5	0	0	10	*** H,	-4,	11	***
0	0	0	7	*** H,	1,	10	***	-3	5	4	10
1	4	4	10	-4	2	3	10	-2	0	0	1
2	0	0	10	-3	19	15	2	-1	9	11	1
*** H,	-6,	10	***	-2	49	42	3	0	0	0	5
-1	1	1	10	-1	34	33	2	1	15	10	1
0	0	0	7	0	110	116	2	2	0	0	10
1	0	0	10	1	5	2	7	3	2	2	10
*** H,	-5,	10	***	2	80	62	14	*** H,	-3,	11	***
-3	0	0	10	3	10	11	1	-4	2	1	10
-2	2	2	10	4	1	1	10	-3	8	4	1
-1	0	0	10	5	0	0	10	-2	19	14	1
0	2	1	7	*** H,	2,	10	***	-1	1	1	7
1	1	2	10	-4	3	3	10	0	18	17	1
2	4	3	10	-3	9	8	7	1	15	13	2
*** H,	-4,	10	***	-2	2	1	7	2	82	55	11
-3	4	3	10	-1	35	31	1	3	4	3	10
-2	0	0	1	0	4	5	5	4	1	1	10
-1	3	3	7	1	55	56	1	*** H,	-2,	11	***
0	9	10	1	2	2	3	7	-4	0	1	10
1	16	12	1	3	4	5	7	-3	0	0	7
2	0	0	7	4	2	2	10	-2	13	10	1
3	4	3	10	*** H,	3,	10	***	-1	154	164	39
*** H,	-3,	10	***	-4	1	1	10	0	4	5	5
-4	1	1	10	-3	11	12	1	1	0	0	7
-3	0	0	7	-2	4	4	7	2	20	15	7
-2	39	32	2	-1	36	35	1	3	4	4	7
-1	0	0	1	0	68	57	4	4	15	15	1
0	1	1	5	1	11	13	1	*** H,	-1,	11	***
1	13	12	7	2	1	0	7	-4	0	0	7
2	14	10	7	3	2	2	7	-3	0	0	7
3	32	24	1	4	0	1	10	-2	9	9	7
4	1	0	10	*** H,	4,	10	***	-1	57	59	5
*** H,	-2,	10	***	-3	1	3	10	0	346	400	3
-4	0	0	10	-2	14	15	2	1	28	23	5
-3	2	2	7	-1	0	0	7	2	23	25	6
-2	26	20	2	0	1	0	5	3	2	2	7
-1	55	52	13	1	0	0	7	4	0	0	10
0	74	72	1	2	14	15	1	*** H,	0,	11	***
1	34	31	6	3	1	1	10	-4	0	0	10
2	13	9	7	4	0	0	10	-3	1	1	7
3	1	0	7	*** H,	5,	10	***	-2	0	1	7
4	15	15	1	-2	2	3	10	-1	210	246	12
*** H,	-1,	10	***	-1	5	5	10	0	488	512	4

1	1296	1057	241	0	0	0	7	-3	0	0	7
2	22	27	7	1	0	0	10	-2	14	14	1
3	6	6	7	2	0	0	10	-1	0	1	7
4	1	1	10	*** H,	-4,	12	***	0	1	1	5
5	0	0	10	-3	2	1	10	1	72	62	2
*** H,	1,	11	***	-2	0	1	1	2	0	0	7
-4	1	2	10	-1	12	12	1	3	43	50	4
-3	28	21	2	0	25	22	0	4	0	1	10
-2	1	1	7	1	2	0	7	*** H,	3,	12	***
-1	0	0	7	2	0	0	10	-4	0	0	10
0	202	202	2	3	0	0	10	-3	0	0	7
1	10	10	7	*** H,	-3,	12	***	-2	20	18	4
2	32	32	6	-4	0	0	10	-1	5	8	7
3	5	5	7	-3	13	10	10	0	3	4	5
4	1	0	10	-2	29	27	4	1	3	4	7
5	0	0	10	-1	4	3	7	2	2	2	7
*** H,	2,	11	***	0	19	19	1	3	0	0	7
-4	1	0	10	1	5	3	7	4	5	5	10
-3	5	4	7	2	22	19	3	*** H,	4,	12	***
-2	60	52	7	3	0	0	10	-3	0	0	10
-1	37	38	2	4	0	0	10	-2	4	4	7
0	18	19	0	*** H,	-2,	12	***	-1	1	1	7
1	31	30	1	-4	0	0	10	0	43	45	5
2	0	0	7	-3	7	8	2	1	9	11	1
3	37	39	4	-2	31	27	4	2	1	2	7
4	15	15	1	-1	94	102	25	3	0	0	10
*** H,	3,	11	***	0	1	1	5	4	0	0	10
-4	1	1	10	1	56	47	7	*** H,	5,	12	***
-3	7	5	7	2	2	1	7	-2	1	1	10
-2	3	4	7	3	114	108	26	-1	6	6	10
-1	82	72	3	4	6	4	10	0	1	1	6
0	37	34	2	*** H,	-1,	12	***	1	37	49	1
1	2	4	7	-4	0	1	10	2	14	14	1
2	6	7	7	-3	0	0	7	3	1	0	10
3	0	0	7	-2	2	1	7	*** H,	6,	12	***
4	0	0	10	-1	169	181	12	-1	0	0	10
*** H,	4,	11	***	0	256	284	3	0	3	2	7
-3	1	1	10	1	1	1	7	1	0	0	10
-2	11	13	2	2	3	4	7	*** H,	-6,	13	***
-1	3	3	7	3	8	6	7	0	0	0	7
0	50	45	5	4	0	0	10	*** H,	-5,	13	***
1	31	33	3	*** H,	0,	12	***	-2	1	1	10
2	2	3	7	-4	0	0	10	-1	18	12	10
3	0	0	10	-3	1	0	7	0	1	0	7
4	0	0	10	-2	1	1	7	1	0	0	10
*** H,	5,	11	***	-1	42	44	2	2	1	1	10
-2	1	1	10	0	354	372	3	*** H,	-4,	13	***
-1	8	7	10	1	147	121	21	-3	1	1	10
0	0	0	6	2	1	0	7	-2	0	0	1
1	0	0	10	3	4	6	7	-1	18	20	3
2	3	4	10	4	0	0	10	0	10	10	1
3	4	4	10	*** H,	1,	12	***	1	0	0	7
*** H,	6,	11	***	-4	0	0	10	2	1	0	10
-1	1	1	10	-3	0	0	7	3	0	0	10
0	2	2	7	-2	3	3	7	*** H,	-3,	13	***
1	0	0	10	-1	15	14	1	-4	2	2	10
2	0	0	10	0	172	171	2	-3	1	0	10
*** H,	-6,	12	***	1	366	284	11	-2	8	8	1
-1	0	0	10	2	407	386	76	-1	0	0	1
0	0	0	7	3	1	1	7	0	45	42	2
*** H,	-5,	12	***	4	2	2	10	1	103	91	10
-2	4	2	10	*** H,	2,	12	***	2	30	20	3
-1	1	1	10	-4	0	2	10	3	1	0	10

17-0511-7

4	0	0	10	-2	0	0	7	-3	7	5	7
*** H,	-2,	13	***	-1	28	28	1	-2	3	6	7
-4	0	1	10	0	5	4	5	-1	485	528	15
-3	8	8	3	1	0	0	7	0	23	25	1
-2	12	13	2	2	0	0	7	1	96	93	6
-1	88	94	23	3	0	0	10	2	17	12	7
0	26	26	1	*** H,	5,	13	***	3	11	13	2
1	17	14	7	-2	0	0	10	4	2	1	10
2	1	0	7	-1	0	0	10	*** H,	1,	14	***
3	1	2	7	0	1	1	6	-4	22	24	1
4	0	0	10	1	5	7	10	-3	5	4	7
*** H,	-1,	13	***	2	1	2	10	-2	4	2	7
-4	1	1	10	3	0	0	10	-1	8	11	7
-3	0	1	7	*** H,	6,	13	***	0	34	31	0
-2	50	65	7	-1	0	0	10	1	351	301	7
-1	42	42	2	0	2	1	7	2	66	72	9
0	183	216	4	1	0	0	10	3	2	2	7
1	5	3	7	*** H,	-5,	14	***	4	2	2	10
2	39	30	8	-2	14	10	10	*** H,	2,	14	***
3	1	0	7	-1	19	15	10	-4	1	1	10
4	49	45	1	0	0	0	7	-3	40	32	8
*** H,	0,	13	***	1	0	0	10	-2	1	1	7
-4	1	2	10	2	1	0	10	-1	9	10	7
-3	2	1	7	*** H,	-4,	14	***	0	0	0	5
-2	1	2	7	-3	0	0	10	1	14	12	1
-1	41	43	2	-2	1	0	1	2	269	274	4
0	971	1066	14	-1	0	0	1	3	0	1	7
1	172	157	16	0	102	94	4	4	0	0	10
2	3	2	7	1	1	0	7	*** H,	3,	14	***
3	4	6	7	2	0	0	10	-3	9	11	10
4	0	0	10	3	1	0	10	-2	65	47	10
*** H,	1,	13	***	*** H,	-3,	14	***	-1	0	0	7
-4	10	12	1	-4	0	0	10	0	2	2	5
-3	0	0	7	-3	0	0	10	1	2	3	7
-2	6	4	7	-2	4	6	1	2	0	0	7
-1	0	0	7	-1	2	2	7	3	1	0	10
0	49	51	1	0	29	31	2	4	14	12	1
1	547	452	8	1	105	87	8	*** H,	4,	14	***
2	16	21	3	2	0	0	7	-3	4	5	10
3	0	0	7	3	0	0	10	-2	6	5	7
4	0	1	10	4	0	0	10	-1	8	8	7
*** H,	2,	13	***	*** H,	-2,	14	***	0	0	0	5
-4	1	2	10	-4	1	2	10	1	0	0	7
-3	9	7	7	-3	3	4	7	2	0	0	7
-2	0	0	7	-2	1	1	7	3	0	1	10
-1	0	0	7	-1	19	24	4	*** H,	5,	14	***
0	13	15	1	0	0	0	5	-2	1	1	10
1	18	16	1	1	104	87	10	-1	1	1	10
2	52	45	1	2	99	83	14	0	17	19	3
3	99	120	12	3	35	32	8	1	14	17	1
4	0	0	10	4	1	0	10	2	0	0	10
*** H,	3,	13	***	*** H,	-1,	14	***	3	0	0	10
-4	1	2	10	-4	2	1	10	*** H,	6,	14	***
-3	3	4	10	-3	1	2	7	0	0	0	7
-2	0	0	7	-2	48	67	10	1	1	1	10
-1	2	3	7	-1	3	4	7	*** H,	-5,	15	***
0	0	0	5	0	80	87	2	-2	21	15	10
1	1	1	7	1	31	26	2	-1	13	10	10
2	10	11	1	2	10	10	7	0	0	0	7
3	3	3	7	3	0	0	7	1	0	0	10
4	20	20	1	4	3	2	10	2	3	1	10
*** H,	4,	13	***	*** H,	0,	14	***	*** H,	-4,	15	***
-3	0	1	10	-4	2	2	10	-3	0	0	10

