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The Crystal Structures of 2,2′,4,4′,6,6′-Hexanitroazobenzene (HNAB), Forms I and II*

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The crystal structures of two polymorphic forms of hexanitroazobenzene, or HNAB, $C_{12}H_4N_8O_{12}$, have been determined by direct methods and refined by analysis of three-dimensional Mo $K\alpha$ intensity data. The unit cell for HNAB, form I, is monoclinic ($a=10{\cdot}149$, $b=8{\cdot}263$, $c=10{\cdot}055$ Å, $\beta=97{\cdot}29°$), space group $P2_1/c$, with 2 molecules per cell. HNAB, form II, is monoclinic ($a=10{\cdot}632$, $b=21{\cdot}869$, $c=7{\cdot}585$ Å, $\beta=102{\cdot}56°$), space group $P2_1/a$, with 4 molecules per cell. Least-squares refinement of all positional and thermal parameters (hydrogen atoms isotropic) with 1335/1635 reflections of non-zero weight, gave a final R index of 0·063/0·047 for form I/form II, respectively. Only one of the substituent groups is coplanar with the benzene rings, and both forms display a *trans* configuration. The following ranges of interatomic separations were obtained: C=C, 1·380–1·397/1·357–1·398 Å; C–N(O), 1·472–1·487/1·473–1·490 Å; C–N(N), 1·426/1·430–1·438 Å; N–O, 1·209–1·232/1·197–1·220 Å; N=N, 1·244/1·243 Å for form I/form II respectively.

Introduction

Five crystalline polymorphs of 2,2′,4,4′,6,6′-hexanitroazobenzene (HNAB) have been identified by hot-stage optical microscopy (McCrone, 1967). Forms I and III are stable from room temperature to 185°C and form II from room temperature to 205°C. The very unstable forms IV and V are formed only from the melt on supercooling during recrystallization. Forms II and III also transform rapidly through the solution phase into form I. Bulk samples of HNAB, regardless of polymorphic forms present, melt at 223°C.

HNAB is extremely complex in its crystallographic behavior as evidenced by the relationships among the various phase transformations. In order to understand some of these relationships and as part of an effort to elucidate fundamental properties of explosives, it has been desirable to determine the crystal structures of several HNAB forms. Efforts to grow single crystals of form III suitable for X-ray measurements are currently underway, and we now report on the crystal structures of HNAB-I and HNAB-II.

Experimental

A sample of hexanitroazobenzene was obtained from the Explosive Component Division of our Laboratories; the compound was prepared by reacting purified picryl chloride with hydrazine and potassium acetate in ethanol followed by acidification with hydrochloric acid. This yield of crude hexanitrohydrazobenzene is subsequently oxidized with nitric acid to give orange-colored crystals of HNAB. About 70% of the crystals from this preparation were form I crystals with the balance being form II. Larger crystals of the two forms were obtained by recrystallizations from nitromethane and have the morphological characteristics shown in Fig. 1. Equant crystals of form I consisted of 'rhombohedra' with monoclinic symmetry and well developed dipyramid {111} faces and {100} basal pinacoids. Form II consisted of long, obliquely truncated rods with {110} prism and {001} basal pinacoids. The crystals used for the collection of X-ray data were approximately equi-dimensional and chosen with appropriate dimensions such that absorption corrections (for Mo $K\alpha$, $\mu=1{\cdot}76$–$1{\cdot}82$ cm^{-1}) would be unnecessary.

Precession and Weissenberg photographs were used to determine preliminary unit-cell dimensions and space-group extinctions and to inspect the diffraction images for satellites. Systematic absences and the symmetry of the reciprocal lattice indicated the space groups to be $P2_1/c$ and $P2_1/a$ for forms I and II, respectively. Cell dimensions for both polymorphs were obtained by least-squares fit of 11 zonal reflections (λMo $K\alpha=0{\cdot}71069$ Å) which were measured on a single-crystal diffractometer at 23°C. Table 1 sum-

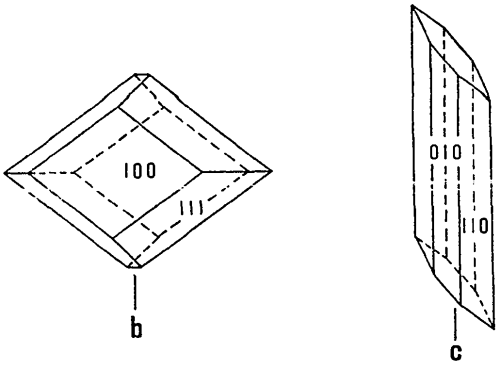

Fig. 1. Perspective drawings of HNAB. Left, form I; right, form II.

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marizes the crystallographic data for forms I and II. The calculated densities agree within a third of a percent with the observed densities as measured by flotation in an aqueous barium perchlorate solution.

