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Allan Zalkin

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University of California
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Crystal Structure of Monoclinic Sulfur¹

Lieselotte K. Templeton, David H. Templeton,
and Allan Zalkin

Received

Monoclinic sulfur is the form which is stable at normal pressure from 95°C to the melting point (115°). Below 95° the orthorhombic form ("rhombic sulfur") is stable, but pure crystals of the metastable monoclinic form can be preserved for weeks at room temperature. Sands² determined the structure of the monoclinic crystals from photographic x-ray diffraction patterns and reported preliminary atomic coordinates, but the data were not accurate enough for good refinement.³ In this note we report more precise parameters, derived from diffractometer data, which confirm Sands' conclusion about the structure.

Experimental

Crystals of monoclinic sulfur were produced accidentally by Dr. R. Gradl in an attempt to make a substituted diethietene complex of uranium, and their identity was not recognized until one of them, (a nine-faced crystal with dimensions about $0.3 \times 0.3 \times 0.2$ mm mounted in a quartz capillary) was examined by x-ray diffraction. Unit cell dimensions were derived from the setting angles of twelve reflections

(with $40^\circ < 2\theta < 45^\circ$) measured with a Picker FACS-I diffractometer with a graphite monochromator and Mo radiation ($\lambda = 0.70926\text{\AA}$ for $K\alpha_1$). The same instrument was used to measure intensities using a $\theta - 2\theta$ scan technique with a scanning rate of $2^\circ/\text{min}$ from 1° below 2θ for $K\alpha_1$ to 1° above 2θ for $K\alpha_2$. Background was counted for 4 sec with an offset of 0.5° from each end of the scan. Three strong reflections (333, 060, $22\bar{4}$) checked at intervals of 200 measurements indicated no decay within the accuracy of the experiment.

Absorption corrections calculated by an analytical integration⁴ ranged from 1.338 to 1.808. Their validity was verified by multiple measurements of several reflections at various azimuthal angles.

Measurements were made of 4577 reflections not excluded by the space group in the hemisphere $\pm h, k, \pm l$ and up to $2\theta = 50^\circ$. These reflections represent 2254 unique reflections; for 1627, $F^2 > \sigma(F^2)$; and for 1140, $F^2 > 3\sigma(F^2)$.

Crystal data:

The space group is $P2_1/c$; at 24°C , $a = 10.926(2)$, $b = 10.855(2)$, $c = 10.790(3)\text{\AA}$, $\beta = 95.92(2)^\circ$, $Z = 48$ atoms, $d_x = 2.008\text{ g cm}^{-3}$.

Determination of the Structure:

The structure was solved with the MULTAN program,⁵ to give an independent check of the previous work. With anisotropic thermal parameters (for the 16 atoms in the asymmetric unit) the full matrix least squares refinement reduced $R_1 = \sum |F| / \sum |F_o|$ to 0.030 for 1140 reflections with $F^2 > 3\sigma(F^2)$ and using $(.035F^2)^2$ as the additional term in $\sigma^2(F^2)$ to reduce the effect of strong reflections. Scattering

factors for neutral S were taken from Doyle and Turner⁶ and the dispersion corrections from Cromer and Liberman.⁷ The standard deviation of observation of unit weight was 0.998. In the last cycle, no parameter changed more than 0.0002σ . Final parameters are listed in Table I.⁸

Discussion

The structure (Fig. 1) consists of crown-shaped S_8 rings in two kinds of positions. Two-thirds of them (atoms 1-8) are in general positions without any disorder. The others (atoms 9-16) are located around centers of symmetry. The crown lacks centric symmetry, and the molecules gain this symmetry by disorder between two orientations, each occupied with 50% probability. The entropy of this disorder, if it is completely random, is $(R/24) \ln 2 = 0.057$ e.u./g-atom. Montgomery⁹ obtained 0.007 ± 0.020 e.u./g-atom for the residual entropy at low temperature relative to orthorhombic sulfur, and he discovered a lambda-type heat capacity anomaly (peaking at about 198°K) which is estimated to involve 0.05 e.u./g-atom of extra entropy. An earlier check of the entropy by Eastman and McGavock¹⁰ appears to have omitted some of the entropy of the lambda anomaly, but within its claimed accuracy of 0.06 e.u./g-atom is in agreement with Montgomery's result. As pointed out by Montgomery, the entropy data imply the disorder exists down to about 200°K but disappears gradually at lower temperatures. An ordered structure requires a change to lower symmetry of the crystal, with either a different space group or larger unit cell. The gradual nature of the transition makes it likely that the general molecular packing stays the same.

The bond distances (Table II) are all equal nearly to the estimated precision of the determination. A weighted average is $2.045(1)\text{\AA}$. The bond angles (Table III), with a weighted average of $107.9(1)^\circ$ range from 106.5° to 109.3° . It is plausible that this variation is the result of packing forces. These results are very similar to those reported by Abrahams¹¹ for S_8 molecules in orthorhombic sulfur: average distance $2.037(5)\text{\AA}$ and average angle $107.8(4)^\circ$.

Supplementary Material Available: A listing of structure factor amplitudes (9 pages). Ordering information is given on any current masthead page.

References and Notes

1. Work done in part under the auspices of the U.S. Energy Research and Development Administration.
2. D. E. Sands, J. Amer. Chem. Soc., 87, 1395 (1965).
3. D. E. Sands, private communication.
4. L. K. Templeton and D. H. Templeton, Amer. Crystallogr. Assoc. Prog. Abstr., Ser. 2, 1, 143 (1973).
5. G. Germain, P. Main and M. M. Woolfson, Acta Crystallogr., Sect. A, 27, 368 (1971).
6. P. A. Doyle and P. S. Turner, Acta Crystallogr., Sect. A, 24, 390 (1968).
7. D. T. Cromer and D. Liberman, J. Chem. Phys., 53, 1891 (1970).
8. See note at end of paper concerning supplementary material.
9. R. L. Montgomery, Science, 184, 562 (1974).
10. E. D. Eastman and W. C. McGavock, J. Amer. Chem. Soc., 59, 145 (1937).
11. S. C. Abrahams, Acta Crystallogr., 8, 661 (1955).

Table I. Atomic Parameters and Esd's

Atom	x ^a	y	z	B ₁₁ ^b	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
1	.2333(1)	.5251(1)	.0299(1)	4.70(7)	3.85(7)	4.89(7)	.57(6)	.17(6)	.63(6)
2	.1538(1)	.3555(2)	.0070(1)	3.44(6)	5.88(8)	6.05(8)	-1.00(6)	-.31(6)	.62(7)
3	.2572(1)	.2523(1)	-.1022(1)	5.89(8)	4.61(7)	4.06(7)	-.69(6)	-1.79(6)	-.32(7)
4	.3720(1)	.1439(1)	.0134(1)	6.08(8)	2.90(6)	5.02(7)	-.82(6)	-1.16(6)	.08(6)
5	.5398(1)	.2283(1)	.0381(1)	4.25(7)	3.87(6)	3.46(6)	.43(5)	.20(5)	-.23(5)
6	.5531(1)	.3154(1)	.2075(1)	4.65(7)	4.08(6)	2.89(5)	-.06(6)	-.79(5)	.24(5)
7	.5133(1)	.4979(1)	.1780(1)	4.52(7)	3.40(6)	4.19(6)	-.94(5)	.02(5)	-.62(5)
8	.3317(1)	.5246(1)	.2023(1)	5.35(8)	4.48(7)	3.79(6)	.05(6)	.92(5)	-1.11(6)
9	.1783(3)	-.1083(4)	.0823(4)	3.6(2)	5.6(2)	8.9(3)	.3(1)	-1.5(2)	.7(2)
10	.0505(4)	-.0710(4)	.2039(3)	7.6(2)	6.7(2)	5.4(2)	-.6(2)	-1.3(2)	2.8(2)
11	.0674(4)	.1125(4)	.1880(3)	8.1(3)	5.8(2)	3.8(2)	-.2(2)	-1.8(2)	-.8(1)
12	-.1953(3)	.1273(4)	.0790(3)	4.6(2)	6.3(2)	4.6(2)	.7(2)	1.2(1)	-.1(2)
13	-.1199(3)	.1709(3)	-.0981(3)	5.1(2)	4.5(2)	4.3(1)	.4(1)	-.3(1)	1.2(1)
14	-.1266(3)	.0105(4)	-.1966(3)	4.9(2)	7.8(2)	4.1(1)	.2(2)	-1.0(1)	-1.5(2)
15	.0510(4)	-.0466(5)	-.2030(4)	5.5(2)	8.1(3)	5.7(2)	-.0(2)	2.1(2)	-1.3(2)
16	.0899(4)	-.1822(4)	-.0743(4)	4.7(2)	4.2(2)	9.5(3)	.2(1)	.3(2)	-1.3(2)

^aEstimated standard deviation of the last digit is enclosed in parentheses. ^bThe form of the temperature factor

is $\exp[-0.25(B_{11}h^2a^2 + \dots + 2B_{12}hka^*b^* + \dots)]$.