-2	0	0	10	4	0	0	10	-2	4	5	7
-1	87	95	23	*** H,	3,	15	***	-1	9	9	7
0	45	44	2	-3	4	4	10	0	1	1	5
1	0	0	10	-2	43	39	9	1	29	25	1
2	0	0	10	-1	6	4	7	2	0	0	7
3	1	0	10	0	4	4	5	3	222	226	50
*** H,	-3,	15	***	1	0	0	7	4	2	1	10
-3	0	1	10	2	4	5	7	*** H,	0,	16	***
-2	0	0	7	3	85	98	2	-4	2	2	10
-1	1	1	7	4	0	0	10	-3	4	2	7
0	3	3	5	*** H,	4,	15	***	-2	86	96	12
1	268	236	14	-3	6	7	10	-1	35	36	1
2	3	1	7	-2	15	15	1	0	25	23	1
3	0	0	10	-1	81	76	4	1	10	12	7
*** H,	-2,	15	***	0	1	1	5	2	5	6	7
-4	0	0	10	1	1	1	7	3	24	27	4
-3	1	1	10	2	0	0	10	4	1	2	10
-2	0	0	7	3	0	0	10	*** H,	1,	16	***
-1	7	8	7	*** H,	5,	15	***	-4	11	12	1
0	22	22	1	-2	4	4	10	-3	9	7	7
1	5	4	7	-1	7	6	10	-2	6	3	7
2	294	224	36	0	18	20	4	-1	24	27	2
3	1	0	7	1	0	0	10	0	20	19	1
4	0	1	10	2	0	0	10	1	0	0	7
*** H,	-1,	15	***	3	0	0	10	2	14	16	1
-4	2	1	10	*** H,	6,	15	***	3	2	3	7
-3	19	18	1	0	0	0	7	4	3	2	10
-2	0	2	7	1	3	4	10	*** H,	2,	16	***
-1	2	1	7	*** H,	-5,	16	***	-4	4	5	10
0	20	24	1	-2	6	5	10	-3	29	24	7
1	3	4	7	-1	6	5	10	-2	18	17	4
2	76	52	12	0	1	0	7	-1	19	17	1
3	8	8	1	1	3	4	10	0	0	0	5
4	17	14	1	2	1	1	10	1	473	353	60
*** H,	0,	15	***	*** H,	-4,	16	***	2	29	32	1
-4	2	2	10	-3	0	0	10	3	1	2	7
-3	5	2	7	-2	0	0	10	4	1	1	10
-2	9	10	7	-1	72	71	23	*** H,	3,	16	***
-1	134	142	3	0	36	36	3	-3	16	16	1
0	0	0	1	1	0	0	10	-2	37	34	8
1	38	37	1	2	2	1	10	-1	15	11	7
2	12	9	7	3	2	0	10	0	4	4	5
3	7	7	2	*** H,	-3,	16	***	1	3	2	7
4	1	0	10	-3	1	0	10	2	21	24	1
*** H,	1,	15	***	-2	0	0	1	3	1	2	10
-4	16	17	1	-1	6	6	7	4	1	1	10
-3	5	4	7	0	372	371	28	*** H,	4,	16	***
-2	22	17	2	1	56	53	1	-3	6	6	10
-1	0	2	7	2	0	1	7	-2	17	15	1
0	1130	1010	28	3	1	1	10	-1	18	15	1
1	76	58	5	*** H,	-2,	16	***	0	6	5	5
2	20	24	2	-4	8	8	1	1	0	1	7
3	6	5	7	-3	5	5	10	2	0	0	10
4	2	2	10	-2	3	3	7	3	0	0	10
*** H,	2,	15	***	-1	3	2	7	*** H,	5,	16	***
-4	6	7	10	0	2	2	5	-2	3	3	10
-3	40	32	8	1	0	1	7	-1	5	5	10
-2	12	9	7	2	241	206	25	0	39	37	9
-1	4	4	7	3	4	2	10	1	2	2	10
0	13	14	1	4	0	0	10	2	0	0	10
1	6	5	7	*** H,	-1,	16	***	*** H,	5,	17	***
2	34	37	1	-4	0	0	10	-1	1	1	10
3	10	13	1	-3	4	4	7	0	1	1	7

88-1105-28

1	2	3	10	2	0	0	7	-4	4	5	10
*** H,	-4,	17	***	3	3	2	7	-3	2	2	7
-3	1	1	10	4	0	0	10	-2	208	224	33
-2	33	27	1	*** H,	3,	17	***	-1	35	38	1
-1	5	8	1	-3	0	1	10	0	10	9	5
0	10	12	1	-2	29	24	5	1	4	1	7
1	2	1	10	-1	28	23	2	2	0	0	7
2	4	5	10	0	4	4	5	3	41	49	5
3	0	0	10	1	0	0	7	4	22	26	1
*** H,	-3,	17	***	2	100	102	7	*** H,	1,	18	***
-3	0	0	10	3	6	7	10	-4	1	1	10
-2	1	1	7	4	0	0	10	-3	13	16	4
-1	0	0	7	*** H,	4,	17	***	-2	14	14	2
0	104	109	8	-2	13	12	10	-1	324	304	15
1	58	56	1	-1	25	21	1	0	3	2	5
2	0	0	10	0	10	7	5	1	2	1	7
3	3	3	10	1	1	1	7	2	1	0	7
*** H,	-2,	17	***	2	0	0	10	3	0	1	7
-4	15	16	1	3	8	9	10	4	2	2	10
-3	7	9	10	*** H,	5,	17	***	*** H,	2,	18	***
-2	2	1	7	-2	3	2	10	-3	5	5	10
-1	0	0	7	-1	22	15	10	-2	17	16	4
0	48	50	3	0	4	3	7	-1	10	9	7
1	789	767	10	1	2	2	10	0	29	24	1
2	45	38	3	2	0	0	10	1	52	41	8
3	1	1	10	*** H,	-5,	18	***	2	10	11	1
4	2	2	10	-1	0	0	10	3	0	0	10
*** H,	-1,	17	***	0	1	1	7	4	0	0	10
-4	1	1	10	1	9	12	10	*** H,	3,	18	***
-3	59	40	20	*** H,	-4,	18	***	-3	0	0	10
-2	14	18	3	-2	2	2	10	-2	12	9	7
-1	8	8	7	-1	1	1	10	-1	24	21	1
0	5	3	5	0	2	4	6	0	0	0	5
1	1	0	7	1	2	2	10	1	20	19	4
2	26	24	2	2	5	6	10	2	30	33	3
3	87	96	17	*** H,	-3,	18	***	3	0	0	10
4	2	1	10	-3	0	0	10	4	0	1	10
*** H,	0,	17	***	-2	4	4	1	*** H,	4,	18	***
-4	3	5	10	-1	128	135	38	-2	1	1	10
-3	2	1	7	0	0	0	5	-1	13	10	7
-2	60	67	9	1	5	6	7	0	15	15	1
-1	6	5	7	2	3	1	10	1	0	1	10
0	13	12	1	3	3	5	10	2	0	0	10
1	1	0	7	*** H,	-2,	18	***	3	6	6	10
2	4	4	7	-3	6	9	10	*** H,	5,	18	***
3	0	1	7	-2	0	0	7	-1	3	2	10
4	82	87	2	-1	6	6	7	0	9	7	7
*** H,	1,	17	***	0	15	18	2	1	4	4	10
-4	5	5	10	1	41	41	2	2	0	0	10
-3	6	6	7	2	40	39	2	*** H,	-5,	19	***
-2	9	7	7	3	0	0	10	-1	0	0	10
-1	161	154	10	4	2	2	10	0	0	1	7
0	100	85	5	*** H,	-1,	18	***	1	1	2	10
1	29	25	3	-4	12	16	1	*** H,	-4,	19	***
2	1	1	7	-3	49	60	2	-2	3	2	10
3	1	2	7	-2	17	22	3	-1	2	2	10
4	4	4	10	-1	5	4	7	0	0	0	7
*** H,	2,	17	***	0	1	1	5	1	1	2	10
-3	15	13	1	1	49	48	2	2	9	10	10
-2	23	20	5	2	452	394	10	*** H,	-3,	19	***
-1	2	1	7	3	25	23	1	-3	1	1	10
0	31	29	1	4	0	0	10	-2	7	6	10
1	11	10	1	*** H,	0,	18	***	-1	1	1	7

0	0	0	5	2	3	3	10	1	40	31	7
1	2	4	7	3	9	12	10	2	2	1	7
2	1	0	10	*** H,	5,	19	***	3	0	0	10
3	4	6	10	-1	1	1	10	4	0	0	10
*** H,	-2,	19	***	0	3	1	7	*** H,	3,	20	***
-3	5	5	10	1	5	5	10	-3	2	3	10
-2	2	2	7	2	0	0	10	-2	0	0	10
-1	6	5	7	*** H,	-5,	20	***	-1	16	15	1
0	281	289	20	0	0	0	7	0	9	7	5
1	1	2	7	*** H,	-4,	20	***	1	184	130	37
2	1	1	7	-2	2	1	10	2	11	12	1
3	2	1	10	-1	3	2	10	3	0	0	10
*** H,	-1,	19	***	0	0	0	7	*** H,	4,	20	***
-4	15	23	1	1	0	1	10	-2	1	1	10
-3	43	61	2	2	0	0	10	-1	1	1	10
-2	14	15	2	*** H,	-3,	20	***	0	10	10	6
-1	0	0	7	-3	3	2	10	1	0	0	10
0	10	10	5	-2	16	14	10	2	6	9	10
1	81	72	8	-1	9	11	2	3	6	8	10
2	1	2	7	0	15	18	1	*** H,	5,	20	***
3	11	10	1	1	1	1	10	-1	0	0	10
4	0	0	10	2	0	1	10	0	1	1	7
*** H,	0,	19	***	3	5	5	10	1	3	4	10
-4	9	12	10	*** H,	-2,	20	***	2	0	0	10
-3	65	56	13	-3	1	1	10	*** H,	-4,	21	***
-2	101	108	17	-2	4	3	7	-2	3	2	10
-1	23	22	1	-1	42	42	5	-1	3	3	10
0	2	1	5	0	36	39	3	0	0	1	7
1	5	6	7	1	7	6	7	1	0	0	10
2	4	2	7	2	1	3	7	2	15	18	1
3	113	123	3	3	0	0	10	*** H,	-3,	21	***
4	7	9	1	*** H,	-1,	20	***	-3	2	2	10
*** H,	1,	19	***	-3	25	37	1	-2	24	20	1
-3	11	11	10	-2	9	9	1	-1	4	5	7
-2	0	0	7	-1	8	5	7	0	8	6	6
-1	292	273	7	0	5	3	5	1	0	0	10
0	57	47	4	1	168	157	18	2	0	0	10
1	7	6	7	2	1	1	7	3	2	2	10
2	2	1	7	3	0	1	10	*** H,	-2,	21	***
3	0	0	10	4	0	1	10	-3	0	0	10
4	17	21	1	*** H,	0,	20	***	-2	8	7	7
*** H,	2,	19	***	-3	28	33	1	-1	12	14	1
-3	0	0	10	-2	98	119	19	0	11	11	1
-2	23	24	6	-1	26	24	1	1	29	29	4
-1	21	18	2	0	2	1	5	2	3	2	10
0	375	299	16	1	4	3	7	3	0	0	10
1	13	11	2	2	58	46	5	*** H,	-1,	21	***
2	0	0	7	3	0	0	10	-3	12	16	1
3	0	0	10	4	1	2	10	-2	1	2	7
4	0	0	10	*** H,	1,	20	***	-1	13	12	1
*** H,	3,	19	***	-3	25	26	1	0	76	68	6
-3	0	1	10	-2	176	173	36	1	64	56	11
-2	3	2	7	-1	110	111	3	2	15	15	1
-1	21	20	2	0	20	17	1	3	0	0	10
0	1	1	5	1	0	0	7	4	0	0	10
1	1	1	7	2	2	1	7	*** H,	0,	21	***
2	22	23	3	3	1	1	10	-3	1	2	10
3	2	3	10	4	15	17	1	-2	42	47	7
*** H,	4,	19	***	*** H,	2,	20	***	-1	15	13	1
-2	0	0	10	-3	0	0	10	0	10	6	5
-1	5	4	10	-2	14	14	3	1	0	1	7
0	11	9	6	-1	6	6	7	2	23	21	3
1	0	0	10	0	155	121	7	3	1	1	10

I-1105-29

Table with 12 columns and 48 rows of numerical data. Includes labels like '*** H, -1, 23 ***' and '*** H, 1, 22 ***' interspersed with the numbers.

Table with 12 columns and 48 rows of numerical data. Includes labels like '*** H, 0, 25 ***' and '*** H, 1, 25 ***' interspersed with the numbers.