Table 1. *Crystallographic data for HNAB**

Form	I	II
Space group	$P2_1/c$	$P2_1/a$
a (Å)	10·149 (4)	10·632 (4)
b	8·263 (3)	21·869 (7)
c	10·055 (4)	7·585 (3)
β (°)	97·29 (4)	102·56 (4)
Cell contents	$2[C_{12}H_4N_8O_{12}]$	$4[C_{12}H_4N_8O_{12}]$
D (g cm^{-3}), calc.	1·795	1·744
obs.	1·799	1·750

* Standard error in parentheses.

The θ–2θ scan technique with a scintillation detector employing pulse-height discrimination was used to measure the Mo $K\alpha$ intensity data at room temperature. Reflections within a sphere limited by $2\theta = 54°$ (form I) and $2\theta = 42°$ (form II) were measured with a β-filter (Zr). Background radiation was measured at each end of the scan with crystal and counter stationary, and was assumed to be a linear function of 2θ between these points. Unique sets of 1824 and 1859 reflections were measured for forms I and II respectively; from these sets 489 and 224 reflections were less than 3σ and considered unobserved. $\sigma = \sqrt{(N_{sc} + K^2N_b)}$, where N_{sc}, N_b and K are the total scan counts, background counts and the time ratio of scan to background, respectively. Intensities were corrected for Lorentz and polarization effects to obtain the observed structure amplitudes; no corrections for absorption or extinction were applied. Atomic scattering factors for C, N and O were taken from Table 3.3.1A of *International Tables for X-ray Crystallography* (1962); for hydrogen, the factors of Stewart, Davidson & Simpson (1965) were used.

Determination and refinement of the structures

Each structure was solved by direct methods through the symbolic addition procedure (Karle & Karle, 1966). The data were corrected for vibrational motion and placed on an absolute scale by means of a K curve. Statistical averages for the normalized structure factors and the distribution of E magnitudes favored the centrosymmetric space groups as shown in Table 2. Phases were determined by hand application of the $\sum_2$

Table 2. *Statistical averages and distribution of* $|E|$ *for HNAB*

	Experimental		Theoretical	
	Form I	Form II	Centro-symmetric	Noncentro-symmetric
$\langle \lvert E \rvert \rangle$	0·795	0·778	0·798	0·866
$\langle \lvert E^2-1 \rvert \rangle$	0·989	1·015	0·968	0·736
$\langle \lvert E \rvert^2 \rangle$	1·000	1·000	1·000	1·000
$\lvert E \rvert > 3·0$	0·005	0·006	0·003	0·0001
$\lvert E \rvert > 2·0$	0·040	0·046	0·050	0·018
$\lvert E \rvert > 1·0$	0·308	0·296	0·320	0·368

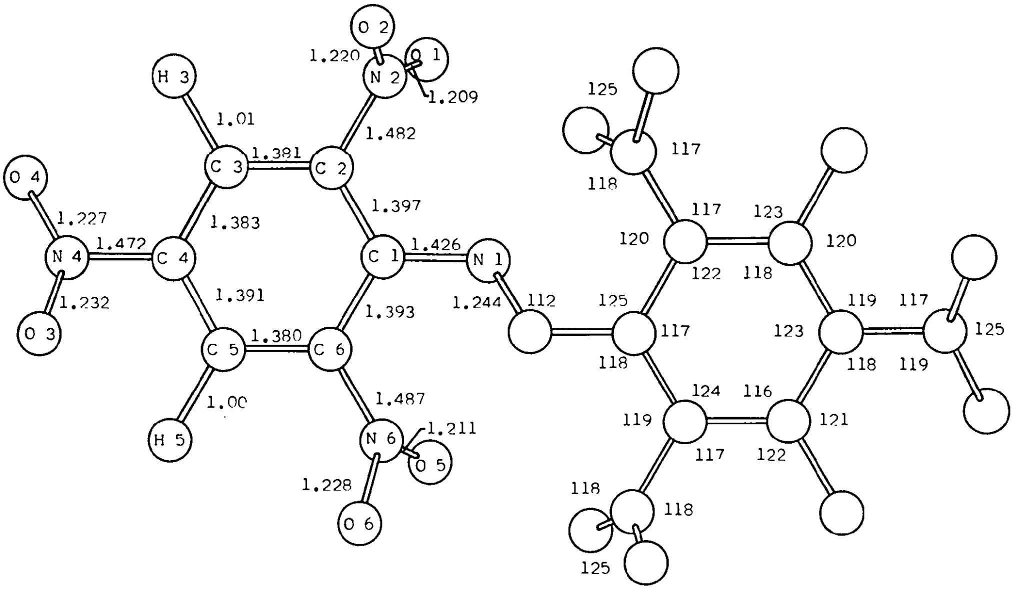

Fig. 2. Bond lengths (Å) and angles (°) in HNAB, form I.

expression where the origin was specified by assigning signs to three linearly independent reflections (Hauptman & Karle, 1953). Other reflections were also specified with letter symbols as shown in Table 3. From the list of 186 values of $|E| > 1·6$ for the form I polymorph, 133 were found (34 being either 0 or π and 99 phases in terms of the symbols a and b). Accordingly, four E maps were computed. Only one of these maps resolved the expected molecular features ($a=0$, $b=0$) and the 16 largest peaks selected from this map completely defined the entire heavy-atom molecule. The positions of these peaks were used as input to the least-squares refinement. For the 133 phases assigned consistent with a and b values of zero, there were no incorrect phases as shown by the final structure.