Table II. Bond Distances ($\text{\AA}$) with Esd's

Atoms	Distance	Atoms	Distance
1-2	2.040(2)	9-10	2.053(6)
2-3	2.048(2)	10-11	2.050(5)
3-4	2.047(2)	11-12	2.034(5)
4-5	2.042(2)	12-13	2.044(5)
5-6	2.050(2)	13-14	2.038(5)
6-7	2.047(2)	14-15	2.045(5)
7-8	2.048(2)	15-16	2.038(6)
8-1	2.050(2)	16-9	2.024(6)

Table III. Bond Angles (deg) with Esd's

Central Atom	Angle	Central Atom	Angle
1	106.5(1)	9	108.3(2)
2	108.1(1)	10	107.7(3)
3	107.7(1)	11	107.7(3)
4	107.9(1)	12	108.7(2)
5	107.7(1)	13	106.8(2)
6	108.2(1)	14	107.1(2)
7	108.1(1)	15	109.1(3)
8	108.0(1)	16	109.3(3)

Figure Caption

Figure 1. Structure of monoclinic sulfur, viewed up the b axis. Numbers designate the atoms listed in the tables. The two alternate positions for the disordered molecules are both shown.

XBL 761-433

Fig. 1

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL $\times 1.0$)
MONOCLINIC SULFUR. $F(0,0,0) = 773$

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FCB. DEL = $|F_{OB}| - |F_{CA}|$.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,	0		5	10	1	1	8	6	6	2*-10	33	1	-1	-9	13	2	2	
2	67	1	3	6	4	6	3*	9	3	9	1*-9	7	10	-3*	-8	4	6	1*	
4	104	2	3	7	7	3	-0*	10	0	6	-3*-8	42	1	0	-7	10	2	-2	
6	50	1	1	8	32	1	1	H,K=	0,	9	-7	90	2	1	-6	7	9	3*	
8	52	1	-1	9	22	1	0	1	0	8	-3*-6	72	1	2	-5	53	1	0	
10	70	1	1	10	4	7	2*	2	22	2	1	-5	30	1	1	-4	46	1	0
12	18	2	-1	11	15	1	0	3	17	3	-0*-4	21	1	-0	-3	15	2	-1	
H,K=	0,	1		12	20	1	2	4	11	4	-1*-3	103	3	-2	-2	18	2	-1	
1	3	6	-3*	H,K=	0,	5	5	5	3	7	1*-2	88	2	0	-1	2	10	1*	
2	10	4	1*	1	40	1	-0	6	4	6	-5*-1	24	1	0	0	82	2	-0	
3	4	10	-2*	2	59	1	-0	7	2	9	-4*0	7	2	-1*	1	87	2	0	
4	9	3	1*	3	68	2	1	8	15	1	-1	1	68	3	3	2	44	1	-1
5	63	1	2	4	3	6	-2*	9	3	10	-3*2	24	1	3	3	13	1	-0	
6	96	2	2	5	63	1	-1	H,K=	0,	10	3	171	3	4	4	40	1	0	
7	20	1	-0	6	28	1	0	0	11	4	2*4	3	5	-0*	5	93	3	1	
8	33	1	-1	7	24	1	2	1	32	1	1	5	91	2	3	6	69	2	1
9	8	10	3*	8	17	2	0	2	40	1	1	6	21	1	1	7	48	1	1
10	13	1	-2	9	2	6	-5*	3	3	7	-0*7	43	1	1	8	20	1	1	
11	8	2	4*	10	7	7	-2*	4	12	1	1	8	35	1	-0	9	2	9	-2*
12	3	8	1*	11	13	2	1	5	18	2	1	9	4	9	2*	10	12	2	-1
H,K=	0,	2		H,K=	0,	6	6	6	0	6	-2*10	12	2	2	11	27	2	2	
0	31	1	0	0	85	2	1	7	18	1	-0	11	20	1	-1	12	5	10	-1*
1	5	8	2*	1	6	3	2*	8	23	1	2	12	6	6	0*	H,K=	1,	4	
2	140	4	-0	2	10	1	-0	H,K=	0,	11		H,K=	1,	2	-12	7	5	2*	
3	36	1	2	3	30	1	-0	1	15	2	1	-12	11	2	3	-11	4	8	-4*
4	36	1	1	4	45	1	-0	2	3	6	-1*-11	6	9	1*	-10	6	7	2*	
5	16	1	-1	5	21	2	-0	3	3	6	2*-10	13	2	-1	-9	23	1	-1	
6	64	1	3	6	38	1	-1	4	5	6	2*-9	23	1	0	-8	32	2	1	
7	31	1	0	7	18	2	-1	5	26	2	1	-8	15	1	-1	-7	6	7	4*
8	40	1	-0	8	6	6	-1*	6	15	2	1	-7	11	1	1	-6	20	1	0
9	10	2	-1	9	17	1	-0	H,K=	0,	12	-6	40	1	1	-5	8	1	2	
10	5	6	-1*	10	18	5	1*	0	13	2	1	-5	54	1	0	-4	25	1	0
11	8	8	3*	11	0	7	-4*	1	0	8	-3*-4	62	1	0	-3	18	1	0	
12	3	10	2*	H,K=	0,	7	2	2	10	4	2*-3	31	2	-0	-2	17	1	-0	
H,K=	0,	3		1	24	1	-1	3	7	4	3*-2	116	2	-1	-1	81	1	-0	
1	136	2	-0	2	8	2	2*	4	10	3	-0*-1	85	2	-1	0	107	2	1	
2	1	9	-2*	3	8	2	2*	H,K=	1,	0	0	51	1	0	1	6	2	2*	
3	20	1	0	4	7	7	-0*-12	22	3	-2	1	13	1	2	2	25	1	-1	
4	4	5	3*	5	33	1	-0	-10	25	1	-0	2	90	2	2	3	59	1	1
5	8	1	-1*	6	24	2	-0	-8	37	1	1	3	41	1	2	4	51	1	0
6	57	2	1	7	7	8	1*	-6	21	1	1	4	50	2	1	5	5	4	4*
7	5	7	3*	8	25	1	-1	-4	71	1	3	5	31	1	1	6	52	1	1
8	23	2	2	9	10	2	-0*-2	16	2	1	6	50	1	0	7	9	2	2*	
9	26	2	1	10	4	6	0*	0	0	125	-24*	7	12	1	1	8	27	2	-0
10	12	2	-1	H,K=	0,	8	2	7	9	5*	8	14	3	-0*	9	19	1	2	
11	12	3	0*	0	60	1	-0	4	24	2	2	9	25	1	-0	10	6	4	5*
12	9	4	3*	1	10	4	-1*	6	104	2	1	10	10	2	-2	11	5	8	0*
H,K=	0,	4		2	35	1	-0	8	20	1	-2	11	0	7	-8*	12	8	3	0*
0	63	1	1	3	5	6	3*	10	7	3	0*12	36	1	0		H,K=	1,	5	
1	51	1	-0	4	4	6	1*12	7	4	1*	H,K=	1,	3	-11	4	6	1*		
2	67	2	0	5	8	5	4*	H,K=	1,	1	-12	11	3	8*-10	0	10	-1*		
3	43	1	-1	6	22	1	-0	-12	10	2	-3*-11	15	2	1	-9	0	7	-1*	
4	14	1	-0	7	11	2	-0	-11	7	3	1*-10	17	2	-0	-8	16	5	1*	

STRUCTURE FACTORS CONTINUED FOR
MONOCLINIC SULFUR.

PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	36	1	0	3	36	1	-0	-1	22	1	-1	-3	2	7	-3*	2	49	1	1
-6	53	1	-1	4	22	1	-0	0	9	2	1	-2	136	3	-4	3	45	2	1
-5	12	1	-1	5	7	4	2*	1	0	8	-4*	-1	97	2	-1	4	53	2	2
-4	57	2	-1	6	0	10	-0*	2	16	3	0	0	33	1	-0	5	0	6	-5*
-3	61	2	-0	7	13	2	-2	3	7	10	5*	1	11	1	2	6	13	1	-0
-2	31	1	0	8	22	1	0	4	4	7	3*	2	68	1	1	7	54	1	0
-1	4	4	0*	9	23	1	-0	5	4	6	1*	3	77	1	2	8	15	2	-2
0	48	1	-0	10	18	2	1	6	2	8	-4*	4	60	1	1	9	39	1	0
1	21	1	0	H,K=	1,	8	7	9	4	-1*	5	58	1	0	10	6	6	-4*	
2	33	1	1	-10	10	2	-1*	H,K=	1,	11	6	67	1	1	11	30	1	-2	
3	39	1	-0	-9	10	2	4*	-6	8	4	1*	7	4	6	4*	12	4	7	2*
4	112	3	-2	-8	10	2	0*	-5	22	1	1	8	20	1	-0	H,K=	2,	4	
5	54	1	0	-7	9	3	-2*	-4	10	2	2*	9	36	1	0	-12	9	7	1*
6	67	1	-1	-6	15	1	-0	-3	9	3	7*	10	6	8	-1*	-11	8	3	4*
7	0	6	-1*	-5	9	11	-1*	-2	16	1	-2	11	12	2	-1	-10	17	1	-0
8	17	2	1	-4	13	2	1	-1	42	1	1	12	6	3	6*	-9	28	1	0
9	20	1	-1	-3	4	8	3*	0	38	1	1	H,K=	2,	2	-8	9	6	1*	
10	5	7	2*	-2	20	1	-1	1	25	1	0	-12	19	1	0	-7	27	1	-1
11	14	2	1	-1	29	1	-2	2	9	2	0*	-11	11	2	1	-6	24	1	-1
H,K=	1,	6	0	24	1	-0	3	2	6	1*	-10	6	3	0*	-5	13	1	1	
-11	6	11	4*	1	29	1	-0	4	15	1	3	-9	33	1	1	-4	41	1	-0
-10	5	7	2*	2	5	5	1*	5	20	2	-0	-8	19	1	-1	-3	69	2	0
-9	0	9	-1*	3	17	2	-1	6	5	7	4*	-7	9	2	-1	-2	14	1	-1
-8	16	1	-2	4	16	2	1	H,K=	1,	12	-6	24	1	-1	-1	33	1	-0	
-7	9	4	3*	5	31	1	-0	-4	0	6	-3*	-5	39	1	1	0	6	3	1*
-6	18	1	0	6	30	1	-1	-3	6	6	0*	-4	58	1	-0	1	58	1	1
-5	16	1	0	7	6	7	3*	-2	6	8	5*	-3	52	1	0	2	4	2	3*
-4	2	5	-6*	8	10	6	2*	-1	4	9	-1*	-2	92	2	-1	3	6	2	2*
-3	7	7	0*	9	4	9	1*	0	12	2	5*	-1	148	3	-3	4	12	1	1
-2	103	2	0	H,K=	1,	9	1	14	2	-1	0	16	1	1	5	29	1	1	
-1	33	1	0	-9	11	2	0*	2	16	1	1	1	173	4	-2	6	7	3	-1*
0	33	1	-0	-8	29	1	1	3	7	3	6*	2	54	1	3	7	8	3	1*
1	29	1	0	-7	11	2	2*	4	8	9	6*	3	4	5	-1*	8	32	2	2
2	31	1	-0	-6	6	6	-2*	H,K=	2,	0	4	92	3	2	9	7	7	4*	
3	7	2	1*	-5	0	6	-0*	-12	5	9	-0*	5	41	12	-8*	10	21	1	1
4	26	1	-1	-4	16	1	-1	-10	3	9	-1*	6	11	2	-1	11	7	4	-1*
5	12	1	1	-3	17	2	0	-8	45	1	-0	7	13	1	-0	H,K=	2,	5	
6	34	1	-1	-2	9	6	-0*	-6	48	1	0	8	8	7	-1*	-11	7	6	-4*
7	15	1	0	-1	7	8	-2*	-4	19	1	1	9	27	1	2	-13	11	3	3*
8	21	1	-0	0	11	3	1*	-2	101	2	-5	10	26	1	-0	-9	5	6	2*
9	5	10	4*	1	7	3	2*	0	45	1	1	11	25	2	0	-8	14	1	-1
10	28	1	1	2	25	1	-1	2	171	3	1	12	21	3	-1	-7	8	2	1*
11	6	6	-0*	3	18	1	-1	4	37	1	1	H,K=	2,	3	-6	23	1	-2	
H,K=	1,	7	4	29	1	0	6	34	1	0	-12	8	3	2*	-5	26	1	-1	
-10	14	2	-1	5	16	2	-2	8	47	1	0	-11	5	7	1*	-4	49	2	-1
-9	17	1	1	6	0	7	-3*	10	8	2	-1*	-10	11	2	0*	-3	74	3	-3
-8	11	3	0*	7	10	5	0*	12	18	1	0	-9	7	7	-3*	-2	12	1	-0
-7	3	10	-4*	8	7	7	5*	H,K=	2,	1	-8	5	16	5*	-1	33	1	-1	
-6	1	8	-5*	9	9	7	5*	-12	24	1	1	-7	8	2	2*	0	37	1	0
-5	14	3	-1*	H,K=	1,	10	-11	7	4	5*	-6	6	2	6*	1	28	1	-1	
-4	23	1	-1	-8	4	6	0*	-10	17	1	1	-5	39	1	-1	2	77	1	1
-3	28	1	-1	-7	9	2	-1*	-9	10	5	3*	-4	27	1	1	3	74	1	1
-2	9	2	-1*	-6	12	3	0*	-8	8	2	1*	-3	19	1	-0	4	32	1	0
-1	7	2	2*	-5	25	1	-0	-7	11	1	-0	-2	15	3	-0*	5	40	1	-0
0	64	1	-1	-4	9	4	2*	-6	5	2	0*	-1	65	1	-1	6	7	9	2*
1	9	2	-1*	-3	7	8	2*	-5	25	1	-0	0	56	1	0	7	4	9	-1*
2	2	7	1*	-2	32	1	0	-4	28	1	-0	1	59	1	2	8	6	7	1*