I-1105-30

-1	0	0	10	*** H,	-1,	30	***
0	1	1	7	-1	0	0	10
1	13	20	1	0	1	1	7
2	8	17	10	1	0	1	10
*** H,	-1,	28	***	2	4	7	10
-2	1	0	10	*** H,	0,	30	***
-1	2	1	10	-1	3	3	10
0	0	0	7	0	0	0	7
1	1	1	10	1	0	0	10
2	0	0	10	2	0	0	10
*** H,	0,	28	***	*** H,	1,	30	***
-2	0	0	10	-1	0	0	10
-1	1	0	10	0	2	3	7
0	0	0	7	1	0	0	10
1	0	1	10	2	0	0	10
2	0	0	10	*** H,	2,	30	***
*** H,	1,	28	***	-1	1	0	10
-2	0	0	10	0	7	4	7
-1	3	3	10	1	4	5	10
0	4	6	7	*** H,	-1,	31	***
1	0	0	10	-1	0	0	10
2	0	1	10	0	1	1	7
*** H,	2,	28	***	1	4	10	10
-1	1	1	10	*** H,	0,	31	***
0	3	2	7	-1	4	4	10
1	4	5	10	0	0	0	7
2	1	0	10	1	2	3	10
*** H,	3,	28	***	*** H,	1,	31	***
-1	0	0	10	-1	4	3	10
0	1	1	7	0	3	3	7
1	2	3	10	1	0	0	10
*** H,	-2,	29	***	*** H,	2,	31	***
-1	1	0	10	0	0	0	7
0	0	0	7	1	2	3	10
1	0	0	10	*** H,	0,	32	***
*** H,	-1,	29	***	0	0	0	7
-1	0	0	10	1	0	1	10
0	0	0	7	*** H,	1,	32	***
1	0	0	10	0	4	6	7
2	18	28	1	1	0	0	10
*** H,	0,	29	***				
-2	0	0	10				
-1	0	0	10				
0	2	1	7				
1	0	0	10				
2	1	1	10				
*** H,	1,	29	***				
-2	0	0	10				
-1	1	1	10				
0	0	0	7				
1	0	0	10				
2	0	0	10				
*** H,	2,	29	***				
-1	0	0	10				
0	3	2	7				
1	5	8	10				
2	0	0	10				
*** H,	3,	29	***				
0	1	0	7				
1	1	2	10				
*** H,	-2,	30	***				
0	3	5	7				
1	8	20	1				

L.I.S.T.I.N.G O.F

O.B.S.E.R.V.E.D A.N.D C.A.L.C.U.L.A.T.E.D

S.T.R.U.C.T.U.R.E. F.A.C.T.O.R.S

F.O.R

S641E C(26) H(44) O(4)

BELONGING TO THE PAPER

Self-Organization of 2,5-Di-n-Alkoxy-1,4-Benzoquinones in
the Solid State: Molecular Recognition involving
Intermolecular Dipole-Dipole-, Weak C-H...O=C Hydrogen Bond-
and Van der Waals Interactions.

b y

Erik M.D. Keegstra, Valentijn van der Mieden, Jan W. Zwikker,
Leonardus W. Jenneskens, Arie Schouten, Huub Kooijman,
Nora Veldman and Anthony L. Spek

----- C O M P O U N D 1(10) -----

Fo/Fc - LISTING: S641E C(26) H(44) O(4)

Page 1

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	0	0	251	225	0	6	0	16	7	5	-1	1	16	23
2	0	0	115	106	1	6	0	10	3	-5	0	1	16	15
3	0	0	30	24	2	6	0	17	20	-4	0	1	14	12
4	0	0	14	2	-2	-6	1	32	29	-3	0	1	14	9
5	0	0	17	26	-1	-6	1	12	10	-2	0	1	59	53
-5	1	0	16	13	0	-6	1	15	5	-1	0	1	87	79
-4	1	0	18	14	1	-6	1	17	21	1	0	1	28	21
-3	1	0	32	30	2	-6	1	37	34	2	0	1	119	109
-2	1	0	125	134	-3	-5	1	40	38	3	0	1	47	47
-1	1	0	1149	1211	-2	-5	1	13	6	4	0	1	38	32
0	1	0	163	166	-1	-5	1	14	6	5	0	1	16	18
1	1	0	230	236	0	-5	1	64	66	-5	1	1	16	4
2	1	0	11	10	1	-5	1	72	73	-4	1	1	5	5
3	1	0	34	34	2	-5	1	16	1	-3	1	1	28	33
4	1	0	56	54	3	-5	1	17	4	-2	1	1	26	17
5	1	0	17	1	-4	-4	1	39	34	-1	1	1	230	234
-5	2	0	17	8	-3	-4	1	14	2	0	1	1	33	33
-4	2	0	14	9	-2	-4	1	14	8	1	1	1	132	136
-3	2	0	40	45	-1	-4	1	129	133	2	1	1	52	52
-2	2	0	391	402	0	-4	1	86	89	3	1	1	53	51
-1	2	0	70	71	1	-4	1	14	4	4	1	1	35	30
0	2	0	184	185	2	-4	1	14	14	5	1	1	15	1
1	2	0	34	32	3	-4	1	28	25	-5	2	1	17	4
2	2	0	146	154	4	-4	1	31	35	-4	2	1	7	17
3	2	0	86	86	-4	-3	1	15	4	-3	2	1	35	30
4	2	0	14	1	-3	-3	1	17	13	-2	2	1	129	130
5	2	0	17	1	-2	-3	1	180	187	-1	2	1	46	51
-5	3	0	20	2	-1	-3	1	62	66	0	2	1	124	127
-4	3	0	16	19	0	-3	1	15	9	1	2	1	79	80
-3	3	0	129	135	1	-3	1	33	32	2	2	1	127	127
-2	3	0	16	35	2	-3	1	45	44	3	2	1	55	55
-1	3	0	63	66	3	-3	1	99	106	4	2	1	14	6
0	3	0	36	34	4	-3	1	14	16	5	2	1	13	5
1	3	0	217	221	5	-3	1	17	1	-5	3	1	18	5
2	3	0	90	89	-5	-2	1	11	1	-4	3	1	34	34
3	3	0	14	7	-4	-2	1	14	13	-3	3	1	67	70
4	3	0	17	0	-3	-2	1	122	128	-2	3	1	29	28
-4	4	0	44	42	-2	-2	1	36	42	-1	3	1	83	85
-3	4	0	15	21	-1	-2	1	19	16	0	3	1	87	83
-2	4	0	19	22	0	-2	1	51	50	1	3	1	207	203
-1	4	0	14	8	1	-2	1	87	90	2	3	1	68	73
0	4	0	128	128	2	-2	1	237	248	3	3	1	14	14
1	4	0	71	72	3	-2	1	39	39	4	3	1	15	2
2	4	0	12	15	4	-2	1	14	10	-4	4	1	30	37
3	4	0	14	1	5	-2	1	16	15	-3	4	1	19	12
4	4	0	32	30	-5	-1	1	15	6	-2	4	1	38	45
-3	5	0	14	11	-4	-1	1	55	56	-1	4	1	42	45
-2	5	0	15	7	-3	-1	1	25	26	0	4	1	155	150
-1	5	0	58	57	-2	-1	1	30	32	1	4	1	65	68
0	5	0	47	47	-1	-1	1	55	57	2	4	1	22	17
1	5	0	15	14	0	-1	1	20	21	3	4	1	15	3
2	5	0	15	1	1	-1	1	447	452	4	4	1	24	19
3	5	0	22	25	2	-1	1	60	58	-3	5	1	16	19
-2	6	0	18	15	3	-1	1	44	46	-2	5	1	22	14
-1	6	0	17	18	4	-1	1	17	29	-1	5	1	91	87

I-1105-32

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	5	1	41	38	-1	-1	2	145	153	1	4	2	14	11
1	5	1	16	10	0	-1	2	319	333	2	4	2	14	19
2	5	1	15	1	1	-1	2	18	11	3	4	2	8	6
3	5	1	42	37	2	-1	2	86	84	4	4	2	16	1
-2	6	1	28	33	3	-1	2	42	48	-3	5	2	16	11
-1	6	1	16	17	4	-1	2	38	41	-2	5	2	17	36
0	6	1	14	7	5	-1	2	17	12	-1	5	2	59	60
1	6	1	16	4	-5	0	2	24	13	0	5	2	18	12
2	6	1	62	51	-4	0	2	30	22	1	5	2	10	17
-2	-6	2	47	45	-3	0	2	14	15	2	5	2	16	1
-1	-6	2	16	14	-2	0	2	70	69	3	5	2	17	13
0	-6	2	16	1	-1	0	2	588	535	-2	6	2	17	26
1	-6	2	17	8	0	0	2	9	72	-1	6	2	14	8
2	-6	2	17	10	1	0	2	197	184	0	6	2	11	8
-3	-5	2	50	46	2	0	2	139	129	1	6	2	16	7
-2	-5	2	12	11	3	0	2	89	84	2	6	2	27	15
-1	-5	2	14	2	4	0	2	46	42	-2	-6	3	44	42
0	-5	2	14	1	5	0	2	11	2	-1	-6	3	24	19
1	-5	2	15	2	-5	1	2	22	8	0	-6	3	16	11
2	-5	2	15	3	-4	1	2	10	2	1	-6	3	65	64
3	-5	2	16	1	-3	1	2	14	14	2	-6	3	11	12
-4	-4	2	40	38	-2	1	2	297	300	-3	-5	3	51	48
-3	-4	2	10	6	-1	1	2	240	243	-2	-5	3	16	18
-2	-4	2	14	7	0	1	2	177	178	-1	-5	3	23	15
-1	-4	2	24	4	1	1	2	241	242	0	-5	3	133	129
0	-4	2	10	3	2	1	2	122	124	1	-5	3	29	25
1	-4	2	14	15	3	1	2	94	95	2	-5	3	16	10
2	-4	2	14	2	4	1	2	22	6	3	-5	3	16	2
3	-4	2	15	26	5	1	2	15	1	-4	-4	3	39	40
4	-4	2	25	25	-5	2	2	17	4	-3	-4	3	17	12
-4	-3	2	15	2	-4	2	2	15	7	-2	-4	3	14	15
-3	-3	2	14	14	-3	2	2	162	163	-1	-4	3	190	192
-2	-3	2	31	17	-2	2	2	131	138	0	-4	3	49	48
-1	-3	2	22	16	-1	2	2	59	57	1	-4	3	17	27
0	-3	2	70	71	0	2	2	254	248	2	-4	3	15	9
1	-3	2	13	1	1	2	2	53	53	3	-4	3	15	13
2	-3	2	51	51	2	2	2	199	198	4	-4	3	17	9
3	-3	2	28	22	3	2	2	14	8	-4	-3	3	16	6
4	-3	2	16	15	4	2	2	12	5	-3	-3	3	15	3
5	-3	2	12	1	5	2	2	17	6	-2	-3	3	205	215
-5	-2	2	15	1	-5	3	2	18	3	-1	-3	3	66	65
-4	-2	2	26	12	-4	3	2	66	65	0	-3	3	56	56
-3	-2	2	44	35	-3	3	2	50	59	1	-3	3	13	21
-2	-2	2	52	57	-2	3	2	16	16	2	-3	3	90	92
-1	-2	2	116	118	-1	3	2	119	116	3	-3	3	16	14
0	-2	2	52	53	0	3	2	37	36	4	-3	3	16	16
1	-2	2	112	115	1	3	2	208	203	-5	-2	3	17	4
2	-2	2	13	1	2	3	2	16	5	-4	-2	3	15	11
3	-2	2	28	29	3	3	2	8	11	-3	-2	3	129	135
4	-2	2	8	11	4	3	2	15	7	-2	-2	3	51	51
5	-2	2	20	20	-4	4	2	18	28	-1	-2	3	67	68
-5	-1	2	10	7	-3	4	2	11	6	0	-2	3	44	47
-4	-1	2	28	29	-2	4	2	34	35	1	-2	3	273	279
-3	-1	2	49	52	-1	4	2	58	59	2	-2	3	57	63
-2	-1	2	68	67	0	4	2	113	114	3	-2	3	34	37

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	-2	3	13	16	4	3	3	15	19	-2	-2	4	32	30
5	-2	3	35	32	-4	4	3	14	18	-1	-2	4	95	96
-5	-1	3	16	7	-3	4	3	13	3	0	-2	4	41	40
-4	-1	3	62	66	-2	4	3	38	39	1	-2	4	140	142
-3	-1	3	35	34	-1	4	3	47	47	2	-2	4	13	5
-2	-1	3	51	50	0	4	3	14	6	3	-2	4	20	22
-1	-1	3	71	72	1	4	3	18	7	4	-2	4	15	21
0	-1	3	817	852	2	4	3	22	30	5	-2	4	23	17
1	-1	3	170	176	3	4	3	15	15	-5	-1	4	20	20
2	-1	3	58	60	4	4	3	27	22	-4	-1	4	48	46
3	-1	3	50	52	-3	5	3	15	17	-3	-1	4	29	29
4	-1	3	67	66	-2	5	3	39	39	-2	-1	4	54	55
5	-1	3	27	25	-1	5	3	15	12	-1	-1	4	44	48
-5	0	3	28	29	0	5	3	14	1	0	-1	4	503	506
-4	0	3	24	20	1	5	3	17	19	1	-1	4	30	35
-3	0	3	25	23	2	5	3	15	6	2	-1	4	49	47
-2	0	3	43	42	3	5	3	46	42	3	-1	4	47	49
-1	0	3	822	776	-2	6	3	17	10	4	-1	4	43	42
0	0	3	230	244	-1	6	3	13	1	5	-1	4	23	20
1	0	3	52	52	0	6	3	17	10	-5	0	4	28	30
2	0	3	127	122	1	6	3	16	11	-4	0	4	23	17
3	0	3	112	105	2	6	3	52	47	-3	0	4	12	9
4	0	3	46	43	-2	-6	4	47	41	-2	0	4	36	12
5	0	3	18	4	-1	-6	4	22	19	-1	0	4	615	579
-5	1	3	16	10	0	-6	4	20	23	0	0	4	32	49
-4	1	3	14	0	1	-6	4	54	55	1	0	4	155	149
-3	1	3	17	7	2	-6	4	17	15	2	0	4	104	102
-2	1	3	235	230	-3	-5	4	45	46	3	0	4	109	104
-1	1	3	137	137	-2	-5	4	28	23	4	0	4	14	16
0	1	3	10	6	-1	-5	4	35	29	5	0	4	8	7
1	1	3	128	131	0	-5	4	82	83	-5	1	4	10	8
2	1	3	131	132	1	-5	4	22	19	-4	1	4	5	11
3	1	3	46	46	2	-5	4	15	7	-3	1	4	20	6
4	1	3	19	15	3	-5	4	16	1	-2	1	4	185	180
5	1	3	17	6	-4	-4	4	40	38	-1	1	4	38	39
-5	2	3	17	6	-3	-4	4	12	23	0	1	4	196	195
-4	2	3	10	5	-2	-4	4	35	20	1	1	4	156	157
-3	2	3	88	90	-1	-4	4	76	80	2	1	4	271	268
-2	2	3	74	74	0	-4	4	10	18	3	1	4	8	6
-1	2	3	19	20	1	-4	4	11	16	4	1	4	15	20
0	2	3	97	97	2	-4	4	14	9	5	1	4	16	10
1	2	3	21	20	3	-4	4	15	2	-5	2	4	17	9
2	2	3	28	14	4	-4	4	11	0	-4	2	4	20	19
3	2	3	30	27	-4	-3	4	25	20	-3	2	4	49	51
4	2	3	15	14	-3	-3	4	31	15	-2	2	4	40	42
5	2	3	17	13	-2	-3	4	54	55	-1	2	4	52	53
-5	3	3	16	1	-1	-3	4	14	21	0	2	4	197	196
-4	3	3	36	38	0	-3	4	54	55	1	2	4	586	573
-3	3	3	35	35	1	-3	4	37	38	2	2	4	14	14
-2	3	3	14	14	2	-3	4	12	31	3	2	4	37	37
-1	3	3	78	76	3	-3	4	10	3	4	2	4	20	18
0	3	3	31	26	4	-3	4	14	13	5	2	4	16	6
1	3	3	25	21	-5	-2	4	14	13	-5	3	4	18	13
2	3	3	24	25	-4	-2	4	33	21	-4	3	4	15	2
3	3	3	25	28	-3	-2	4	57	58	-3	3	4	14	17