Table 3. *Initial phase assignments for HNAB*

	h	k	l	$\lvert E_{hkl}\rvert$	φ_{hkl}
Form I	5	1	$\bar{7}$	4·074	0
	4	7	$\bar{9}$	3·867	0
	2	5	6	2·923	0
	7	5	$\bar{1}$	3·632	a
	8	4	0	3·542	b
Form II	6	9	3	4·191	0
	2	4	1	3·275	0
	3	2	$\bar{2}$	3·106	π
	8	9	2	4·667	a
	2	5	1	3·118	b
	0	5	1	2·947	c

Table 4. *Final positional and thermal parameters for HNAB*

The standard deviations apply to the rightmost digits of the least-squares parameters. The anisotropic temperature factor is of the form:

$$\exp\left(-\tfrac{1}{4}\sum_{i=1}^{3}\sum_{j=1}^{3}B_{ijn}h_ih_ja_i^*a_j^*\right).$$

(a) Form I

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	B_{iso}
N 1	0.49915±26	0.96215±34	0.05338±27	1.56± 9	2.07±10	1.93± 9	-0.09± 9	0.17± 9	0.07± 9	
N 2	0.47629±29	0.00025±38	0.32674±29	2.43±11	2.71±12	1.88±10	-0.29±11	0.73±10	-0.01±10	
N 4	0.94506±31	0.15109±37	0.41357±32	2.43±12	2.20±12	2.86±13	-0.03±12	-0.74±11	-0.23±10	
N 6	0.76979±26	0.94211±37	0.96885±28	1.60±10	2.67±12	2.15±11	0.20±10	0.42± 9	-0.37±11	
C 1	0.61816±30	0.98687±36	0.14281±30	1.95±11	1.39±10	1.65±11	0.04±11	0.20± 9	0.06±11	
C 2	0.60726±31	0.01719±38	0.27766±31	2.10±12	1.70±11	1.74±11	-0.01±12	0.49±10	0.12±11	
C 3	0.71188±34	0.06897±42	0.36903±34	2.51±13	2.12±13	2.03±13	-0.10±13	-0.05±11	-0.14±13	
C 4	0.83302±31	0.08690±38	0.32142±32	1.89±12	1.71±11	2.17±12	-0.06±12	-0.38±10	-0.11±10	
C 5	0.85360±32	0.04762±41	0.19113±34	1.82±12	2.08±12	2.38±12	0.17±12	0.32±11	0.01±12	
C 6	0.74527±31	0.99577±38	0.10475±31	1.84±11	1.77±11	1.82±11	0.11±11	0.30±10	0.04±13	
O 1	0.41836±31	0.87305±40	0.30661±34	3.81±13	3.77±14	4.43±15	-1.91±13	1.97±11	-1.43±13	
O 2	0.43776±31	0.11296±37	0.39001±34	3.92±13	3.16±12	4.30±14	0.05±13	2.33±12	-0.79±10	
O 3	0.04268±29	0.19721±44	0.36273±34	2.57±12	4.81±16	4.45±15	-1.31±13	-0.13±11	-0.50±15	
O 4	0.93490±31	0.15653±39	0.53376±28	4.07±13	3.38±12	2.46±12	0.33±13	-0.93±10	-0.62±12	
O 5	0.71112±27	0.92363±33	0.92169±28	2.34±11	2.71±11	3.04±11	-0.30±11	0.78±10	-1.03±11	
O 6	0.94988±30	0.02066±42	0.91332±30	3.76±13	4.76±15	3.36±13	-1.60±14	2.31±11	-0.90±13	
H 3	0.7011 ±33	0.0934 ±43	0.4651 ±36							1.37±81
H 5	0.9430 ±33	0.0628 ±41	0.1621 ±32							0.89±41