STRUCTURE FACTORS CONTINUED FOR
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PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL			
9	5	6	3*	-2	6	3	2*	2	7	3	2*-11	16	2	-1	-4	19	1	-0				
10	11	2	1*	-1	24	1	1	3	4	7	1*-10	9	2	-1*	-3	23	1	1				
11	20	1	3	0	24	1	-1	4	4	11	-3*	-9	14	2	-1	-2	10	1	-0			
H,K= 2,				6	1	58	1	-1	5	19	2	2	-8	8	3	1*	-1	11	2	-2		
-11	14	2	2	2	7	3	2*	6	21	1	-1	-7	8	2	-0*	0	14	1	1			
-10	4	10	-1*	3	22	1	1	H,K= 2,				12	-6	12	2	1*	1	3	4	-1*		
-9	11	3	-0*	4	10	2	0	-4	2	8	-1*	-5	22	1	0	2	6	5	3*			
-8	11	3	-1*	5	54	1	-0	-3	16	2	-1	-4	8	2	-2*	3	22	1	1			
-7	41	1	-1	6	31	1	-0	-2	0	6	-1*	-3	13	2	-0	4	4	5	2*			
-6	23	1	-2	7	22	2	-0	-1	14	2	1	-2	34	1	-1	5	57	1	0			
-5	11	3	1*	8	21	1	-2	0	7	4	0*	-1	80	1	0	6	0	9	-5*			
-4	62	2	-3	9	17	1	-1	1	7	8	3*	0	38	1	-1	7	21	1	1			
-3	51	2	-1	H,K= 2,				9	2	13	2	0	1	30	1	1	8	59	1	-0		
-2	39	1	1	-9	9	3	3*	3	19	3	0	2	22	1	1	9	19	1	-1			
-1	75	1	-0	-8	11	2	-1*	4	1	9	-5*	3	14	1	1	10	21	1	1			
0	17	1	-0	-7	11	3	4*	H,K= 3,				0	4	72	1	2	11	0	7	-1*		
1	14	1	0	-6	4	6	-4*-12	8	9	6*	5	26	1	1	H,K= 3,				5			
2	32	1	-1	-5	9	7	-4*-10	4	6	4*	6	53	1	1	-11	11	2	-2*				
3	82	1	-1	-4	14	1	-1	-8	17	2	-0	7	23	1	-1	-10	2	8	-2*			
4	28	1	0	-3	16	2	-1	-6	67	1	-1	8	6	4	1*	-9	17	1	1			
5	2	6	-5*	-2	26	1	0	-4	2	4	1*	9	5	8	4*	-8	0	9	-1*			
6	8	3	-0*	-1	14	1	1	-2	103	2	-2	10	9	3	3*	-7	12	2	0			
7	24	2	2	0	4	9	3*	0	115	2	-0	11	18	1	1	-6	6	7	2*			
8	0	8	-3*	1	4	10	-1*	2	81	1	2	H,K= 3,				3	-5	16	2	-1		
9	14	1	4	2	11	5	0*	4	7	1	2	-12	0	7	-6*	-4	14	2	1			
10	14	2	-3	3	19	3	-1	6	70	1	-1	-11	8	5	1*	-3	26	1	-0			
H,K= 2,				7	4	6	3	2*	8	36	1	-0	-10	9	2	-0*	-2	9	1	0		
-10	3	6	-3*	5	7	4	1*	10	14	1	-2	-9	16	1	-1	-1	28	1	1			
-9	0	6	-1*	6	5	6	2*	12	13	3	-1*	-8	8	5	2*	0	41	1	0			
-8	10	2	2*	7	5	6	-5*	H,K= 3,				1	-7	14	2	-2	1	23	1	-1		
-7	7	8	1*	8	8	4	4*-12	13	3	2*	-6	22	1	0	2	34	1	0				
-6	24	1	-1	H,K= 2,				10	-11	21	2	0	-5	52	1	-0	3	6	2	2*		
-5	20	1	-1	-8	4	7	-1*-10	4	6	-3*	-4	14	1	0	4	4	6	-1*				
-4	24	1	-1	-7	0	6	-5*	-9	3	7	2*	-3	18	1	-1	5	17	1	1			
-3	6	7	2*	-6	14	2	-2	-8	21	1	0	-2	53	1	-1	6	16	1	-3			
-2	26	1	1	-5	11	4	0*	-7	65	1	-0	-1	16	1	-0	7	3	11	-1*			
-1	10	1	0	-4	17	1	2	-6	69	1	-0	0	88	2	0	8	13	2	-1			
0	8	3	1*	-3	6	9	0*	-5	70	2	-1	1	8	2	2*	9	7	11	3*			
1	21	1	1	-2	6	6	5*	-4	40	1	0	2	102	3	4	10	12	2	-2			
2	34	1	0	-1	7	3	4*	-3	13	1	0	3	57	1	2	11	0	10	-5*			
3	43	1	-1	0	30	2	0	-2	34	1	-1	4	19	1	-1	H,K= 3,				6		
4	22	1	1	1	5	5	-1*	-1	83	2	0	5	84	2	-1	-11	0	8	-3*			
5	13	1	0	2	14	2	-1	0	123	2	-0	6	6	3	1*-10	12	3	1*				
6	36	1	-1	3	7	3	2*	1	7	9	-1*	7	23	1	-1	-9	31	1	0			
7	19	1	-0	4	6	10	3*	2	4	7	-0*	8	18	2	-2	-8	24	1	-1			
8	10	4	2*	5	10	2	2*	3	24	1	0	9	44	1	0	-7	8	6	-1*			
9	28	1	1	6	0	8	-1*	4	32	1	1	10	11	4	-1*	-6	21	1	-0			
10	15	2	2	7	8	4	8*	5	49	1	1	11	6	7	2*	-5	5	5	5*			
H,K= 2,				8	H,K= 2,				11	6	17	2	0	H,K= 3,				4	-4	20	1	-0
-10	18	2	-0	-6	16	1	2	7	1	7	-4*-12	3	9	-2*	-3	7	2	3*				
-9	6	4	0*	-5	17	2	1	8	18	2	-0	-11	5	6	2*	-2	3	7	0*			
-8	6	6	-1*	-4	8	9	-0*	9	5	8	1*-10	0	10	-1*	-1	60	1	-1				
-7	23	1	0	-3	14	2	1	10	28	1	0	-9	6	5	-2*	0	38	1	-0			
-6	20	1	0	-2	14	1	1	11	5	7	-3*	-8	24	1	1	1	27	1	0			
-5	6	7	-0*	-1	22	2	0	12	15	3	-1*	-7	0	5	-1*	2	56	1	-1			
-4	7	8	2*	0	10	5	-0*	H,K= 3,				2	-6	83	3	-2	3	65	1	0		
-3	4	6	3*	1	14	2	-8	-12	28	2	1	-5	53	1	-1	4	2	8	1*			