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	3	4	14	3	2	-3	5	87	88	3	2	5	48	47
-1	3	4	115	117	3	-3	5	7	3	4	2	5	12	16
0	3	4	465	459	4	-3	5	16	8	5	2	5	16	5
1	3	4	12	12	-5	-2	5	18	12	-5	3	5	13	17
2	3	4	47	47	-4	-2	5	122	124	-4	3	5	16	4
3	3	4	22	25	-3	-2	5	86	90	-3	3	5	10	5
4	3	4	14	9	-2	-2	5	20	23	-2	3	5	14	11
-4	4	4	16	9	-1	-2	5	12	4	-1	3	5	34	38
-3	4	4	10	2	0	-2	5	75	79	0	3	5	149	144
-2	4	4	37	38	1	-2	5	202	202	1	3	5	83	83
-1	4	4	234	234	2	-2	5	16	15	2	3	5	58	59
0	4	4	14	6	3	-2	5	14	15	3	3	5	29	34
1	4	4	42	39	4	-2	5	10	17	4	3	5	15	2
2	4	4	21	27	5	-2	5	13	3	-4	4	5	17	5
3	4	4	15	3	-5	-1	5	59	65	-3	4	5	15	11
4	4	4	46	40	-4	-1	5	56	60	-2	4	5	33	32
-3	5	4	16	4	-3	-1	5	13	5	-1	4	5	64	61
-2	5	4	102	105	-2	-1	5	10	6	0	4	5	40	47
-1	5	4	28	1	-1	-1	5	293	292	1	4	5	38	41
0	5	4	22	19	0	-1	5	307	308	2	4	5	31	42
1	5	4	20	25	1	-1	5	13	10	3	4	5	10	10
2	5	4	32	30	2	-1	5	33	34	4	4	5	40	35
3	5	4	55	51	3	-1	5	30	33	-3	5	5	17	9
-2	6	4	17	5	4	-1	5	17	12	-2	5	5	29	27
-1	6	4	17	3	5	-1	5	17	0	-1	5	5	21	17
0	6	4	12	16	-5	0	5	35	33	0	5	5	22	17
1	6	4	40	41	-4	0	5	14	7	1	5	5	15	28
2	6	4	52	46	-3	0	5	8	4	2	5	5	16	4
-2	-6	5	36	33	-2	0	5	269	244	3	5	5	46	41
-1	-6	5	18	17	-1	0	5	211	199	-2	6	5	17	3
0	-6	5	55	55	0	0	5	12	52	-1	6	5	11	5
1	-6	5	13	34	1	0	5	66	69	0	6	5	11	12
2	-6	5	17	14	2	0	5	75	73	1	6	5	17	9
-3	-5	5	40	38	3	0	5	71	73	2	6	5	44	38
-2	-5	5	28	24	4	0	5	14	4	-2	-6	6	20	23
-1	-5	5	106	106	5	0	5	17	6	-1	-6	6	17	15
0	-5	5	49	50	-5	1	5	8	5	0	-6	6	69	71
1	-5	5	20	17	-4	1	5	14	0	1	-6	6	46	44
2	-5	5	16	4	-3	1	5	132	130	2	-6	6	23	17
3	-5	5	16	11	-2	1	5	70	67	-3	-5	6	14	30
-4	-4	5	29	34	-1	1	5	8	2	-2	-5	6	11	22
-3	-4	5	30	25	0	1	5	26	31	-1	-5	6	135	135
-2	-4	5	163	163	1	1	5	74	72	0	-5	6	83	82
-1	-4	5	75	76	2	1	5	193	189	1	-5	6	15	21
0	-4	5	21	22	3	1	5	14	15	2	-5	6	14	9
1	-4	5	14	11	4	1	5	14	21	3	-5	6	29	27
2	-4	5	15	4	5	1	5	19	7	-4	-4	6	31	29
3	-4	5	15	7	-5	2	5	12	4	-3	-4	6	12	26
4	-4	5	17	2	-4	2	5	59	61	-2	-4	6	179	182
-4	-3	5	25	20	-3	2	5	14	19	-1	-4	6	121	121
-3	-3	5	174	176	-2	2	5	13	3	0	-4	6	14	8
-2	-3	5	91	93	-1	2	5	18	10	1	-4	6	18	18
-1	-3	5	35	34	0	2	5	42	41	2	-4	6	26	33
0	-3	5	12	21	1	2	5	278	264	3	-4	6	32	28
1	-3	5	25	25	2	2	5	54	60	4	-4	6	17	2

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-4	-3	6	23	22	-3	2	6	35	40	1	-4	7	33	39
-3	-3	6	156	164	-2	2	6	25	23	2	-4	7	10	15
-2	-3	6	118	122	-1	2	6	71	71	3	-4	7	16	22
-1	-3	6	13	10	0	2	6	81	80	4	-4	7	11	4
0	-3	6	30	31	1	2	6	12	5	-4	-3	7	19	6
1	-3	6	13	15	2	2	6	49	53	-3	-3	7	43	40
2	-3	6	51	54	3	2	6	28	30	-2	-3	7	100	101
3	-3	6	14	5	4	2	6	23	23	-1	-3	7	19	22
4	-3	6	16	1	-4	3	6	22	12	0	-3	7	71	70
-5	-2	6	22	12	-3	3	6	14	2	1	-3	7	66	58
-4	-2	6	100	101	-2	3	6	21	15	2	-3	7	36	36
-3	-2	6	81	84	-1	3	6	93	90	3	-3	7	14	11
-2	-2	6	23	22	0	3	6	10	1	4	-3	7	16	2
-1	-2	6	28	21	1	3	6	45	48	-5	-2	7	19	13
0	-2	6	42	37	2	3	6	33	38	-4	-2	7	46	44
1	-2	6	107	107	3	3	6	23	34	-3	-2	7	79	80
2	-2	6	24	23	4	3	6	39	39	-2	-2	7	34	33
3	-2	6	14	6	-4	4	6	17	0	-1	-2	7	117	115
4	-2	6	11	20	-3	4	6	15	2	0	-2	7	132	128
5	-2	6	31	23	-2	4	6	79	81	1	-2	7	86	85
-5	-1	6	54	52	-1	4	6	15	8	2	-2	7	39	37
-4	-1	6	53	53	0	4	6	28	29	3	-2	7	14	3
-3	-1	6	8	13	1	4	6	38	36	4	-2	7	28	31
-2	-1	6	11	8	2	4	6	34	36	5	-2	7	17	15
-1	-1	6	134	143	3	4	6	19	18	-5	-1	7	36	32
0	-1	6	144	138	4	4	6	31	23	-4	-1	7	50	49
1	-1	6	84	83	-3	5	6	42	46	-3	-1	7	28	29
2	-1	6	25	24	-2	5	6	16	4	-2	-1	7	65	65
3	-1	6	32	30	-1	5	6	16	14	-1	-1	7	394	399
4	-1	6	48	51	0	5	6	15	17	0	-1	7	148	153
5	-1	6	19	3	1	5	6	34	38	1	-1	7	86	84
-5	0	6	17	30	2	5	6	16	15	2	-1	7	12	8
-4	0	6	14	1	3	5	6	32	26	3	-1	7	53	51
-3	0	6	16	3	-2	6	6	17	4	4	-1	7	16	12
-2	0	6	43	24	-1	6	6	19	1	5	-1	7	18	2
-1	0	6	178	171	0	6	6	40	39	-5	0	7	17	27
0	0	6	132	139	1	6	6	17	27	-4	0	7	14	13
1	0	6	85	87	2	6	6	18	23	-3	0	7	14	13
2	0	6	48	45	-2	-6	7	12	14	-2	0	7	299	277
3	0	6	72	72	-1	-6	7	17	10	-1	0	7	133	132
4	0	6	14	4	0	-6	7	38	35	0	0	7	20	79
5	0	6	16	1	1	-6	7	40	40	1	0	7	24	27
-5	1	6	17	1	2	-6	7	17	13	2	0	7	79	75
-4	1	6	10	10	-3	-5	7	17	21	3	0	7	14	3
-3	1	6	29	25	-2	-5	7	16	13	4	0	7	14	6
-2	1	6	105	111	-1	-5	7	41	45	5	0	7	17	1
-1	1	6	87	85	0	-5	7	61	66	-5	1	7	20	3
0	1	6	166	164	1	-5	7	15	9	-4	1	7	20	10
1	1	6	60	61	2	-5	7	16	20	-3	1	7	123	122
2	1	6	78	82	3	-5	7	17	3	-2	1	7	70	67
3	1	6	22	25	-4	-4	7	26	25	-1	1	7	55	55
4	1	6	15	15	-3	-4	7	15	9	0	1	7	14	15
5	1	6	20	12	-2	-4	7	39	40	1	1	7	108	96
-5	2	6	19	4	-1	-4	7	88	93	2	1	7	11	2
-4	2	6	26	21	0	-4	7	9	6	3	1	7	8	9