(b) Form II

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	B_{iso}
C 1	0.80905±37	0.58218±17	0.64782±51	2.44±19	1.83±17	1.93±17	0.17±15	[illegible]	0.33±15	
C 2	0.84893±40	0.57238±19	0.45982±53	3.03±20	1.98±18	2.40±19	-0.31±15	0.13±16	0.06±15	
C 3	0.80865±45	0.52275±20	0.37993±57	4.54±24	3.06±21	2.33±20	0.26±19	0.68±19	-0.36±17	
C 4	0.72396±43	0.48319±19	0.42871±56	3.95±23	1.61±18	2.83±20	-0.07±16	-0.44±17	-0.30±16	
C 5	0.67928±42	0.49043±18	0.58188±58	3.28±21	1.80±19	3.39±21	-0.48±16	-0.13±17	0.65±16	
C 6	0.72371±40	0.53948±18	0.69031±53	3.11±20	2.23±19	2.15±19	0.13±16	0.11±15	0.42±15	
C11	0.99581±37	0.69646±17	0.92310±52	2.40±19	1.95±19	2.13±18	-0.36±15	0.36±14	-0.17±15	
C21	0.92694±37	0.75330±18	0.99199±52	2.42±18	2.26±18	2.11±18	-0.12±15	-0.27±15	0.06±16	
C31	0.95434±40	0.80061±19	0.01213±57	2.95±20	1.56±18	3.38±21	0.40±15	0.14±16	0.09±16	
C41	0.04475±38	0.79084±18	0.16976±54	2.63±18	2.04±18	2.53±19	-0.42±15	0.16±15	-0.48±15	
C51	0.10916±37	0.73707±19	0.20719±52	2.06±18	2.97±20	2.01±18	0.02±16	-0.51±14	0.01±15	
C61	0.07967±38	0.69048±18	0.08284±53	2.53±19	1.96±18	2.41±19	0.14±15	0.29±15	0.25±15	
N 1	0.84080±31	0.63498±14	0.76174±42	2.93±16	1.77±15	1.87±15	-0.25±13	0.04±12	0.01±12	
N 2	0.93237±36	0.61730±17	0.42394±46	4.02±19	3.71±19	2.41±17	-0.55±15	1.16±14	-0.79±14	
N 4	0.68028±41	0.42964±17	0.31146±52	5.63±23	2.58±18	3.59±19	-0.42±16	-0.54±17	-0.53±15	
N 6	0.67982±40	0.54494±17	0.86210±51	5.38±22	3.23±19	3.41±19	[illegible]	1.10±17	-0.06±15	
N11	0.95954±32	0.64526±14	0.90370±42	2.98±16	1.96±15	1.93±15	-0.02±13	0.02±12	[illegible]	
N21	0.83016±35	0.76535±15	0.72211±47	3.91±19	2.07±16	2.91±17	-0.14±14	-1.01±14	[illegible]	
N41	0.06960±33	0.84075±16	0.30663±48	2.57±16	2.93±17	3.58±18	-0.55±14	0.11±14	-1.19±15	
N61	0.14560±35	0.63148±16	0.12905±45	3.84±19	2.64±17	2.41±16	[illegible]	0.41±14	[illegible]	
O 1	0.87969±38	0.65940±16	0.33704±55	6.93±23	3.55±17	7.85±24	0.34±16	3.61±19	[illegible]	
O 2	0.04590±35	0.60780±20	0.45533±52	4.09±18	9.98±27	5.75±21	-1.10±18	1.19±16	[illegible]	
O 3	0.72026±39	0.42545±16	0.17392±47	7.92±24	4.06±18	4.39±18	[illegible]	0.86±17	[illegible]	
O 4	0.60737±41	0.39399±15	0.36024±50	8.67±26	3.09±16	5.41±20	-2.62±17	0.75±19	[illegible]	
O 5	0.57739±38	0.52268±19	0.87082±53	6.01±22	7.17±24	6.29±22	-2.75±19	3.15±19	[illegible]	
O 6	0.75351±43	0.56959±19	0.99760±46	8.98±26	7.13±24	2.39±15	[illegible]	1.94±16	[illegible]	
O11	0.86330±33	0.75474±14	0.58257±39	5.94±19	3.42±15	[illegible]	-0.15±14	[illegible]	[illegible]	
O21	0.72810±31	0.78665±16	0.73679±47	3.66±16	5.26±19	[illegible]	1.64±15	-1.47±14	[illegible]	
O31	0.04114±32	0.89269±13	0.25384±45	5.29±19	1.81±13	5.15±18	[illegible]	-0.04±14	[illegible]	
O41	0.11630±32	0.92587±15	0.46121±40	4.99±17	4.06±17	2.71±14	0.03±14	[illegible]	[illegible]	
O51	0.25780±29	0.63361±15	0.21000±44	2.98±15	4.02±16	4.62±17	1.21±14	-0.50±13	[illegible]	
O61	0.08334±34	0.58495±13	0.09631±46	5.89±20	1.99±14	5.14±18	0.42±13	-0.98±15	-0.34±13	
H 3	0.8370 ±33	0.5190 ±16	0.2911 ±47							[illegible]
H 5	0.6268 ±31	0.4666 ±15	0.6124 ±44							1.81±74
H31	0.9149 ±31	0.9337 ±15	0.9951 ±43							1.59±71
H51	0.1652 ±28	0.7332 ±13	0.2981 ±39							0.66±62

From the form II data set, 551 values of $|E| > 1·0$ were used in the symbolic addition procedure. Of these, 231 phases were found (57 either 0 or π and 174 phases in terms of the symbols a, b and c). Of the eight E maps computed, seven showed a large anomalous peak and only one appeared reasonable in distribution and intensity of peaks. From this map coordinates for 20 of the 32 non-hydrogen atoms were used as input to refinement. Of the 231 phases assigned with $a=0$, $b=0$ and $c=\pi$, there were two incorrect phases as determined by the final refinement.