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	27	1	-0	-1	16	4	-1*	4	31	1	0	-10	0	7	-0*	-1	76	1	-2
6	15	5	1*	0	25	1	0	6	57	1	0	-9	25	1	-1	0	2	4	1*
7	13	1	-2	1	11	3	2*	8	8	7	-3*	-8	36	1	-1	1	17	1	-0
8	10	2	4*	2	8	8	-1*	10	14	1	-1	-7	33	1	-0	2	47	1	-0
9	17	1	-1	3	18	1	0	H,K=	4,	1	-6	0	5	-3*	3	4	5	-1*	
10	11	5	-1*	4	29	1	0	-12	7	9	-3*	-5	35	1	-1	4	9	3	6*
H,K=	3,	7	5	7	3	-1*	-11	17	1	0	-4	5	5	3*	5	36	1	-1	
-10	14	2	1	6	17	2	-1	-10	7	7	4*	-3	10	1	-0	6	35	1	1
-9	4	7	2*	7	8	8	4*	-9	36	1	-0	-2	4	6	2*	7	9	4	-2*
-8	0	9	-5*	8	3	6	-0*	-8	17	1	-0	-1	20	1	0	8	34	1	0
-7	46	1	0	H,K=	3,	10	-7	12	1	1	0	51	1	-1	9	19	2	-2	
-6	18	2	0	-7	2	6	2*	-6	29	1	0	1	2	4	1*	10	2	8	-6*
-5	38	1	-0	-6	8	3	-0*	-5	7	4	-0*	2	44	1	1	H,K=	4,	6	
-4	39	1	-3	-5	8	3	1*	-4	38	1	-0	3	8	2	2*	-11	6	6	2*
-3	52	1	-1	-4	2	6	2*	-3	30	1	-1	4	55	2	-1	-10	19	1	3
-2	46	1	-1	-3	5	7	-1*	-2	18	1	1	5	52	1	-0	-9	22	2	-0
-1	52	1	-1	-2	6	7	-1*	-1	127	2	-1	6	44	1	-1	-8	30	1	-1
0	0	8	-1*	-1	17	1	2	0	48	1	-0	7	1	6	-0*	-7	0	8	-1*
1	36	1	0	0	22	1	-1	1	13	1	1	8	25	1	0	-6	19	1	1
2	33	1	1	1	0	8	-1*	2	20	1	0	9	24	1	-1	-5	27	1	0
3	17	1	-0	2	22	1	1	3	36	1	1	10	19	2	1	-4	34	1	0
4	31	1	-1	3	25	1	-0	4	33	1	1	11	9	4	2*	-3	26	1	0
5	16	1	-3	4	9	3	5*	5	21	1	1	H,K=	4,	4	-2	20	1	-0	
6	11	3	-1*	5	22	1	-1	6	8	2	3*	-11	4	6	2*	-1	17	2	0
7	15	1	1	6	11	3	2*	7	6	7	5*	-10	7	4	-1*	0	50	1	1
8	26	1	1	7	7	4	1*	8	8	10	-3*	-9	2	6	1*	1	28	1	0
9	18	2	-0	H,K=	3,	11	9	15	1	-0	-8	22	2	-0	2	44	1	-0	
10	9	8	5*	-6	4	10	3*	10	0	9	-4*	-7	32	1	0	3	31	1	1
H,K=	3,	8	-5	6	6	1*	11	0	8	-2*	-6	36	1	0	4	31	1	0	
-9	0	6	-1*	-4	7	4	-2*	H,K=	4,	2	-5	17	1	-0	5	16	1	1	
-8	0	7	-4*	-3	21	1	-1	-12	10	4	-1*	-4	10	2	-0*	6	14	3	-1*
-7	9	6	-2*	-2	13	3	1*	-11	6	7	4*	-3	33	1	-1	7	18	2	1
-6	9	3	0*	-1	12	2	0*	-10	23	1	1	-2	109	2	-2	8	7	4	-2*
-5	0	10	-2*	0	14	4	-1*	-9	12	2	3	-1	13	1	-1	9	9	6	1*
-4	8	4	7*	1	11	2	-2	-8	19	2	1	0	122	3	-0	10	15	2	-2
-3	4	8	-4*	2	7	6	-0*	-7	14	1	-1	1	7	3	1*	H,K=	4,	7	
-2	8	3	-1*	3	12	2	-0	-6	9	2	1*	2	81	3	2	-10	0	6	-2*
-1	27	1	-0	4	2	10	2*	-5	10	1	-0	3	38	1	1	-9	4	9	-3*
0	17	1	-2	5	3	6	-4*	-4	15	2	1	4	16	1	2	-8	32	1	1
1	16	1	0	H,K=	3,	12	-3	42	1	-0	5	6	7	-1*	-7	7	3	-2*	
2	27	1	0	-4	10	5	3*	-2	25	1	-1	6	9	2	-0*	-6	20	2	-1
3	5	4	5*	-3	2	7	-4*	-1	29	1	-0	7	10	2	-0*	-5	20	1	-1
4	3	8	-5*	-2	16	2	0	0	15	1	-1	8	16	1	-0	-4	20	3	1
5	20	1	-0	-1	21	1	-1	1	43	1	-0	9	8	3	-4*	-3	7	4	-1*
6	12	1	1	0	11	4	0*	2	24	1	0	10	4	8	-2*	-2	28	1	0
7	16	1	-0	1	7	3	1*	3	51	1	1	11	11	2	6	-1	46	1	-1
8	22	1	-1	2	7	10	4*	4	53	1	1	H,K=	4,	5	0	27	1	1	
9	3	6	-2*	3	19	1	1	5	26	1	0	-11	20	1	1	1	26	1	0
H,K=	3,	9	H,K=	4,	0	6	57	1	0	-10	17	1	1	1	2	2	10	1	1*
-9	12	3	0*	-12	7	7	1*	7	20	1	-1	-9	30	1	-1	3	8	2	2*
-8	7	8	-1*	-10	12	2	-1	8	13	2	-0*	-8	10	2	2*	4	0	10	-0*
-7	5	7	-3*	-8	34	1	0	9	10	2	1*	-7	5	9	1*	5	19	1	-1
-6	16	2	1	-6	61	1	-2	10	0	9	-2*	-6	19	1	1	6	0	6	-4*
-5	16	1	1	-4	82	1	-2	11	8	3	1*	-5	17	1	1	7	9	4	4*
-4	26	1	1	-2	9	2	-0*	H,K=	4,	3	-4	13	2	1	8	26	1	-0	
-3	30	1	-0	0	13	2	0	-12	8	6	-2*	-3	67	1	-1	9	3	8	-2*
-2	22	1	1	2	81	1	1	-11	2	9	-0*	-2	78	1	-3	H,K=	4,	8	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	5	8	3*	1	10	2	3	-6	20	1	-0	4	25	1	-1	-5	23	2	-0
-8	2	6	2*	2	10	3	-2*	-5	7	3	4*	5	19	1	1	-4	1	14	-5*
-7	6	5	-2*	3	18	1	2	-4	70	1	-2	6	16	1	-1	-3	5	7	5*
-6	4	6	1*	4	0	8	-7*	-3	16	1	1	7	36	1	0	-2	7	3	3*
-5	10	2	-3*	5	9	5	3*	-2	92	2	-0	8	8	4	5*	-1	23	1	0
-4	14	6	-2*	H,K=	4,	12	-1	30	1	-0	9	15	2	0	0	38	1	-1	
-3	13	5	0*	-3	15	1	3	0	10	1	1	10	22	1	-2	1	17	1	1
-2	7	8	2*	-2	3	7	-0*	1	38	1	0	H,K=	5,	5	2	7	8	3*	
-1	0	8	-4*	-1	9	5	-3*	2	26	1	-0	-11	4	6	-2*	3	11	3	-2*
0	18	2	1	0	9	2	-0*	3	4	6	3*-10	22	1	-2	4	7	7	4*	
1	18	1	-0	1	16	1	1	4	71	2	-0	-9	20	1	0	5	11	3	-1*
2	7	9	1*	2	5	7	2*	5	3	7	-5*	-8	28	1	1	6	9	2	1*
3	5	7	1*	H,K=	5,	0	6	41	1	0	-7	5	11	1*	7	3	6	-1*	
4	39	1	1	-12	7	7	-4*	7	1	10	-3*	-6	20	1	-0	8	5	9	-2*
5	10	2	1	-10	21	1	1	8	11	2	-2	-5	10	2	2*	9	7	4	1*
6	6	7	4*	-8	43	1	-0	9	8	2	-0*	-4	21	1	0	H,K=	5,	8	
7	0	6	-1*	-6	46	1	-1	10	28	1	-2	-3	64	1	-1	-9	10	6	-3*
8	19	1	1	-4	64	1	-1	11	12	3	3*	-2	7	3	4*	-8	8	4	7*
H,K=	4,	9	-2	41	1	0	H,K=	5,	3	-1	16	1	0	-7	0	9	-3*		
-8	8	3	-0*	0	33	1	0	-11	4	6	3*	0	20	1	0	-6	8	3	0*
-7	6	8	1*	2	138	2	0	-10	10	2	-0*	1	52	1	-1	-5	12	3	2*
-6	0	7	-3*	4	12	1	1	-9	3	6	0*	2	1	6	-1*	-4	3	6	1*
-5	9	2	7*	6	49	1	-1	-8	23	1	1	3	7	3	1*	-3	6	4	-0*
-4	12	4	-2*	8	7	9	1*	-7	16	2	-1	4	0	6	-3*	-2	17	3	1*
-3	21	1	0	10	5	8	-5*	-6	22	1	-1	5	26	1	0	-1	26	1	1
-2	35	1	-0	H,K=	5,	1	-5	14	2	1	6	3	8	0*	0	0	8	-2*	
-1	9	2	0*-12	8	3	-1*	-4	15	2	1	7	17	2	0	1	21	1	0	
0	1	7	-3*-11	10	6	2*	-3	30	1	-1	8	5	9	-2*	2	35	1	-0	
1	4	6	1*-10	6	6	4*	-2	9	2	1	9	7	8	-1*	3	30	1	-0	
2	3	8	-4*	-9	28	1	-0	-1	5	4	4*	10	17	3	-2*	4	15	2	0
3	10	2	-2*	-8	10	5	1*	0	14	1	1	H,K=	5,	6	5	13	2	1	
4	33	1	1	-7	10	1	2	1	15	1	0	-10	0	6	-4*	6	11	3	0*
5	15	2	1	-6	42	1	-1	2	6	3	1*	-9	3	7	1*	7	4	8	-2*
6	5	9	0*	-5	10	1	1	3	52	1	-0	-8	34	1	1	8	8	7	-2*
7	9	4	-2*	-4	65	2	-3	4	10	1	-0	-7	21	1	1	H,K=	5,	9	
H,K=	4,	10	-3	73	1	-2	5	6	8	6*	-6	16	6	-0*	-8	10	2	-0*	
-7	26	1	0	-2	34	1	-0	6	14	2	2	-5	5	9	3*	-7	13	2	2
-6	24	1	-0	-1	39	1	1	7	7	9	-1*	-4	64	1	-2	-6	18	2	-1
-5	1	10	1*	0	63	1	-0	8	12	2	-2	-3	10	2	9	-5	12	2	3
-4	7	3	7*	1	19	1	1	9	12	2	2	-2	24	1	-1	-4	19	1	-1
-3	15	2	-0	2	19	1	1	10	15	2	1	-1	5	7	-1*	-3	15	2	-1
-2	10	3	2*	3	6	2	5*	H,K=	5,	4	0	26	1	0	-2	46	1	0	
-1	12	2	-1	4	108	2	-3	-11	9	9	2*	1	27	2	-1	-1	11	1	0
0	19	1	0	5	42	1	-1	-10	0	13	-1*	2	35	1	-1	0	5	7	4*
1	20	1	1	6	55	1	-2	-9	22	1	-1	3	3	9	-4*	1	12	1	1
2	0	10	-1*	7	7	2	7*	-8	37	1	-1	4	29	1	0	2	34	1	2
3	5	9	2*	8	3	10	-1*	-7	17	2	1	5	3	11	-6*	3	20	1	1
4	29	1	0	9	15	2	-1	-6	35	1	-0	6	26	1	-1	4	23	1	-3
5	16	4	-1*	10	5	7	2*	-5	40	1	-2	7	10	4	5*	5	11	6	-1*
6	22	1	2	11	13	2	3	-4	17	1	0	8	4	8	-4*	6	20	1	1
H,K=	4,	11	H,K=	5,	2	-3	47	1	-1	9	5	6	2*	7	5	9	3*		
-5	15	2	-1	-12	0	7	-2*	-2	25	1	-1	H,K=	5,	7	H,K=	5,	10		
-4	7	3	-0*-11	3	8	2*	-1	11	1	1	-10	5	6	-1*	-6	16	1	3	
-3	8	3	-1*-10	9	3	1*	0	72	2	-0	-9	7	7	1*	-5	8	3	-1*	
-2	0	7	-1*	-9	3	9	-3*	1	9	3	-1*	-8	0	7	-4*	-4	6	7	2*
-1	17	2	0	-8	33	1	-0	2	61	1	-0	-7	8	5	2*	-3	0	7	-5*
0	6	7	1*	-7	10	2	0	3	49	1	-1	-6	9	4	1*	-2	3	6	0*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	3	6	3*	-8	15	2	-1	3	19	1	0	-3	5	10	-2*	-3	3	7	3*
0	11	3	-1*	-7	22	1	2	4	19	1	-0	-2	4	9	-0*	-2	0	7	-7*
1	5	6	5*	-6	33	1	-0	5	8	3	6*	-1	22	1	0	-1	16	1	-0
2	6	5	3*	-5	6	2	4*	6	17	4	1*	0	11	4	-1*	0	0	6	-3*
3	9	2	-0*	-4	25	1	-0	7	8	3	-4*	1	6	9	3*	1	2	8	-5*
4	20	1	0	-3	71	1	-1	8	26	1	-1	2	39	1	-1	2	20	2	0
5	3	7	0*	-2	65	1	-0	9	4	6	2*	3	14	2	1	H,K=	7,	0	
H,K=	5,	11	-1	29	1	-0	10	11	5	-3*	4	5	6	-1*	-10	8	5	5*	
-5	11	2	2*	0	55	1	0	H,K=	6,	5	5	17	3	2	-8	14	2	-0	
-4	19	1	1	1	63	1	0	-10	18	2	1	6	8	3	-1*	-6	54	1	0
-3	14	2	0	2	32	1	0	-9	21	1	2	7	8	5	4*	-4	12	1	1
-2	2	7	1*	3	30	1	0	-8	6	10	3*	8	15	3	2	-2	4	5	1*
-1	1	8	-4*	4	37	1	-0	-7	10	3	1*	H,K=	6,	8	0	3	6	1*	
0	3	6	2*	5	11	2	0*	-6	12	2	-1	-8	0	7	-4*	2	9	2	3*
1	11	3	-3*	6	15	2	2	-5	6	3	4*	-7	12	6	0*	4	9	2	1*
2	8	3	3*	7	35	1	1	-4	20	1	-1	-6	6	9	4*	6	25	2	1
3	10	5	4*	8	24	2	2	-3	43	1	-1	-5	8	7	3*	8	27	1	1
4	7	4	6*	9	12	4	1*	-2	6	6	5*	-4	20	1	-1	10	24	1	1
H,K=	6,	0	10	28	1	-2	-1	52	1	0	-3	16	1	-1	H,K=	7,	1		
-10	21	1	1	H,K=	6,	3	0	31	1	0	-2	3	8	-0*	-11	8	7	5*	
-8	0	11	-4*	-11	10	4	4*	1	23	1	-1	-1	8	8	1*	-10	6	9	3*
-6	71	1	-1	-10	8	6	5*	2	16	1	1	0	30	1	0	-9	9	2	8*
-4	40	1	1	-9	9	3	2*	3	17	2	-1	1	21	1	0	-8	12	1	1
-2	21	1	1	-8	0	6	-1*	4	21	1	1	2	22	1	0	-7	8	7	2*
0	37	1	1	-7	4	8	4*	5	5	6	3*	3	7	3	1*	-6	15	1	1
2	58	1	-0	-6	17	1	0	6	5	6	-1*	4	11	2	-0	-5	3	5	1*
4	8	3	4*	-5	33	1	0	7	24	1	-1	5	7	8	2*	-4	5	6	-0*
6	11	1	1	-4	26	1	1	8	14	2	1	6	17	2	2	-3	15	1	0
8	31	1	0	-3	50	1	-1	9	10	2	1*	7	4	6	3*	-2	7	7	0*
10	11	3	-2*	-2	3	6	-1*	H,K=	6,	6	6	H,K=	6,	9	-1	2	7	-2*	
H,K=	6,	1	-1	3	4	0*	-10	0	6	6	-7*	5	6	5	5*	0	54	1	-0
-11	15	3	-0*	0	37	1	-1	-9	6	6	-2*	-6	6	4	1*	1	11	2	1*
-10	8	2	8*	1	20	1	-0	-8	2	9	2*	-5	5	7	5*	2	4	5	3*
-9	0	9	-5*	2	25	1	1	-7	4	9	3*	-4	19	3	1	3	43	1	-1
-8	10	4	-0*	3	86	2	-2	-6	19	1	-1	-3	16	1	-2	4	23	1	-1
-7	10	3	2*	4	27	1	-1	-5	12	2	-0	-2	3	6	-2*	5	0	6	-0*
-6	5	7	-2*	5	9	2	5*	-4	14	2	-0	-1	13	3	0*	6	28	1	-1
-5	30	1	-1	6	20	1	1	-3	28	1	-1	0	5	7	5*	7	14	1	-2
-4	0	6	-2*	7	56	1	-1	-2	14	1	-1	1	3	6	-0*	8	9	4	4*
-3	57	1	0	8	28	2	0	-1	12	1	2	2	17	3	-2	9	17	1	2
-2	8	3	5*	9	20	2	1	0	26	1	-1	3	4	8	4*	10	7	4	-3*
-1	28	1	-0	10	8	3	3*	1	4	8	4*	5	22	2	2	H,K=	7,	2	
0	59	1	0	H,K=	6,	4	2	7	4	6*	5	19	2	-1	-11	10	2	-0*	
1	32	1	0	-11	6	7	4*	3	6	10	4*	6	7	11	-1*	-10	3	6	3*
2	34	1	0	-10	0	6	-5*	4	11	5	1*	H,K=	6,	10	-9	0	9	-7*	
3	18	1	1	-9	10	2	0*	5	26	1	1	-6	0	7	-2*	-8	9	2	1*
4	40	1	0	-8	1	7	0*	6	5	8	3*	-5	20	1	1	-7	3	6	1*
5	37	1	-0	-7	0	8	-1*	7	7	8	3*	-4	19	2	-1	-6	6	8	0*
6	9	2	1*	-6	20	1	1	8	6	7	4*	-3	14	3	-1*	-5	4	5	2*
7	4	7	-3*	-5	11	3	1*	9	19	2	1	-2	8	7	2*	-4	17	1	2
8	11	3	1*	-4	16	1	0	H,K=	6,	7	-1	14	2	2	-3	34	1	-0	
9	11	3	-0*	-3	12	2	2*	-9	7	9	2*	0	11	2	1*	-2	6	7	4*
10	0	6	-5*	-2	53	1	-1	-8	20	1	1	1	20	2	0	-1	19	1	-0
H,K=	6,	2	-1	31	1	-0	-7	13	2	2	2	13	1	0	0	55	1	-1	
-11	3	7	0*	0	36	1	0	-6	5	6	5*	3	6	5	-2*	1	41	1	-0
-10	6	6	-2*	1	23	1	-0	-5	20	1	-0	4	0	9	-2*	2	17	1	-1
-9	13	1	-2	2	69	1	-1	-4	28	1	1	H,K=	6,	11	3	40	1	-1	