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	1	7	15	6	-3	-4	8	53	50	0	1	8	81	79
5	1	7	17	8	-2	-4	8	51	52	1	1	8	87	93
-5	2	7	8	11	-1	-4	8	89	91	2	1	8	12	10
-4	2	7	49	52	0	-4	8	15	11	3	1	8	14	2
-3	2	7	25	27	1	-4	8	66	71	4	1	8	11	6
-2	2	7	32	32	2	-4	8	21	17	5	1	8	11	13
-1	2	7	15	4	3	-4	8	17	10	-5	2	8	17	6
0	2	7	328	301	4	-4	8	11	5	-4	2	8	15	13
1	2	7	12	13	-4	-3	8	52	51	-3	2	8	22	20
2	2	7	20	18	-3	-3	8	58	62	-2	2	8	31	35
3	2	7	25	22	-2	-3	8	98	102	-1	2	8	84	88
4	2	7	15	19	-1	-3	8	46	43	0	2	8	188	181
-4	3	7	12	11	0	-3	8	120	128	1	2	8	48	40
-3	3	7	13	10	1	-3	8	62	62	2	2	8	15	0
-2	3	7	14	7	2	-3	8	22	14	3	2	8	19	11
-1	3	7	151	151	3	-3	8	11	12	4	2	8	26	31
0	3	7	18	20	4	-3	8	17	1	-4	3	8	16	7
1	3	7	34	33	-5	-2	8	34	34	-3	3	8	14	2
2	3	7	34	35	-4	-2	8	50	51	-2	3	8	44	48
3	3	7	28	23	-3	-2	8	67	71	-1	3	8	111	109
4	3	7	16	9	-2	-2	8	57	55	0	3	8	33	31
-4	4	7	17	0	-1	-2	8	88	91	1	3	8	14	2
-3	4	7	18	14	0	-2	8	70	70	2	3	8	14	2
-2	4	7	82	83	1	-2	8	14	27	3	3	8	44	53
-1	4	7	11	5	2	-2	8	14	28	4	3	8	17	13
0	4	7	29	29	3	-2	8	17	2	-4	4	8	16	3
1	4	7	30	27	4	-2	8	16	25	-3	4	8	23	16
2	4	7	14	12	5	-2	8	17	5	-2	4	8	49	50
3	4	7	15	9	-5	-1	8	18	32	-1	4	8	14	11
4	4	7	14	10	-4	-1	8	44	41	0	4	8	11	3
-3	5	7	32	36	-3	-1	8	25	27	1	4	8	14	1
-2	5	7	15	0	-2	-1	8	39	40	2	4	8	33	45
-1	5	7	14	11	-1	-1	8	25	20	3	4	8	28	26
0	5	7	16	7	0	-1	8	51	53	4	4	8	17	5
1	5	7	44	43	1	-1	8	75	73	-3	5	8	17	16
2	5	7	15	12	2	-1	8	5	2	-2	5	8	16	6
3	5	7	19	10	3	-1	8	42	41	-1	5	8	14	2
-2	6	7	17	2	4	-1	8	25	10	0	5	8	15	1
-1	6	7	16	2	5	-1	8	17	1	1	5	8	16	13
0	6	7	44	39	-5	0	8	26	23	2	5	8	27	26
1	6	7	17	7	-4	0	8	14	4	3	5	8	17	8
2	6	7	20	11	-3	0	8	45	41	-2	6	8	15	1
-2	-6	8	22	6	-2	0	8	30	23	-1	6	8	17	4
-1	-6	8	10	2	-1	0	8	42	41	0	6	8	17	9
0	-6	8	21	19	0	0	8	109	129	1	6	8	17	16
1	-6	8	30	34	1	0	8	11	3	2	6	8	17	9
2	-6	8	11	7	2	0	8	59	60	-2	-6	9	17	3
-3	-5	8	16	11	3	0	8	7	4	-1	-6	9	17	4
-2	-5	8	24	24	4	0	8	13	3	0	-6	9	17	18
-1	-5	8	25	30	5	0	8	17	0	1	-6	9	19	27
0	-5	8	60	61	-5	1	8	16	1	2	-6	9	19	0
1	-5	8	16	5	-4	1	8	25	26	-3	-5	9	16	7
2	-5	8	38	37	-3	1	8	27	18	-2	-5	9	11	2
3	-5	8	17	2	-2	1	8	41	39	-1	-5	9	35	31
-4	-4	8	24	15	-1	1	8	105	96	0	-5	9	42	45

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	-5	9	16	7	-4	1	9	75	77	-1	-5	10	14	3
2	-5	9	34	30	-3	1	9	38	31	0	-5	10	25	24
3	-5	9	17	30	-2	1	9	13	3	1	-5	10	16	5
-4	-4	9	12	10	-1	1	9	40	41	2	-5	10	16	24
-3	-4	9	14	5	0	1	9	27	29	3	-5	10	17	20
-2	-4	9	40	42	1	1	9	113	108	-4	-4	10	23	9
-1	-4	9	57	61	2	1	9	51	51	-3	-4	10	57	56
0	-4	9	21	23	3	1	9	18	16	-2	-4	10	14	3
1	-4	9	60	62	4	1	9	17	11	-1	-4	10	39	40
2	-4	9	50	53	5	1	9	49	50	0	-4	10	10	8
3	-4	9	11	10	-5	2	9	18	32	1	-4	10	15	7
4	-4	9	17	7	-4	2	9	15	16	2	-4	10	24	24
-4	-3	9	11	6	-3	2	9	14	5	3	-4	10	17	2
-3	-3	9	34	38	-2	2	9	19	21	4	-4	10	17	2
-2	-3	9	63	64	-1	2	9	60	55	-4	-3	10	42	38
-1	-3	9	41	46	0	2	9	188	175	-3	-3	10	8	6
0	-3	9	109	110	1	2	9	36	37	-2	-3	10	46	47
1	-3	9	62	65	2	2	9	47	45	-1	-3	10	14	23
2	-3	9	14	4	3	2	9	10	10	0	-3	10	53	40
3	-3	9	15	12	4	2	9	74	75	1	-3	10	15	30
4	-3	9	17	1	-4	3	9	16	7	2	-3	10	8	13
-5	-2	9	18	2	-3	3	9	14	11	3	-3	10	14	4
-4	-2	9	33	28	-2	3	9	59	58	4	-3	10	22	22
-3	-2	9	45	48	-1	3	9	78	78	-5	-2	10	17	15
-2	-2	9	40	39	0	3	9	14	7	-4	-2	10	15	12
-1	-2	9	151	143	-1	3	9	42	44	-3	-2	10	34	36
0	-2	9	69	69	2	3	9	14	1	-2	-2	10	21	22
1	-2	9	22	24	3	3	9	72	73	-1	-2	10	181	171
2	-2	9	25	26	4	3	9	16	18	0	-2	10	50	47
3	-2	9	14	8	-4	4	9	10	4	1	-2	10	43	47
4	-2	9	45	44	-3	4	9	50	54	2	-2	10	14	14
5	-2	9	17	2	-2	4	9	28	31	3	-2	10	54	55
-5	-1	9	23	19	-1	4	9	14	3	4	-2	10	16	1
-4	-1	9	33	30	0	4	9	17	17	5	-2	10	16	10
-3	-1	9	17	17	1	4	9	7	1	-5	-1	10	16	11
-2	-1	9	200	184	2	4	9	29	34	-4	-1	10	25	21
-1	-1	9	24	24	3	4	9	15	28	-3	-1	10	14	3
0	-1	9	11	13	-3	5	9	11	11	-2	-1	10	260	256
1	-1	9	70	68	-2	5	9	15	3	-1	-1	10	48	47
2	-1	9	13	16	-1	5	9	15	6	0	-1	10	66	63
3	-1	9	46	44	0	5	9	19	14	1	-1	10	20	24
4	-1	9	10	7	1	5	9	15	10	2	-1	10	97	99
5	-1	9	17	1	2	5	9	28	32	3	-1	10	34	39
-5	0	9	14	15	3	5	9	17	6	4	-1	10	26	20
-4	0	9	24	10	-2	6	9	17	5	5	-1	10	17	2
-3	0	9	153	135	-1	6	9	28	25	-5	0	10	13	12
-2	0	9	46	41	0	6	9	12	4	-4	0	10	14	13
-1	0	9	11	4	1	6	9	30	26	-3	0	10	152	139
0	0	9	17	88	-2	-6	10	13	1	-2	0	10	12	7
1	0	9	12	3	-1	-6	10	25	22	-1	0	10	79	79
2	0	9	12	7	0	-6	10	11	1	0	0	10	14	42
3	0	9	15	26	1	-6	10	17	15	1	0	10	196	186
4	0	9	15	4	2	-6	10	25	1	2	0	10	102	105
5	0	9	16	6	-3	-5	10	16	4	3	0	10	11	26
-5	1	9	16	2	-2	-5	10	48	45	4	0	10	15	6

I-1105-35

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
5	0	10	7	2	-3	-5	11	17	14	5	0	11	32	23
-5	1	10	16	14	-2	-5	11	28	21	-5	1	11	17	3
-4	1	10	61	58	-1	-5	11	15	16	-4	1	11	23	1
-3	1	10	8	5	0	-5	11	21	13	-3	1	11	14	2
-2	1	10	45	42	1	-5	11	16	0	-2	1	11	55	58
-1	1	10	55	56	2	-5	11	17	5	-1	1	11	11	8
0	1	10	8	3	3	-5	11	17	9	0	1	11	206	187
1	1	10	143	144	-4	-4	11	20	18	1	1	11	32	39
2	1	10	15	25	-3	-4	11	19	17	2	1	11	55	52
3	1	10	24	26	-2	-4	11	27	17	3	1	11	16	11
4	1	10	15	12	-1	-4	11	26	23	4	1	11	60	60
5	1	10	20	1	0	-4	11	11	3	5	1	11	17	12
-5	2	10	18	21	1	-4	11	34	37	-5	2	11	18	2
-4	2	10	15	6	2	-4	11	12	17	-4	2	11	15	4
-3	2	10	12	5	3	-4	11	10	0	-3	2	11	12	17
-2	2	10	28	28	4	-4	11	19	1	-2	2	11	14	8
-1	2	10	63	59	-4	-3	11	11	11	-1	2	11	12	3
0	2	10	91	93	-3	-3	11	13	11	0	2	11	68	66
1	2	10	22	19	-2	-3	11	27	27	1	2	11	48	51
2	2	10	42	42	-1	-3	11	13	10	2	2	11	47	44
3	2	10	35	28	0	-3	11	85	86	3	2	11	114	119
4	2	10	17	17	1	-3	11	28	29	4	2	11	18	9
-4	3	10	10	2	2	-3	11	26	20	-4	3	11	10	2
-3	3	10	10	3	3	-3	11	18	0	-3	3	11	17	8
-2	3	10	25	30	4	-3	11	18	20	-2	3	11	30	24
-1	3	10	53	50	-4	-2	11	15	4	-1	3	11	35	38
0	3	10	26	22	-3	-2	11	27	27	0	3	11	23	24
1	3	10	41	41	-2	-2	11	45	49	1	3	11	61	61
2	3	10	23	27	-1	-2	11	76	74	2	3	11	132	143
3	3	10	16	24	0	-2	11	49	46	3	3	11	14	2
4	3	10	17	15	1	-2	11	77	78	4	3	11	16	13
-4	4	10	17	3	2	-2	11	14	0	-4	4	11	12	13
-3	4	10	17	14	3	-2	11	56	57	-3	4	11	23	23
-2	4	10	23	22	4	-2	11	7	9	-2	4	11	17	14
-1	4	10	14	13	-5	-1	11	12	2	-1	4	11	17	8
0	4	10	29	25	-4	-1	11	17	21	0	4	11	35	36
1	4	10	10	9	-3	-1	11	35	39	1	4	11	68	82
2	4	10	10	2	-2	-1	11	14	13	2	4	11	15	11
3	4	10	28	30	-1	-1	11	34	25	3	4	11	16	14
-3	5	10	23	8	0	-1	11	139	136	-3	5	11	17	5
-2	5	10	10	4	1	-1	11	11	6	-2	5	11	16	5
-1	5	10	15	12	2	-1	11	147	141	-1	5	11	16	11
0	5	10	20	22	3	-1	11	18	6	0	5	11	18	25
1	5	10	27	21	4	-1	11	15	14	1	5	11	15	10
2	5	10	30	31	5	-1	11	17	4	2	5	11	17	12
3	5	10	12	16	-5	0	11	10	12	3	5	11	21	18
-2	6	10	17	3	-4	0	11	19	17	-2	6	11	14	5
-1	6	10	17	12	-3	0	11	20	11	-1	6	11	17	4
0	6	10	29	22	-2	0	11	10	2	0	6	11	11	12
1	6	10	17	20	-1	0	11	105	112	1	6	11	17	9
-2	-6	11	17	2	0	0	11	14	15	-2	-6	12	17	0
-1	-6	11	17	15	1	0	11	337	320	-1	-6	12	17	11
0	-6	11	15	9	2	0	11	13	9	0	-6	12	15	17
1	-6	11	17	5	3	0	11	16	26	1	-6	12	20	0
2	-6	11	17	0	4	0	11	17	2	2	-6	12	15	19