The least-squares procedure together with analysis of Fourier syntheses proceeded normally through the process of heavy atoms with isotropic thermal parameters (B's), heavy atoms with anisotropic B's, and finally all atoms with anisotropic B's for heavy atoms and isotropic B's for hydrogens. The full-matrix least-squares program was used throughout the refinement with the exception for form II whenever the storage capabilities were exceeded; in those cases the block-diagonal least-squares routine was employed. All hydrogen atoms were determined by difference Fourier syntheses. The final residual R indices (where $R = \sum||F_o| - |F_c||/\sum|F_o|$), omitting less-thans, were 0·063/0·047 for 1335/1635 observed reflections for form I/form II polymorphs, respectively. The parameter shifts in the last cycle of refinement for both forms were all less than two-tenths of the standard deviation. The final least-squares parameters are given in Table 4, and the corresponding values of observed and calculated structure factors are given in Table 5. All numerical calculations were performed on a CDC-6600 computer using the X-RAY 67 or 71 system of crystallographic programs (Stewart, 1971). The program *ORTEP* (Johnson, 1965) was used for the thermal ellipsoid representations.

Discussion of the structures

Form I

There are two molecules of HNAB in the unit cell with space group $P2_1/c$ so that each molecule lies with its midpoint on a center of symmetry. The molecules possess a *trans* configuration with bond lengths and angles shown in Fig. 2 (no correction for thermal motion). The estimated standard deviations (e.s.d.) of the bond distances are less than 0·005 Å for heavy atoms and 0·03 Å for those involving hydrogen atoms. For bond angles with heavy (H) and light hydrogen atoms