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	3	8	3*	-3	7	2	2*	0	4	7	1*	5	4	8	3*	0	10	5	-1*
5	19	3	-0	-2	4	6	0*	1	10	2	-0*	6	9	9	-0*	1	24	1	-1
6	30	1	-1	-1	12	1	1	2	8	7	2*	7	4	9	-5*	2	11	3	1*
7	18	2	-0	0	33	1	-0	3	19	2	-0	8	18	4	-1*	3	25	1	0
8	10	4	3*	1	18	1	0	4	2	8	-2*	9	6	8	-3*	4	27	1	2
9	1	8	-4*	2	3	5	1*	5	6	7	-3*	H,K=	8,	2	5	6	5	-1*	
H,K=	7,	3	3	3	7	11	-0*	6	0	7	-1*	-10	19	1	-2	6	11	3	1*
-11	3	8	1*	4	20	2	-3	H,K=	7,	9	-9	11	4	2*	7	3	8	-1*	
-10	5	11	-1*	5	13	2	-3	-6	6	7	6*	-8	10	3	-2*	8	14	2	-2
-9	24	1	-1	6	14	4	1*	-5	0	10	-2*	-7	10	2	5	H,K=	8,	5	
-8	9	3	1*	7	5	8	0*	-4	5	6	-0*	-6	14	3	-0*	-9	17	2	3
-7	12	2	-1	8	13	2	0*	-3	9	3	1*	-5	28	1	1	-8	5	7	5*
-6	0	10	-0*	H,K=	7,	6	-2	3	6	1	-1*	-4	8	3	5*	-7	8	3	1*
-5	57	1	-2	-9	2	6	-2*	-1	15	1	1	-3	5	6	-1*	-6	3	6	1*
-4	6	3	3*	-8	12	5	2*	0	14	1	2	-2	10	2	-1*	-5	21	2	1
-3	42	1	-0	-7	5	6	3*	1	18	2	2	-1	40	1	1	-4	13	1	1
-2	14	1	2	-6	6	7	4*	2	3	7	1*	0	11	2	-2*	-3	8	3	3*
-1	28	1	-0	-5	4	6	-3*	3	7	5	-0*	1	12	2	0	-2	14	1	-1
0	13	2	1	-4	8	5	-1*	4	14	2	-1	2	5	7	2*	-1	4	10	0*
1	65	1	-1	-3	16	2	-0	5	28	1	1	3	11	3	-0*	0	11	6	0*
2	37	1	-1	-2	28	1	-1	H,K=	7,	10	4	34	1	-0	1	5	8	2*	
3	24	1	1	-1	29	1	1	-5	0	7	-3*	5	14	1	1	2	10	3	2*
4	0	7	-4*	0	14	5	-2*	-4	13	2	2	6	51	1	-0	3	24	2	1
5	48	1	-1	1	12	3	-1*	-3	19	2	1	7	12	2	-0	4	26	1	1
6	0	6	-3*	2	14	3	-1*	-2	11	3	4*	8	9	4	1*	5	19	1	2
7	2	8	1*	3	11	1	-0	-1	19	2	-0	9	8	4	-5*	6	6	6	-2*
8	3	6	-0*	4	5	9	-2*	0	2	8	-4*	H,K=	8,	3	7	19	2	-1	
9	12	5	0*	5	1	6	-2*	1	17	3	1*	-10	3	6	0*	H,K=	8,	6	
H,K=	7,	4	6	10	3	-0*	2	7	4	3*	-9	10	3	5*	-8	10	4	3*	
-10	6	5	-1*	7	9	3	-2*	3	17	1	1	-8	11	2	1	-7	9	2	1*
-9	6	6	4*	8	12	2	-3*	H,K=	8,	0	-7	5	5	4*	-6	5	7	3*	
-8	15	1	-1	H,K=	7,	7	-10	4	8	4*	-6	8	2	-1*	-5	13	3	-1*	
-7	17	2	-1	-8	5	7	-3*	-8	28	1	1	-5	4	7	-2*	-4	4	6	-2*
-6	29	2	-1	-7	7	8	2*	-6	19	1	0	-4	5	8	5*	-3	22	1	-2
-5	5	8	-1*	-6	14	1	-0	-4	11	2	3	-3	3	5	0*	-2	16	2	-0
-4	14	2	1	-5	0	7	-3*	-2	38	1	0	-2	32	1	1	-1	22	1	1
-3	11	1	-1	-4	0	7	-1*	0	24	1	-0	-1	18	1	0	0	18	1	1
-2	5	6	1*	-3	21	1	-1	2	22	1	-1	0	15	1	-2	1	9	2	-1*
-1	18	2	1	-2	45	1	-1	4	5	10	-0*	1	33	1	0	2	7	7	-2*
0	36	1	-2	-1	0	8	-5*	6	0	6	-0*	2	19	2	-1	3	18	2	0
1	3	8	-2*	0	23	1	0	8	3	7	-1*	3	8	9	1*	4	16	1	0
2	5	10	-1*	1	3	6	2*	H,K=	8,	1	4	14	3	0*	5	14	1	0	
3	14	3	-2*	2	46	1	1	-10	2	7	-3*	5	31	1	-1	6	23	1	0
4	7	9	1*	3	40	1	-2	-9	16	1	3	6	18	1	-2	7	0	7	-2*
5	12	4	-0*	4	16	1	0	-8	4	10	-4*	7	1	7	-1*	H,K=	8,	7	
6	12	2	1	5	6	7	5*	-7	4	7	4*	8	5	6	-3*	-8	9	9	-0*
7	17	1	2	6	11	2	1*	-6	14	4	-1*	H,K=	8,	4	-7	11	3	1*	
8	30	1	-2	7	21	1	1	-5	13	3	0*	-10	12	3	3*	-6	7	3	-0*
9	16	3	1*	H,K=	7,	8	-4	22	1	-1	-9	7	9	3*	-5	4	6	1*	
H,K=	7,	5	-8	13	2	2	-3	5	5	1*	-8	3	6	2*	-4	0	6	-2*	
-10	13	1	2	-7	6	6	3*	-2	44	1	-1	-7	14	2	-1	-3	0	10	-1*
-9	1	7	-1*	-6	13	2	1	-1	7	6	-0*	-6	4	5	-1*	-2	0	9	-5*
-8	2	8	-1*	-5	8	3	2*	0	45	1	-1	-5	0	7	-3*	-1	9	2	4*
-7	11	2	0	-4	10	3	3*	1	11	1	-0	-4	12	2	-0	0	19	1	1
-6	4	7	2*	-3	15	1	1	2	2	6	1*	-3	20	1	2	1	16	1	1
-5	11	2	0*	-2	16	2	0	3	8	6	0*	-2	8	4	-0*	2	8	3	-3*
-4	0	9	-2*	-1	14	1	-0	4	14	3	-1	-1	3	6	0*	3	17	2	0