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-3	-5	12	18	5	5	0	12	16	29	0	-5	13	15	7
-2	-5	12	20	14	-5	1	12	22	23	1	-5	13	65	68
-1	-5	12	30	31	-4	1	12	10	16	2	-5	13	14	8
0	-5	12	17	2	-3	1	12	13	1	3	-5	13	16	2
1	-5	12	39	43	-2	1	12	69	66	-3	-4	13	29	19
2	-5	12	42	43	-1	1	12	19	22	-2	-4	13	38	40
3	-5	12	17	11	0	1	12	199	190	-1	-4	13	16	15
-4	-4	12	17	12	1	1	12	62	60	0	-4	13	93	94
-3	-4	12	14	16	2	1	12	36	35	1	-4	13	10	11
-2	-4	12	40	41	3	1	12	15	18	2	-4	13	15	6
-1	-4	12	15	10	4	1	12	62	59	3	-4	13	10	8
0	-4	12	67	70	-5	2	12	18	6	4	-4	13	14	1
1	-4	12	57	60	-4	2	12	14	5	-4	-3	13	20	15
2	-4	12	14	16	-3	2	12	17	17	-3	-3	13	38	36
3	-4	12	7	2	-2	2	12	50	51	-2	-3	13	14	23
4	-4	12	18	0	-1	2	12	96	92	-1	-3	13	94	99
-4	-3	12	22	16	0	2	12	21	23	0	-3	13	22	23
-3	-3	12	32	35	1	2	12	22	24	1	-3	13	17	18
-2	-3	12	14	17	2	2	12	14	20	2	-3	13	25	26
-1	-3	12	76	84	3	2	12	69	71	3	-3	13	16	20
0	-3	12	71	74	4	2	12	15	5	4	-3	13	12	13
1	-3	12	14	17	-4	3	12	10	1	-4	-2	13	24	21
2	-3	12	17	21	-3	3	12	47	55	-3	-2	13	28	31
3	-3	12	10	9	-2	3	12	44	43	-2	-2	13	45	47
4	-3	12	60	62	-1	3	12	14	7	-1	-2	13	50	50
-4	-2	12	28	19	0	3	12	29	26	0	-2	13	34	31
-3	-2	12	24	22	1	3	12	14	5	1	-2	13	75	76
-2	-2	12	13	19	2	3	12	47	46	2	-2	13	52	56
-1	-2	12	74	71	3	3	12	15	13	3	-2	13	15	9
0	-2	12	23	23	4	3	12	16	2	4	-2	13	18	5
1	-2	12	65	66	-4	4	12	17	32	-5	-1	13	17	8
2	-2	12	14	23	-3	4	12	11	17	-4	-1	13	24	25
3	-2	12	130	130	-2	4	12	15	3	-3	-1	13	14	16
4	-2	12	15	4	-1	4	12	26	24	-2	-1	13	42	40
-5	-1	12	15	6	0	4	12	21	2	-1	-1	13	28	23
-4	-1	12	14	16	1	4	12	14	18	0	-1	13	168	156
-3	-1	12	46	38	2	4	12	15	7	1	-1	13	97	106
-2	-1	12	55	51	3	4	12	16	4	2	-1	13	16	23
-1	-1	12	39	32	-3	5	12	17	0	3	-1	13	14	7
0	-1	12	124	117	-2	5	12	16	12	4	-1	13	15	20
1	-1	12	69	70	-1	5	12	16	6	-5	0	13	17	17
2	-1	12	208	204	0	5	12	16	14	-4	0	13	15	9
3	-1	12	14	1	1	5	12	16	5	-3	0	13	19	15
4	-1	12	15	18	2	5	12	10	4	-2	0	13	12	2
5	-1	12	17	5	-2	6	12	22	9	-1	0	13	116	131
-5	0	12	19	8	-1	6	12	16	12	0	0	13	43	54
-4	0	12	41	38	0	6	12	17	10	1	0	13	22	72
-3	0	12	39	34	1	6	12	11	1	2	0	13	40	35
-2	0	12	17	4	-1	-6	13	23	13	3	0	13	31	32
-1	0	12	121	126	0	-6	13	24	21	4	0	13	27	21
0	0	12	119	111	1	-6	13	17	2	5	0	13	28	28
1	0	12	291	284	2	-6	13	42	34	-5	1	13	17	4
2	0	12	31	30	-3	-5	13	13	9	-4	1	13	19	6
3	0	12	33	33	-2	-5	13	10	18	-3	1	13	14	3
4	0	12	14	0	-1	-5	13	38	34	-2	1	13	52	53

J-1105-36

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	1	13	52	49	-2	-4	14	36	34	-4	2	14	15	1
0	1	13	177	166	-1	-4	14	22	21	-3	2	14	14	8
1	1	13	50	49	0	-4	14	16	5	-2	2	14	50	48
2	1	13	59	59	1	-4	14	14	7	-1	2	14	120	113
3	1	13	12	32	2	-4	14	15	6	0	2	14	13	11
4	1	13	62	60	3	-4	14	15	3	1	2	14	57	60
-5	2	13	18	2	4	-4	14	23	28	2	2	14	145	145
-4	2	13	15	1	-4	-3	14	16	11	3	2	14	15	9
-3	2	13	18	20	-3	-3	14	26	31	4	2	14	11	12
-2	2	13	38	40	-2	-3	14	33	35	-4	3	14	16	8
-1	2	13	129	124	-1	-3	14	30	22	-3	3	14	15	12
0	2	13	19	23	0	-3	14	18	11	-2	3	14	59	57
1	2	13	84	85	1	-3	14	14	11	-1	3	14	14	13
2	2	13	29	29	2	-3	14	14	16	0	3	14	48	46
3	2	13	81	86	3	-3	14	79	78	1	3	14	127	131
4	2	13	16	3	4	-3	14	17	5	2	3	14	14	5
-4	3	13	10	7	-4	-2	14	15	17	3	3	14	14	3
-3	3	13	15	14	-3	-2	14	32	35	4	3	14	17	10
-2	3	13	56	54	-2	-2	14	79	77	-4	4	14	17	4
-1	3	13	14	1	-1	-2	14	19	13	-3	4	14	28	25
0	3	13	64	63	0	-2	14	19	16	-2	4	14	15	2
1	3	13	15	7	1	-2	14	37	41	-1	4	14	40	35
2	3	13	67	70	2	-2	14	174	173	0	4	14	44	50
3	3	13	15	3	3	-2	14	26	33	1	4	14	15	1
4	3	13	11	1	4	-2	14	16	9	2	4	14	14	9
-4	4	13	18	2	-5	-1	14	24	6	3	4	14	14	17
-3	4	13	14	22	-4	-1	14	17	18	-3	5	14	17	3
-2	4	13	15	2	-3	-1	14	68	67	-2	5	14	20	21
-1	4	13	33	31	-2	-1	14	21	11	-1	5	14	10	1
0	4	13	28	29	-1	-1	14	18	17	0	5	14	8	6
1	4	13	11	16	0	-1	14	80	75	1	5	14	13	8
2	4	13	16	5	1	-1	14	376	364	2	5	14	17	14
3	4	13	16	10	2	-1	14	109	107	-1	6	14	11	2
-3	5	13	17	1	3	-1	14	22	24	0	6	14	13	1
-2	5	13	12	16	4	-1	14	30	21	1	6	14	13	10
-1	5	13	14	15	-5	0	14	17	4	-1	-6	15	17	5
0	5	13	15	4	-4	0	14	28	32	0	-6	15	17	6
1	5	13	16	1	-3	0	14	14	8	1	-6	15	18	24
2	5	13	25	16	-2	0	14	13	8	-3	-5	15	17	5
-2	6	13	13	5	-1	0	14	16	75	-2	-5	15	11	4
-1	6	13	19	8	0	0	14	504	462	-1	-5	15	16	11
0	6	13	12	0	1	0	14	191	188	0	-5	15	45	41
1	6	13	17	13	2	0	14	30	28	1	-5	15	35	35
-1	-6	14	13	9	3	0	14	42	46	2	-5	15	16	1
0	-6	14	17	16	4	0	14	17	15	3	-5	15	17	1
1	-6	14	13	8	-5	1	14	18	12	-3	-4	15	18	6
2	-6	14	17	7	-4	1	14	14	6	-2	-4	15	15	14
-3	-5	14	17	3	-3	1	14	8	1	-1	-4	15	53	52
-2	-5	14	14	9	-2	1	14	35	30	0	-4	15	16	16
-1	-5	14	17	26	-1	1	14	179	167	1	-4	15	10	6
0	-5	14	15	15	0	1	14	193	180	2	-4	15	10	0
1	-5	14	14	14	1	1	14	13	9	3	-4	15	18	2
2	-5	14	17	2	2	1	14	65	66	-4	-3	15	19	8
3	-5	14	17	1	3	1	14	63	66	-3	-3	15	16	13
-3	-4	14	23	10	4	1	14	24	26	-2	-3	15	40	44

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	-3	15	14	16	-2	3	15	55	53	3	-2	16	17	12
0	-3	15	17	14	-1	3	15	15	12	4	-2	16	16	7
1	-3	15	7	11	0	3	15	106	107	-4	-1	16	14	4
2	-3	15	19	13	1	3	15	171	174	-3	-1	16	14	1
3	-3	15	67	65	2	3	15	27	30	-2	-1	16	16	21
4	-3	15	17	11	3	3	15	10	11	-1	-1	16	12	9
-4	-2	15	15	6	4	3	15	17	6	0	-1	16	116	122
-3	-2	15	14	8	-4	4	15	21	21	1	-1	16	88	92
-2	-2	15	25	23	-3	4	15	16	23	2	-1	16	53	50
-1	-2	15	12	9	-2	4	15	14	6	3	-1	16	15	19
0	-2	15	32	33	-1	4	15	60	61	4	-1	16	30	27
1	-2	15	34	34	0	4	15	108	111	-5	0	16	17	2
2	-2	15	93	94	1	4	15	19	16	-4	0	16	14	1
3	-2	15	23	27	2	4	15	16	12	-3	0	16	7	11
4	-2	15	17	8	3	4	15	17	14	-2	0	16	21	11
-4	-1	15	15	8	-3	5	15	16	6	-1	0	16	23	138
-3	-1	15	14	13	-2	5	15	19	23	0	0	16	14	42
-2	-1	15	13	5	-1	5	15	48	49	1	0	16	97	102
-1	-1	15	29	32	0	5	15	16	5	2	0	16	29	32
0	-1	15	99	96	1	5	15	17	6	3	0	16	55	54
1	-1	15	85	93	2	5	15	16	23	4	0	16	117	117
2	-1	15	48	45	-1	6	15	18	3	-5	1	16	17	2
3	-1	15	14	17	0	6	15	17	0	-4	1	16	12	3
4	-1	15	15	21	-1	-6	16	17	1	-3	1	16	14	3
-5	0	15	18	10	0	-6	16	16	7	-2	1	16	71	69
-4	0	15	14	2	1	-6	16	19	4	-1	1	16	44	40
-3	0	15	14	4	-2	-5	16	16	7	0	1	16	115	108
-2	0	15	21	15	-1	-5	16	12	11	1	1	16	15	21
-1	0	15	17	58	0	-5	16	16	0	2	1	16	74	76
0	0	15	59	56	1	-5	16	16	2	3	1	16	199	201
1	0	15	24	59	2	-5	16	17	8	4	1	16	16	11
2	0	15	48	45	3	-5	16	18	4	-4	2	16	16	5
3	0	15	38	38	-3	-4	16	10	7	-3	2	16	12	28
4	0	15	40	40	-2	-4	16	17	11	-2	2	16	36	38
-5	1	15	20	1	-1	-4	16	14	12	-1	2	16	70	69
-4	1	15	15	4	0	-4	16	15	2	0	2	16	14	2
-3	1	15	14	2	1	-4	16	15	14	1	2	16	43	47
-2	1	15	14	6	2	-4	16	15	4	2	2	16	257	252
-1	1	15	60	58	3	-4	16	11	11	3	2	16	15	2
0	1	15	98	98	-4	-3	16	16	3	4	2	16	24	22
1	1	15	75	75	-3	-3	16	23	12	-4	3	16	17	3
2	1	15	67	68	-2	-3	16	14	22	-3	3	16	15	25
3	1	15	78	83	-1	-3	16	14	9	-2	3	16	30	34
4	1	15	16	18	0	-3	16	15	20	-1	3	16	14	0
-4	2	15	15	1	1	-3	16	10	3	0	3	16	14	13
-3	2	15	20	21	2	-3	16	26	28	1	3	16	196	195
-2	2	15	53	52	3	-3	16	28	33	2	3	16	16	16
-1	2	15	102	100	4	-3	16	18	3	3	3	16	25	23
0	2	15	49	54	-4	-2	16	15	9	4	3	16	17	9
1	2	15	110	114	-3	-2	16	14	15	-3	4	16	16	14
2	2	15	149	155	-2	-2	16	11	1	-2	4	16	16	2
3	2	15	16	29	-1	-2	16	26	22	-1	4	16	15	1
4	2	15	16	10	0	-2	16	13	12	0	4	16	106	109
-4	3	15	16	20	1	-2	16	48	62	1	4	16	16	8
-3	3	15	44	40	2	-2	16	71	72	2	4	16	16	11