Table 5. *Observed and calculated structure factors for HNAB*

(*a*) Form I

L	10FO	10FC
H# 0 K# 0		
2	278	274
4	654	-659
8	162	-161
H# 0 K# 1		
1	223	240
2	350	342
3	507	565
4	60	-74
5	320	-303
6	391	-385
7	94	-84
8	60	-56
9	51	-46
H# 0 K# 2		
0	1158	1296
1	533	-529
2	197	-185
3	447	-462
4	121	-113
5	194	181
6	46	43
7	190	180
8	63	-70
9	61	52
H# 0 K# 3		
1	821	883
2	317	314
3	37	-49
4	191	195
5	194	-185
6	174	-175
7	46	43
8	80	-79
12	59	-45
H# 0 K# 4		
0	94	79
1	62	-59
2	105	-107
3	284	286
4	56	-53
5	42	50
7	192	-199
9	85	-83
10	53	-54
11	105	-108
H# 0 K# 5		
1	321	313
2	202	195
3	101	-93
4	50	50
5	241	-232
6	47	47
7	70	-72
8	39	24
H# 0 K# 6		
0	377	357
1	117	-118
2	83	88
3	186	183
4	84	-94
6	119	-125
7	120	-125
H# 0 K# 7		
1	54	-39
3	99	-96
5	174	-175
6	42	-31
7	113	107
8	40	-34
9	42	41
H# 0 K# 8		
0	49	43
1	61	45
2	98	-94
3	104	104
4	57	-55
5	44	-45
7	70	67
H# 0 K# 9		
3	35	28
4	105	110
5	103	-106
H# 0 K# 10		
1	55	73
2	72	-78
3	92	95
4	68	-64
H# 1 K# 0		
0	392	-247
10	71	69
2	255	249
-2	663	639
12	61	63
4	385	-395
-4	463	455
6	155	-152
-6	106	101
8	78	72
H# 1 K# 1		
1	282	290
-1	490	-469
-2	499	-491
3	657	-749
-3	251	-244
4	101	-116
-4	303	283
5	173	-157
-5	551	515
-6	240	227
7	142	-138
8	95	-101
-8	57	51
9	108	101
-9	81	85
10	64	-63
-10	91	97
11	105	98
-11	77	73
H# 1 K# 2		
0	717	-744
1	808	-826
-1	198	-201
2	67	72
3	124	115
-3	169	-175
4	44	36
-4	162	155
5	54	53
-5	215	-207
6	198	-187
7	40	-40
-7	139	148
8	98	-92
-8	40	22
9	131	139
-9	41	-54
10	32	30
-10	173	176
11	63	54
-11	38	-31
12	67	59
-12	47	17
H# 1 K# 3		
0	397	374
1	763	776
-1	58	-45
2	521	-525
3	46	39
-3	174	-158
4	262	-249
5	43	-50
-5	101	91
6	83	80
7	103	-112
8	111	-118
-8	34	-29
10	36	-32
-10	90	93
11	82	82
H# 1 K# 4		
0	159	-171
1	49	48
-1	42	-37
2	43	37
-2	171	-164
3	99	91
-3	36	19
4	132	-136
-4	73	-62
5	254	-255
-5	32	33
6	175	-173
-6	76	70
7	342	-345
-7	33	32
8	73	72
10	58	52
-10	115	123
-11	68	84
H# 1 K# 5		
0	101	102
1	167	-165
-1	195	-185
2	336	-320
-2	48	43
3	67	-62
-3	104	109
4	101	-102
-4	191	-191
5	120	112
-5	154	148
6	109	-106
7	146	-150
8	56	47
-8	57	-59
9	33	7
-9	87	-81
10	97	88
11	116	116
H# 1 K# 6		
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6	182	-183
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7	84	-87
8	175	172
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9	86	-88
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H# 1 K# 7		
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7	64	-62
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-8	77	78
-9	50	-50
H# 1 K# 8		
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1	61	-53
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2	259	265
3	126	-126
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6	135	-137
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H# 1 K# 9		
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3	68	75
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6	98	-90
H# 1 K# 10		
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2	63	40
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H# 2 K# 0		
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H# 2 K# 1		
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5	87	-92
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6	212	-210
7	172	174
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8	134	-137
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11	106	-95
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H# 2 K# 2		
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3	241	-238
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4	50	-50
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5	264	259
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6	80	90
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7	215	211
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8	205	-253
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9	68	77
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H# 2 K# 3		
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4	52	41
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H# 2 K# 4		
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8	166	-167
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9	131	129
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10	77	-85
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H# 2 K# 5		
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3	156	157
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5	85	94
6	332	332
-6	136	-132
-7	46	-50
8	76	79
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H# 2 K# 6		
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1	183	189
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3	44	41
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-5	181	-184
6	271	267
9	42	33
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H# 2 K# 7		
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6	88	87
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9	42	-27
H# 2 K# 8		
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H# 2 K# 9		
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3	93	91
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-6	45	-16
H# 2 K# 10		
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H# 3 K# 0		
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8	518	514
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H# 3 K# 1		
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-2	214	203
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-4	490	421
5	233	229
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6	164	-163
-6	41	41
7	203	193
-7	107	100
8	127	-131
-8	205	-205
9	39	-30
-9	93	-102
10	68	67
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H# 3 K# 2		
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2	230	-220
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3	355	-329
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4	46	-38
-4	250	235
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-6	56	44
7	226	228
8	332	321
-8	54	50
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-12	70	-61
H# 3 K# 3		
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2	149	-148
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3	361	-339
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4	157	151
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5	29	26
-5	145	145
6	42	47
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7	360	350
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8	90	-89
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9	133	153
-9	189	-202
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H# 3 K# 4		
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3	81	87
-3	155	148
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-4	40	40
5	50	-48
-5	156	157
-6	129	130
7	67	78
8	194	189
9	72	-75
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10	73	-75
-10	54	62
11	42	2
H# 3 K# 5		
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2	52	-42