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	9	2	1*	3	0	3	-1*	4	28	1	1	1	3	9	-5*	-4	10	2	1*
5	7	8	1*	4	11	1	0	5	7	4	6*	2	11	2	-1	-3	1	7	-5*
6	13	5	-1*	5	8	3	2*	6	8	3	2*	3	7	9	3*	-2	8	2	5*
H,K= 8, 8				6	12	2	-1	7	10	3	5*	H,K= 9, 9				-1	27	1	0
-7	6	7	1*	7	8	9	1*	H,K= 9, 5				-3	16	2	-1	0	3	7	-2*
-6	8	3	-2*	8	0	7	-3*	-8	5	6	-2*	-2	10	2	1*	1	7	3	2*
-5	27	2	-0	H,K= 9, 2				-7	0	6	-3*	-1	0	8	-1*	2	8	7	-2*
-4	0	11	-0*	-9	10	2	2	-6	11	6	7*	0	3	8	1*	3	15	1	-0
-3	16	1	-0	-8	11	3	-1*	-5	18	2	-1	1	4	10	-0*	4	21	1	-0
-2	12	2	1	-7	9	5	2*	-4	44	1	1	H,K= 10, 0				5	15	2	2
-1	18	4	2*	-6	7	3	-2*	-3	4	5	2*	-8	6	6	3*	6	7	4	0*
0	30	1	2	-5	0	8	-1*	-2	20	2	1	-6	15	2	-1	H,K= 10, 4			
1	31	1	-1	-4	22	2	0	-1	24	1	2	-4	32	1	1	-8	8	3	2*
2	6	6	-0*	-3	3	7	-4*	0	21	1	-1	-2	9	2	-1*	-7	6	7	4*
3	5	6	-1*	-2	16	2	-1	1	9	2	4*	0	50	1	1	-6	24	2	-1
4	5	8	-2*	-1	5	7	2*	2	20	2	2	2	42	1	0	-5	5	6	4*
5	8	4	-2*	0	4	9	-2*	3	0	6	0*	4	16	1	0	-4	1	9	-1*
H,K= 8, 9				1	3	6	-0*	4	10	4	-0*	6	13	3	-1*	-3	11	3	3*
-5	1	6	-7*	2	5	6	1*	5	8	3	1*	H,K= 10, 1				-2	21	1	1
-4	13	2	-4*	3	3	8	-1*	6	27	1	-1	-9	0	9	-6*	-1	17	1	2
-3	4	6	2*	4	9	9	-2*	H,K= 9, 6				-8	7	3	4*	0	1	7	-1*
-2	10	2	2*	5	0	8	-1*	-8	7	8	5*	-7	11	2	3	1	7	3	1*
-1	13	2	-1	6	5	7	1*	-7	3	6	-0*	-6	12	3	0*	2	21	1	1
0	16	1	2	7	4	6	0*	-6	9	3	0*	-5	5	5	3*	3	7	8	1*
1	13	2	-0	8	11	4	-1*	-5	9	4	1*	-4	3	6	2*	4	8	10	2*
2	0	7	-3*	H,K= 9, 3				15	1	1	-3	16	2	0	5	10	2	3*	3*
3	0	8	-1*	-9	10	6	-1*	-3	0	8	-7*	-2	5	8	-1*	6	4	7	0*
H,K= 8, 10				-8	7	7	5*	-2	1	6	-1*	-1	3	6	1*	H,K= 10, 5			
-2	3	7	1*	-7	4	7	0*	-1	4	5	0*	0	6	3	1*	-7	11	3	-2*
-1	7	4	6*	-6	25	1	-0	0	10	2	0*	1	19	1	-0	-6	0	7	-4*
0	10	3	3*	-5	14	1	1	1	3	6	2*	2	6	3	3*	-5	4	6	2*
1	10	4	2*	-4	18	2	1	2	24	1	-0	3	17	1	0	-4	4	7	1*
H,K= 9, 0				-3	27	2	0	3	12	2	2*	4	3	6	1*	-3	7	8	2*
-10	7	8	2*	-2	24	1	-0	4	24	1	-2	5	5	9	-5*	-2	7	7	5*
-8	3	8	-2*	-1	6	9	-1*	5	8	4	-1*	6	21	1	-2	-1	4	6	0*
-6	6	8	1*	0	0	11	-3*	6	16	1	2	7	12	2	2	0	6	4	4*
-4	15	2	3	1	20	1	-1	H,K= 9, 7				H,K= 10, 2				1	1	8	-0*
-2	29	1	0	2	4	5	4*	-7	14	2	3	-8	4	9	3*	2	17	1	0
0	8	3	1*	3	15	1	0	-6	9	9	2*	-7	0	7	-7*	3	13	1	-1
2	0	9	-4*	4	6	6	-4*	-5	3	6	-1*	-6	20	2	1	4	8	8	-1*
4	11	1	-1	5	10	3	2*	-4	2	7	-3*	-5	4	6	1*	5	9	3	2*
6	12	2	0	6	2	7	2*	-3	13	6	-1*	-4	24	1	1	H,K= 10, 6			
8	22	1	-2	7	15	1	-0	-2	12	2	-0	-3	9	2	0*	-6	5	6	4*
H,K= 9, 1				H,K= 9, 4				-1	5	8	-0*	-2	12	1	-0	-5	16	2	1
-10	3	10	1*	-9	4	8	1*	0	11	2	-1	-1	0	7	-2*	-4	19	2	1
-9	16	2	1	-8	8	3	3*	1	8	5	-1*	0	17	1	-0	-3	7	6	-3*
-8	6	6	-2*	-7	6	6	4*	2	12	6	3*	1	13	1	0	-2	10	2	-0
-7	22	1	1	-6	4	6	3*	3	15	3	-0	2	6	5	4*	-1	14	1	4
-6	7	3	-0*	-5	5	8	3*	4	7	4	3*	3	12	2	-2	0	6	6	2*
-5	26	1	2	-4	24	1	-0	5	0	7	-5*	4	18	2	-2	1	11	3	1*
-4	4	8	-0*	-3	13	2	0	H,K= 9, 8				5	6	8	3*	2	8	6	-1*
-3	12	4	0*	-2	15	3	-2*	-5	9	2	4*	6	14	1	-1	3	9	6	3*
-2	4	8	3*	-1	10	4	1*	-4	0	8	-0*	H,K= 10, 3				4	11	4	4*
-1	7	10	6*	0	30	1	-0	-3	9	3	-2*	-8	4	7	-2*	H,K= 10, 7			
0	12	1	-2	1	27	1	1	-2	12	2	0	-7	9	2	0*	-5	9	2	8*
1	26	1	1	2	44	1	1	-1	13	1	1	-6	18	3	1	-4	20	1	1
2	24	1	-0	3	1	6	-1*	0	16	1	1	-5	20	2	1	-3	8	3	-2*