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	4	16	17	13	-1	0	17	225	245	-1	-4	18	68	70
-3	5	16	16	6	0	0	17	15	3	0	-4	18	27	28
-2	5	16	19	13	1	0	17	18	10	1	-4	18	10	14
-1	5	16	59	55	2	0	17	26	27	2	-4	18	16	3
0	5	16	16	4	3	0	17	10	3	3	-4	18	14	1
1	5	16	12	4	4	0	17	61	60	-4	-3	18	29	22
2	5	16	17	4	-4	1	17	21	6	-3	-3	18	18	21
-1	6	16	18	5	-3	1	17	14	9	-2	-3	18	70	74
0	6	16	16	5	-2	1	17	87	86	-1	-3	18	28	34
-1	-6	17	22	9	-1	1	17	8	8	0	-3	18	21	24
0	-6	17	16	18	0	1	17	14	11	1	-3	18	15	4
1	-6	17	52	48	1	1	17	56	59	2	-3	18	15	4
-2	-5	17	22	16	2	1	17	25	35	3	-3	18	14	9
-1	-5	17	27	29	3	1	17	71	75	4	-3	18	17	7
0	-5	17	89	83	4	1	17	16	6	-4	-2	18	15	1
1	-5	17	12	16	-4	2	17	17	4	-3	-2	18	69	68
2	-5	17	16	3	-3	2	17	26	32	-2	-2	18	31	33
3	-5	17	17	1	-2	2	17	14	9	-1	-2	18	34	31
-3	-4	17	16	17	-1	2	17	25	29	0	-2	18	14	4
-2	-4	17	31	34	0	2	17	52	53	1	-2	18	15	22
-1	-4	17	110	106	1	2	17	52	51	2	-2	18	33	30
0	-4	17	25	23	2	2	17	78	87	3	-2	18	15	5
1	-4	17	15	13	3	2	17	15	5	4	-2	18	16	1
2	-4	17	14	0	4	2	17	17	20	-4	-1	18	47	43
3	-4	17	40	39	-4	3	17	17	11	-3	-1	18	13	24
-4	-3	17	14	12	-3	3	17	17	13	-2	-1	18	30	34
-3	-3	17	27	30	-2	3	17	25	22	-1	-1	18	14	6
-2	-3	17	89	94	-1	3	17	26	15	0	-1	18	51	70
-1	-3	17	23	21	0	3	17	16	14	1	-1	18	61	65
0	-3	17	27	28	1	3	17	93	98	2	-1	18	14	3
1	-3	17	14	10	2	3	17	15	3	3	-1	18	12	7
2	-3	17	120	118	3	3	17	29	25	4	-1	18	59	53
3	-3	17	13	10	-3	4	17	17	8	-4	0	18	20	14
4	-3	17	14	10	-2	4	17	15	5	-3	0	18	23	23
-4	-2	17	10	14	-1	4	17	48	47	-2	0	18	7	26
-3	-2	17	52	49	0	4	17	87	87	-1	0	18	26	48
-2	-2	17	19	13	1	4	17	15	5	0	0	18	72	75
-1	-2	17	31	33	2	4	17	34	29	1	0	18	11	19
0	-2	17	36	33	3	4	17	14	8	2	0	18	14	18
1	-2	17	231	232	-3	5	17	14	5	3	0	18	119	121
2	-2	17	10	1	-2	5	17	41	38	4	0	18	44	40
3	-2	17	20	21	-1	5	17	51	52	-4	1	18	15	12
4	-2	17	16	8	0	5	17	16	0	-3	1	18	14	19
-4	-1	17	30	22	1	5	17	29	26	-2	1	18	14	1
-3	-1	17	10	12	2	5	17	17	6	-1	1	18	16	30
-2	-1	17	31	27	0	6	17	18	15	0	1	18	32	30
-1	-1	17	40	38	0	-6	18	19	21	1	1	18	14	10
0	-1	17	361	355	1	-6	18	40	38	2	1	18	247	245
1	-1	17	14	12	-2	-5	18	26	25	3	1	18	79	79
2	-1	17	14	22	-1	-5	18	30	35	4	1	18	17	1
3	-1	17	16	13	0	-5	18	59	58	-4	2	18	23	11
4	-1	17	17	19	1	-5	18	16	19	-3	2	18	16	10
-4	0	17	24	10	2	-5	18	14	4	-2	2	18	8	3
-3	0	17	13	13	-3	-4	18	33	28	-1	2	18	14	15
-2	0	17	25	29	-2	-4	18	33	39	0	2	18	16	16

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	2	18	365	351	-4	-1	19	44	43	2	5	19	18	23
2	2	18	114	117	-3	-1	19	27	25	-2	-5	20	24	21
3	2	18	15	7	-2	-1	19	32	35	-1	-5	20	55	52
4	2	18	29	25	-1	-1	19	135	133	0	-5	20	33	35
-4	3	18	16	10	0	-1	19	76	75	1	-5	20	29	28
-3	3	18	17	2	1	-1	19	14	15	2	-5	20	7	3
-2	3	18	12	3	2	-1	19	17	4	-3	-4	20	28	25
-1	3	18	13	19	3	-1	19	7	3	-2	-4	20	58	54
0	3	18	279	275	4	-1	19	52	55	-1	-4	20	56	56
1	3	18	115	113	-4	0	19	19	14	0	-4	20	45	43
2	3	18	23	22	-3	0	19	14	19	1	-4	20	15	0
3	3	18	42	37	-2	0	19	92	96	2	-4	20	16	1
-3	4	18	16	1	-1	0	19	15	26	3	-4	20	18	27
-2	4	18	19	6	0	0	19	16	20	-4	-3	20	23	18
-1	4	18	151	149	1	0	19	25	28	-3	-3	20	42	41
0	4	18	76	73	2	0	19	17	4	-2	-3	20	62	64
1	4	18	16	25	3	0	19	113	114	-1	-3	20	57	57
2	4	18	39	34	4	0	19	17	23	0	-3	20	10	7
3	4	18	48	43	-4	1	19	14	10	1	-3	20	16	17
-2	5	18	60	62	-3	1	19	41	45	2	-3	20	30	32
-1	5	18	36	41	-2	1	19	14	7	3	-3	20	16	0
0	5	18	16	13	-1	1	19	28	30	-4	-2	20	24	25
1	5	18	25	21	0	1	19	42	42	-3	-2	20	54	55
2	5	18	75	65	1	1	19	44	47	-2	-2	20	50	50
0	-6	19	18	15	2	1	19	160	162	-1	-2	20	17	17
-2	-5	19	24	27	3	1	19	32	33	0	-2	20	25	36
-1	-5	19	35	25	4	1	19	16	6	1	-2	20	32	28
0	-5	19	26	26	-4	2	19	16	10	2	-2	20	14	6
1	-5	19	25	21	-3	2	19	14	7	3	-2	20	17	2
2	-5	19	17	0	-2	2	19	22	19	4	-2	20	11	10
-3	-4	19	39	31	-1	2	19	14	22	-4	-1	20	36	38
-2	-4	19	36	34	0	2	19	82	82	-3	-1	20	31	31
-1	-4	19	48	51	1	2	19	151	153	-2	-1	20	14	16
0	-4	19	38	39	2	2	19	30	33	-1	-1	20	17	35
1	-4	19	15	7	3	2	19	10	14	0	-1	20	21	25
2	-4	19	11	9	4	2	19	17	23	1	-1	20	30	32
3	-4	19	37	40	-4	3	19	16	5	2	-1	20	17	8
-4	-3	19	32	25	-3	3	19	16	7	3	-1	20	16	8
-3	-3	19	31	33	-2	3	19	13	1	4	-1	20	16	12
-2	-3	19	68	68	-1	3	19	50	59	-4	0	20	18	15
-1	-3	19	53	53	0	3	19	92	97	-3	0	20	11	11
0	-3	19	13	21	1	3	19	12	36	-2	0	20	17	3
1	-3	19	33	35	2	3	19	15	13	-1	0	20	16	44
2	-3	19	86	82	3	3	19	33	31	0	0	20	53	53
3	-3	19	16	12	-3	4	19	11	4	1	0	20	14	11
4	-3	19	15	5	-2	4	19	17	23	2	0	20	15	5
-4	-2	19	28	20	-1	4	19	53	62	3	0	20	15	4
-3	-2	19	65	65	0	4	19	41	40	4	0	20	17	6
-2	-2	19	43	44	1	4	19	16	9	-4	1	20	10	6
-1	-2	19	30	36	2	4	19	45	43	-3	1	20	14	16
0	-2	19	79	78	3	4	19	18	13	-2	1	20	38	40
1	-2	19	99	97	-2	5	19	41	38	-1	1	20	42	39
2	-2	19	25	16	-1	5	19	30	28	0	1	20	14	2
3	-2	19	15	6	0	5	19	15	11	1	1	20	16	13
4	-2	19	11	4	1	5	19	49	49	2	1	20	16	23

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	1	20	18	15	3	-2	21	16	3	-2	-5	22	47	47
4	1	20	20	1	4	-2	21	16	8	-1	-5	22	17	13
-4	2	20	16	11	-4	-1	21	15	29	0	-5	22	27	14
-3	2	20	29	23	-3	-1	21	29	29	1	-5	22	17	25
-2	2	20	17	16	-2	-1	21	14	2	2	-5	22	18	2
-1	2	20	14	2	-1	-1	21	249	248	-3	-4	22	51	47
0	2	20	16	23	0	-1	21	82	80	-2	-4	22	16	7
1	2	20	16	16	1	-1	21	10	3	-1	-4	22	13	22
2	2	20	36	35	2	-1	21	14	12	0	-4	22	37	42
3	2	20	15	3	3	-1	21	45	46	1	-4	22	16	9
4	2	20	27	23	4	-1	21	17	6	2	-4	22	73	70
-4	3	20	16	11	-4	0	21	8	14	3	-4	22	25	23
-3	3	20	11	7	-3	0	21	11	6	-3	-3	22	11	1
-2	3	20	15	1	-2	0	21	162	160	-2	-3	22	24	28
-1	3	20	52	53	-1	0	21	43	62	-1	-3	22	54	54
0	3	20	16	22	0	0	21	15	2	0	-3	22	23	23
1	3	20	42	44	1	0	21	34	32	1	-3	22	126	125
2	3	20	12	14	2	0	21	123	125	2	-3	22	39	37
3	3	20	38	38	3	0	21	16	9	3	-3	22	17	0
-3	4	20	17	1	4	0	21	17	5	-4	-2	22	20	7
-2	4	20	48	47	-4	1	21	7	6	-3	-2	22	15	25
-1	4	20	25	32	-3	1	21	80	78	-2	-2	22	50	51
0	4	20	28	30	-2	1	21	43	41	-1	-2	22	45	51
1	4	20	17	24	-1	1	21	14	4	0	-2	22	159	157
2	4	20	41	39	0	1	21	48	47	1	-2	22	45	46
-2	5	20	19	23	1	1	21	237	235	2	-2	22	8	9
-1	5	20	17	13	2	1	21	10	3	3	-2	22	14	2
0	5	20	22	20	3	1	21	15	7	4	-2	22	17	5
1	5	20	17	18	4	1	21	17	1	-4	-1	22	17	19
-2	-5	21	17	4	-4	2	21	31	32	-3	-1	22	36	37
-1	-5	21	7	1	-3	2	21	35	27	-2	-1	22	49	56
0	-5	21	23	22	-2	2	21	14	11	-1	-1	22	140	147
1	-5	21	24	25	-1	2	21	32	32	0	-1	22	49	48
2	-5	21	15	1	0	2	21	247	239	1	-1	22	14	10
-3	-4	21	18	6	1	2	21	15	0	2	-1	22	14	10
-2	-4	21	10	3	2	2	21	15	1	3	-1	22	16	7
-1	-4	21	33	34	3	2	21	19	4	4	-1	22	13	15
0	-4	21	43	42	-4	3	21	25	15	-4	0	22	21	20
1	-4	21	17	2	-3	3	21	15	6	-3	0	22	12	28
2	-4	21	66	63	-2	3	21	10	3	-2	0	22	92	110
3	-4	21	35	25	-1	3	21	138	137	-1	0	22	17	47
-3	-3	21	10	7	0	3	21	11	1	0	0	22	15	1
-2	-3	21	38	43	1	3	21	10	8	1	0	22	15	9
-1	-3	21	56	55	2	3	21	12	7	2	0	22	15	11
0	-3	21	16	3	3	3	21	17	19	3	0	22	40	30
1	-3	21	132	132	-3	4	21	17	8	4	0	22	23	1
2	-3	21	46	44	-2	4	21	61	62	-4	1	22	16	6
3	-3	21	17	5	-1	4	21	10	3	-3	1	22	67	66
-4	-2	21	20	15	0	4	21	12	4	-2	1	22	42	43
-3	-2	21	38	40	1	4	21	16	5	-1	1	22	14	1
-2	-2	21	47	48	2	4	21	17	9	0	1	22	16	23
-1	-2	21	5	14	-2	5	21	13	7	1	1	22	18	18
0	-2	21	221	213	-1	5	21	17	2	2	1	22	58	59
1	-2	21	73	70	0	5	21	17	6	3	1	22	15	7
2	-2	21	15	7	1	5	21	18	19	4	1	22	17	1