-2	70	-70
3	46	-44
-3	32	40
-4	195	177
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6	38	16
-6	32	31
7	33	30
-7	85	94
8	38	40
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10	53	65
-10	41	-52
H# 3 K# 6		
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2	34	-32
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3	121	-120
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4	41	-37
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-5	101	107
-6	43	-42
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8	113	106
-8	120	-125
9	69	-63
-9	51	-42
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H# 3 K# 7		
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1	49	40
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2	113	116
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3	112	-112
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6	92	-90
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H# 3 K# 8		
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3	41	-32
-3	85	83
4	41	-32
-4	155	155
5	60	-55
-5	54	62
-6	34	34
-7	42	-19
-8	47	-47
H# 3 K# 9		
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-5	35	53
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H# 4 K# 0		
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2	235	219
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4	72	-71
-4	199	-166
6	57	54
-6	106	-152
8	166	172
-8	146	-147
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-10	157	-158
H# 4 K# 1		
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1	256	269
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3	468	522
-3	75	77
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-5	152	148
6	97	-92
7	247	-239
-7	69	-57
8	59	63
-8	92	83
-9	73	86
11	43	-30
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H# 4 K# 2		
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3	357	-346
4	206	211
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6	94	93
-6	30	-23
7	117	109
8	100	-118
-8	106	107
9	86	-84
-9	40	-36
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H# 4 K# 3		
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2	259	243
-2	220	214
3	401	384
-3	22	-22
4	115	-115
-4	157	-143
5	35	16
-5	85	-79
6	40	-29
-6	106	-107
-7	112	-105
8	78	68
-8	171	169
9	166	157
-9	46	42
11	40	-48
-11	48	-54
-12	42	-24
H# 4 K# 4		
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1	218	214
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2	226	213
-2	212	-205
3	197	184
-3	197	193
4	71	65
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5	103	97
-5	30	35
-6	163	156
7	52	-58
-7	127	-131
8	190	-194
-8	101	104
9	128	-132
-9	44	48
-11	47	51
H# 4 K# 5		
0	78	-82
1	163	-160
-1	88	83
-2	90	-87
3	42	29
-3	264	258
-4	36	-34
5	90	-96
-5	79	-72
6	41	39
-6	60	58
-7	170	-174
-9	128	135
10	61	-59
H# 4 K# 6		
1	110	107
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2	61	-59
3	32	-30
-3	129	132
-4	89	-94
-5	140	-139
6	42	-30
7	63	64
8	65	-54
-8	70	-69
-9	89	98
-10	44	-47
H# 4 K# 7		
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1	52	51
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3	37	-34
-3	41	-27
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5	100	-93
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-7	70	-63
-8	51	-46
-9	179	185
H# 4 K# 8		
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2	84	-85
3	46	-26
4	34	19
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5	51	53
H# 4 K# 9		
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2	38	32
-2	46	33
3	43	-34
-3	60	-62
-4	59	-59
H# 4 K# 10		
0	51	-26
H# 5 K# 0		
0	28	-72
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-4	163	150
6	52	48
-6	239	241
8	89	94
-8	148	174
-12	109	-109
H# 5 K# 1		
0	135	-124
1	306	-288
-1	298	274
2	168	175
-2	37	-30
3	113	129
-3	196	-170
4	168	214
-4	54	54
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6	48	-48
7	45	-48
-7	560	556
8	43	-34
-8	35	-12
9	84	-49
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11	42	-30
H# 5 K# 2		
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1	98	-100
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2	46	46
-2	162	-145
3	174	-172
-3	199	-187
4	183	166
-4	51	-43
5	115	-110
6	71	-73
7	30	15
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8	110	-106
-8	240	242
9	41	-42
-9	109	106
10	75	-70
-10	134	131
-12	49	-47
H# 5 K# 3		
0	168	-160
1	187	182
2	99	-99
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6	68	-61
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-7	219	217
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-9	39	-36
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H# 5 K# 4		
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1	50	-45
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3	37	-25
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4	100	100
-4	106	-96
5	151	-152
-5	158	162
6	105	-107
7	109	-103
-8	200	208
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H# 5 K# 5		
0	279	-271
1	33	-34
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2	117	-117
3	53	-54
-3	227	-227
4	250	-245
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5	125	119
6	36	-37
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8	48	41
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9	120	-110
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H# 5 K# 6		
0	90	-88
1	85	-85
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-3	55	-56
-4	33	-21
5	95	-86
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6	36	39
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8	119	112
-8	81	76
-9	46	-40
H# 5 K# 7		
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2	50	42
3	51	60
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4	52	-60
-4	39	34
5	45	45
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-8	86	94
H# 5 K# 8		
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1	110	-118
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2	51	52
-2	121	-128
3	51	54
-4	60	-53
5	87	-80
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-6	64	-61
-7	75	77
H# 5 K# 9		
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H# 6 K# 0		
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2	67	56
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4	73	85
-4	165	-169
6	73	-79
-6	215	217
8	32	-40
-8	234	-238
-10	62	-59
-12	186	178
H# 6 K# 1		
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1	293	281
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3	82	85
-3	85	-79
-4	52	46
5	44	-27
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-6	322	-323
7	187	-189
-7	93	-90
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9	59	-61
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10	61	39
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H# 6 K# 2		
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3	88	83
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-4	80	-81
-5	127	-120
6	64	-84
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7	62	-59