PAGE 9

L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL	L	F08	SG	DEL
-2	3	6	0*	2	7	6	4*	0	5	9	-5*				
-1	5	7	4*	3	4	8	3*	1	13	2	-0				
0	17	1	G	4	13	2	0	2	8	3	3*				
1	10	2	-3*	5	5	6	-2*	3	0	6	-0*				
2	9	6	0*	H,K= 11,	4	H,K= 12,	3								
3	15	2	-1	-6	14	1	2	-5	8	4	4*				
H,K= 10,	8	-5	2	8	-0*	-4	11	3	5*						
-3	7	3	3*	-4	4	6	2*	-3	22	1	2				
-2	11	3	-2*	-3	7	7	2*	-2	8	4	-1*				
-1	0	6	-2*	-2	5	8	3*	-1	4	8	-3*				
0	0	8	-2*	-1	6	7	4*	0	3	9	3*				
1	8	4	4*	0	12	2	0	1	12	2	1				
H,K= 11,	0	1	0	7	-3*	2	0	8	-3*						
-6	21	3	2	2	12	3	0*	H,K= 12,	4						
-4	4	10	0*	3	20	1	-1	-4	12	3	0*				
-2	15	2	G	4	5	6	-3*	-3	2	10	-1*				
0	5	6	2*	H,K= 11,	5	-2	6	5	-4*						
2	7	4	0*	-5	7	5	4*	-1	4	9	-2*				
4	8	3	1*	-4	4	6	3*	0	4	6	3*				
H,K= 11,	1	-3	0	7	-0*	1	5	7	-4*						
-7	15	1	1	-2	7	3	5*	H,K= 12,	5						
-6	16	3	0	-1	12	4	0*	-1	13	2	3				
-5	4	9	-3*	0	5	8	3*	H,K= 13,	0						
-4	0	9	-3*	1	4	9	4*	-2	19	1	-1				
-3	12	2	2	2	8	5	4*								
-2	22	1	2	3	7	4	-0*								
-1	36	1	0	H,K= 11,	6										
0	9	3	1*	-4	6	10	1*								
1	0	6	-4*	-3	14	1	0								
2	9	2	2*	-2	9	2	1*								
3	10	3	-1*	-1	9	2	-0*								
4	4	6	4*	0	11	2	0*								
5	5	9	2*	1	23	1	3								
H,K= 11,	2	2	7	3	7*										
-7	0	10	-4*	H,K= 12,	0										
-6	13	2	2	-6	5	8	1*								
-5	0	7	-2*	-4	9	2	0*								
-4	2	7	-3*	-2	2	8	-3*								
-3	9	2	2*	0	0	9	-5*								
-2	16	1	2	2	4	6	4*								
-1	17	1	-1	H,K= 12,	1										
0	40	1	0	-6	10	3	5*								
1	9	9	1*	-5	4	9	-2*								
2	16	1	2	-4	9	2	4*								
3	15	1	0	-3	11	5	0*								
4	15	1	-0	-2	6	9	2*								
5	6	6	-0*	-1	9	3	1*								
H,K= 11,	3	0	9	6	3*										
-7	6	6	-1*	1	8	9	-3*								
-6	5	6	3*	2	2	8	-6*								
-5	5	7	2*	3	0	9	-5*								
-4	7	3	3*	H,K= 12,	2										
-3	22	1	-1	-5	11	3	2*								
-2	0	8	-8*	-4	4	6	-1*								
-1	11	2	1	-3	4	7	-0*								
0	15	3	2*	-2	5	9	-2*								
1	20	1	2	-1	0	9	-1*								

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