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-4	2	22	42	35	1	-1	23	15	23	-1	-3	24	41	37
-3	2	22	32	27	2	-1	23	15	7	0	-3	24	95	90
-2	2	22	10	4	3	-1	23	32	26	1	-3	24	71	71
-1	2	22	15	34	4	-1	23	17	15	2	-3	24	19	32
0	2	22	17	50	-4	0	23	20	19	3	-3	24	17	0
1	2	22	73	72	-3	0	23	61	61	-3	-2	24	15	2
2	2	22	12	6	-2	0	23	105	113	-2	-2	24	47	47
3	2	22	17	2	-1	0	23	36	58	-1	-2	24	136	134
-3	3	22	16	6	0	0	23	30	41	0	-2	24	112	111
-2	3	22	21	23	1	0	23	10	24	1	-2	24	42	41
-1	3	22	28	36	2	0	23	50	56	2	-2	24	17	9
0	3	22	48	45	3	0	23	31	30	3	-2	24	18	24
1	3	22	15	2	4	0	23	17	2	4	-1	24	13	3
2	3	22	17	1	-4	1	23	42	36	-3	-1	24	42	43
3	3	22	53	51	-3	1	23	75	71	-2	-1	24	129	128
-3	4	22	22	6	-2	1	23	39	35	-1	-1	24	122	120
-2	4	22	14	11	-1	1	23	36	38	0	-1	24	46	42
-1	4	22	17	16	0	1	23	62	65	1	-1	24	17	26
0	4	22	17	2	1	1	23	70	75	2	-1	24	10	7
1	4	22	11	13	2	1	23	44	41	3	-1	24	22	29
2	4	22	82	78	3	1	23	13	4	-4	0	24	26	27
-2	5	22	16	4	-4	2	23	39	36	-3	0	24	79	78
-1	5	22	17	3	-3	2	23	16	22	-2	0	24	82	92
0	5	22	24	20	-2	2	23	15	17	-1	0	24	17	32
1	5	22	90	86	-1	2	23	84	83	0	0	24	17	32
-1	-5	23	23	4	0	2	23	60	56	1	0	24	17	39
0	-5	23	15	5	1	2	23	35	39	2	0	24	33	31
1	-5	23	23	19	2	2	23	13	8	3	0	24	27	19
-3	-4	23	28	26	3	2	23	17	0	-4	1	24	18	39
-2	-4	23	10	6	-3	3	23	17	5	-3	1	24	60	57
-1	-4	23	16	5	-2	3	23	62	65	-2	1	24	27	22
0	-4	23	33	34	-1	3	23	29	25	-1	1	24	24	25
1	-4	23	22	15	0	3	23	32	32	0	1	24	79	90
2	-4	23	34	42	1	3	23	17	15	1	1	24	16	28
3	-4	23	22	19	2	3	23	16	2	2	1	24	39	37
-3	-3	23	15	6	3	3	23	49	48	3	1	24	11	7
-2	-3	23	15	7	-3	4	23	34	32	-4	2	24	27	30
-1	-3	23	50	46	-2	4	23	17	12	-3	2	24	16	15
0	-3	23	20	27	-1	4	23	17	22	-2	2	24	25	19
1	-3	23	70	69	0	4	23	16	14	-1	2	24	57	66
2	-3	23	28	30	1	4	23	27	15	0	2	24	31	32
3	-3	23	19	1	2	4	23	75	68	1	2	24	56	53
-4	-2	23	17	2	-1	5	23	18	6	2	2	24	13	10
-3	-2	23	14	9	0	5	23	28	25	3	2	24	17	18
-2	-2	23	52	48	1	5	23	65	57	-3	3	24	17	15
-1	-2	23	45	50	-1	-5	24	21	13	-2	3	24	23	26
0	-2	23	100	102	0	-5	24	17	4	-1	3	24	30	32
1	-2	23	45	50	1	-5	24	17	10	0	3	24	49	47
2	-2	23	14	7	-2	-4	24	24	17	1	3	24	15	6
3	-2	23	11	1	-1	-4	24	16	7	2	3	24	17	2
-4	-1	23	12	9	0	-4	24	16	24	3	3	24	17	15
-3	-1	23	37	36	1	-4	24	45	44	-2	4	24	17	20
-2	-1	23	65	71	2	-4	24	26	36	-1	4	24	22	25
-1	-1	23	121	123	-3	-3	24	13	14	0	4	24	16	2
0	-1	23	68	67	-2	-3	24	19	7	1	4	24	24	15

I-1105-39

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	4	24	17	4	3	2	25	17	2	-3	2	26	12	7
-1	5	24	18	4	-3	3	25	17	7	-2	2	26	32	37
0	5	24	15	5	-2	3	25	67	65	-1	2	26	49	52
-1	-5	25	15	14	-1	3	25	33	27	0	2	26	11	7
0	-5	25	17	7	0	3	25	14	15	1	2	26	16	2
1	-5	25	17	4	1	3	25	16	14	2	2	26	26	21
-2	-4	25	13	17	2	3	25	28	23	3	2	26	21	7
-1	-4	25	16	11	-2	4	25	11	17	-3	3	26	21	27
0	-4	25	20	14	-1	4	25	19	13	-2	3	26	30	29
1	-4	25	13	14	0	4	25	25	16	-1	3	26	16	12
2	-4	25	16	24	1	4	25	61	55	0	3	26	20	9
-3	-3	25	7	16	2	4	25	18	6	1	3	26	11	14
-2	-3	25	21	10	0	-5	26	21	12	2	3	26	15	7
-1	-3	25	24	30	-2	-4	26	22	19	-2	4	26	12	11
0	-3	25	18	16	-1	-4	26	16	16	0	4	26	17	8
1	-3	25	45	43	0	-4	26	10	10	0	4	26	12	5
2	-3	25	22	22	1	-4	26	17	7	1	4	26	17	6
3	-3	25	19	4	2	-4	26	17	15	-2	-4	27	17	15
-3	-2	25	15	4	-3	-3	26	27	19	-1	-4	27	11	13
-2	-2	25	29	41	-2	-3	26	7	15	0	-4	27	23	12
-1	-2	25	10	8	-1	-3	26	29	28	1	-4	27	17	6
0	-2	25	63	63	0	-3	26	16	15	2	-4	27	17	7
1	-2	25	32	28	1	-3	26	28	26	-3	-3	27	24	14
2	-2	25	16	13	2	-3	26	19	21	-2	-3	27	19	10
3	-2	25	18	25	3	-3	26	18	13	-1	-3	27	35	30
-4	-1	25	15	3	-3	-2	26	16	7	0	-3	27	13	9
-3	-1	25	16	28	-2	-2	26	45	46	1	-3	27	16	9
-2	-1	25	14	10	-1	-2	26	14	12	2	-3	27	17	12
-1	-1	25	69	72	0	-2	26	44	44	-3	-2	27	16	1
0	-1	25	40	34	1	-2	26	36	30	-2	-2	27	36	36
1	-1	25	30	32	2	-2	26	25	24	-1	-2	27	15	9
2	-1	25	41	47	3	-2	26	17	12	0	-2	27	16	10
3	-1	25	27	24	-3	-1	26	40	44	1	-2	27	15	18
-4	0	25	11	11	-2	-1	26	14	3	2	-2	27	33	37
-3	0	25	16	19	-1	-1	26	54	53	3	-2	27	29	31
-2	0	25	53	62	0	-1	26	22	28	-3	-1	27	28	24
-1	0	25	16	27	1	-1	26	40	35	-2	-1	27	10	8
0	0	25	51	58	2	-1	26	37	45	-1	-1	27	15	11
1	0	25	21	86	3	-1	26	17	15	0	-1	27	15	20
2	0	25	28	34	-4	0	26	16	27	1	-1	27	43	42
3	0	25	11	14	-3	0	26	22	14	2	-1	27	51	48
-4	1	25	18	17	-2	0	26	26	41	3	-1	27	17	8
-3	1	25	42	41	-1	0	26	15	17	-3	0	27	11	3
-2	1	25	15	12	0	0	26	18	19	-2	0	27	15	11
-1	1	25	58	57	1	0	26	19	73	-1	0	27	10	18
0	1	25	122	132	2	0	26	16	17	0	0	27	18	32
1	1	25	36	44	3	0	26	16	0	1	0	27	18	53
2	1	25	16	22	-4	1	26	15	13	2	0	27	16	4
3	1	25	16	13	-3	1	26	30	26	3	0	27	17	4
-3	2	25	16	5	-2	1	26	15	10	-3	1	27	11	9
-2	2	25	32	31	-1	1	26	15	25	-2	1	27	10	9
-1	2	25	114	114	0	1	26	58	77	-1	1	27	11	28
0	2	25	39	41	1	1	26	10	11	0	1	27	37	48
1	2	25	16	21	2	1	26	16	3	1	1	27	15	5
2	2	25	16	12	3	1	26	17	14	2	1	27	14	7

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	1	27	30	30	-2	2	28	69	68	-1	3	29	10	10
-3	2	27	16	1	-1	2	28	30	34	0	3	29	15	10
-2	2	27	27	28	0	2	28	18	13	1	3	29	23	21
-1	2	27	44	43	1	2	28	17	15	2	3	29	17	13
0	2	27	16	8	2	2	28	18	22	-1	4	29	16	11
1	2	27	14	9	-2	3	28	8	19	0	4	29	14	4
2	2	27	35	32	-1	3	28	16	9	-1	-4	30	17	10
3	2	27	26	25	0	3	28	15	8	0	-4	30	16	3
-3	3	27	26	21	1	3	28	17	14	1	-4	30	18	14
-2	3	27	33	29	2	3	28	11	1	-2	-3	30	17	7
-1	3	27	17	8	-1	4	28	20	2	-1	-3	30	12	1
0	3	27	16	8	0	4	28	43	38	0	-3	30	23	23
1	3	27	17	24	1	4	28	17	2	1	-3	30	23	20
2	3	27	17	4	-1	-4	29	16	3	2	-3	30	18	0
-2	4	27	13	6	0	-4	29	13	6	-3	-2	30	17	6
-1	4	27	17	3	1	-4	29	19	14	-2	-2	30	15	2
0	4	27	18	22	-2	-3	29	29	18	-1	-2	30	31	31
1	4	27	17	13	-1	-3	29	16	8	0	-2	30	25	27
-1	-4	28	16	8	0	-3	29	26	23	1	-2	30	17	5
0	-4	28	17	8	1	-3	29	17	11	2	-2	30	20	14
1	-4	28	17	13	2	-3	29	17	9	-3	-1	30	14	6
-2	-3	28	17	9	-3	-2	29	24	25	-2	-1	30	25	30
-1	-3	28	16	18	-2	-2	29	15	7	-1	-1	30	26	26
0	-3	28	32	24	-1	-2	29	17	27	0	-1	30	13	11
1	-3	28	10	7	0	-2	29	24	16	1	-1	30	17	5
2	-3	28	18	3	1	-2	29	14	7	2	-1	30	17	9
-3	-2	28	16	10	2	-2	29	11	13	-3	0	30	17	20
-2	-2	28	16	27	-3	-1	29	16	5	-2	0	30	20	18
-1	-2	28	26	31	-2	-1	29	16	24	-1	0	30	15	4
0	-2	28	18	10	-1	-1	29	21	16	0	0	30	16	6
1	-2	28	16	9	0	-1	29	15	5	1	0	30	17	12
2	-2	28	17	9	1	-1	29	15	2	2	0	30	17	3
3	-2	28	23	20	2	-1	29	17	21	3	0	30	18	7
-3	-1	28	20	20	3	-1	29	18	2	-3	1	30	17	10
-2	-1	28	16	25	-3	0	29	17	16	-2	1	30	16	12
-1	-1	28	15	8	-2	0	29	15	10	-1	1	30	15	5
0	-1	28	15	11	-1	0	29	24	30	0	1	30	22	16
1	-1	28	16	12	0	0	29	16	5	1	1	30	16	6
2	-1	28	28	30	1	0	29	19	28	2	1	30	18	14
3	-1	28	17	2	2	0	29	13	12	-3	2	30	12	17
-3	0	28	16	13	3	0	29	10	6	-2	2	30	17	2
-2	0	28	16	5	-3	1	29	10	3	-1	2	30	16	12
-1	0	28	14	10	-2	1	29	16	37	0	2	30	21	9
0	0	28	43	59	-1	1	29	16	4	1	2	30	10	21
1	0	28	17	44	0	1	29	14	23	2	2	30	61	49
2	0	28	16	1	1	1	29	10	20	-2	3	30	15	6
3	0	28	17	4	2	1	29	17	9	-1	3	30	17	9
-3	1	28	17	1	3	1	29	17	7	0	3	30	17	11
-2	1	28	15	11	-3	2	29	29	24	1	3	30	30	26
-1	1	28	90	91	-2	2	29	13	3	0	-4	31	17	6
0	1	28	34	47	-1	2	29	15	16	-2	-3	31	30	23
1	1	28	16	7	0	2	29	11	18	-1	-3	31	14	7
2	1	28	16	11	1	2	29	17	8	0	-3	31	22	16
3	1	28	34	29	2	2	29	20	23	1	-3	31	11	20
-3	2	28	19	11	-2	3	29	17	10	-2	-2	31	19	7

2-105-48