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8	102	-132
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-9	81	-81
-10	37	-24
H# 6 K# 3		
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1	38	-36
-1	219	-208
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6	59	65
-6	216	-207
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8	69	63
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9	84	92
-9	108	-106
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H# 6 K# 4		
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6	88	-96
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7	50	54
-7	48	51
8	75	-72
-8	80	-77
9	97	95
-9	48	-53
H# 6 K# 5		
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2	62	-63
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3	74	68
-3	72	75
4	189	191
-4	79	-82
5	85	84
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-7	92	-81
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H# 6 K# 6		
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3	31	20
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4	106	115
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-5	215	-219
6	41	6
7	64	74
-7	54	-53
H# 6 K# 7		
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-5	124	126
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-6	46	-44
-8	42	-47
H# 6 K# 8		
0	80	-85
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-2	114	114
-5	49	-58
H# 6 K# 9		
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-3	49	35
H# 7 K# 0		
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2	246	-251
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4	203	-206
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-8	88	-92
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H# 7 K# 1		
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3	48	-55
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4	43	52
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5	49	40
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-6	62	52
-7	231	-235
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-10	95	-90
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H# 7 K# 2		
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2	186	-183
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3	134	-128
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-4	49	-38
6	132	136
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-9	69	63
-10	119	118
-11	40	-29
H# 7 K# 3		
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1	318	-311
2	119	116
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3	151	-151
-3	189	-188
4	30	-7
-4	138	-138
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-5	46	39
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7	51	52
-7	42	-46
9	75	74
-10	93	-83
H# 7 K# 4		
0	82	-87
1	48	-43
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2	90	94
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3	99	90
-3	33	31
4	58	-68
-4	182	179
5	103	106
-5	117	-126
6	39	43
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7	43	-47
-10	66	64
H# 7 K# 5		
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1	89	-85
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2	90	94
-2	61	-59
3	97	-99
-3	60	-70
-4	56	-55
5	51	60
-5	128	-128
6	38	-33
-6	91	91
7	38	-36
-8	60	44
H# 7 K# 6		
0	96	-94
-1	159	160
-2	53	56
-3	44	-60
4	74	-74
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-5	38	-4
-6	161	-168
-7	76	71
H# 7 K# 7		
-1	199	205
2	48	-50
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3	44	28
-3	41	38
-5	71	-75
H# 7 K# 8		
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3	52	-42
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-4	75	74
-5	67	70
H# 8 K# 0		
0	65	-21
2	112	-113
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-4	172	174
8	42	55
-8	130	-134
-10	149	-148
H# 8 K# 1		
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1	482	473
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2	103	-115
3	57	-69
4	64	60
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5	108	-119
-5	31	-43
6	110	105
-6	44	-44
7	99	98
-7	122	-121
-8	54	-54
-9	89	-84
-10	53	47
H# 8 K# 2		
0	360	346
1	48	41
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3	201	204
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4	46	46
-4	126	-136
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6	33	21
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7	49	-44
-7	168	166
-8	69	-62
-10	36	-42
H# 8 K# 3		
0	285	286
1	204	193
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2	84	-85
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-4	29	-34
5	107	-103
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6	71	68
7	49	55
-7	78	-82
-8	53	-61
-10	38	35
H# 8 K# 4		
0	367	363
1	35	49
-1	46	47
2	41	45
3	121	120
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-4	179	-180
-5	36	-8
6	77	-73
7	40	-24
-7	110	-118
-8	39	-49
H# 8 K# 5		
0	139	149
1	51	46
2	36	41
3	91	-89
-3	131	129
4	62	55
-4	53	-57
5	65	-60
-5	53	-52
-6	50	49
7	38	36
H# 8 K# 6		
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1	45	57
-1	53	53
2	82	-79
-3	60	-57
4	95	-98
-4	44	-40
5	38	30
-5	39	37
-6	75	68
-7	55	-64
H# 8 K# 7		
1	66	60
-1	66	58
2	52	52
-2	57	-64
4	62	64
-5	78	-76
H# 8 K# 8		
0	52	47
-3	71	-78
H# 9 K# 0		
0	396	-409
2	156	151
-2	83	-95
4	41	33
-4	200	206
6	53	-53
-6	128	121
-8	65	55
-10	53	49
H# 9 K# 1		
0	56	-61
1	44	28
-1	53	-48
2	54	-60
-2	74	77
-3	39	19
4	36	38
-4	55	-56
5	82	83
-5	162	173
-6	48	-66
-7	42	51
-9	55	52
-10	51	18
H# 9 K# 2		
0	128	-129
1	146	152
2	168	160
-2	52	53
3	61	-66
-3	30	-43
4	53	-52
-4	163	170
5	50	-62
-5	119	127
7	59	-55
-9	57	45
H# 9 K# 3		
1	135	-131
2	120	-115
-2	66	64
-3	39	25
4	49	-56
-5	137	113
6	42	-40
-6	64	56
7	80	-77
-8	51	48
H# 9 K# 4		
0	81	-81
1	67	-66
2	148	151
-2	72	-76
3	171	-176
-3	112	114
4	47	-51
-4	147	152
5	42	-42
-5	115	120
-8	58	-53
H# 9 K# 5		
1	99	-96
2	112	-112
-2	44	47
3	60	63
-4	107	119
-6	51	66
H# 9 K# 6		
0	117	-119
1	43	28
2	35	-18
-2	115	-119
3	96	-95
-4	44	25
-5	54	27
-6	80	81
H# 9 K# 7		
-1	61	-62
2	84	-81
-2	49	52
-4	66	53
H# 10 K# 0		
0	98	-102
2	32	28
-2	84	-88
4	35	25
-4	151	161
6	41	-36
-6	43	35
-8	113	109
H# 10 K# 1		
0	55	-65
1	79	-76
-1	105	103
2	95	-109
-2	50	55
3	40	24
-3	118	123
-4	45	45
-5	45	-61
-6	65	-67
-8	99	-98
H# 10 K# 2		
1	132	133
2	93	-89
-2	66	69
-3	72	-67
-4	57	54
5	36	-40
-5	43	-44
-6	37	33
-7	40	-20
-8	106	100
-9	46	30
H# 10 K# 3		
0	89	-90
1	130	-128
-1	147	-151
-2	87	-80
-3	134	141
-5	139	144
-6	42	-32
-7	43	33
-8	65	-65
H# 10 K# 4		
0	47	33
-1	77	-73
2	93	-95
-2	107	120
3	96	-100
-3	102	-102
4	83	78
-4	34	-21
5	71	68
-5	40	-38
-7	80	-76
H# 10 K# 5		
0	53	-65
1	47	45
2	94	104
-2	95	-101
-3	40	12
4	48	22
-5	62	36
H# 10 K# 6		
2	118	-112
-2	44	43
-3	65	-64
H# 11 K# 0		
0	157	-159
2	60	-66
4	93	-94
H# 11 K# 1		
0	80	-82
1	79	-73
-1	79	-79
2	39	-45
3	47	-32
-3	65	-65
4	43	-35
-4	47	44
-6	36	-31
-7	77	84
-8	47	50
H# 11 K# 2		
0	57	-54
-2	66	-70
3	38	39
4	89	-90
-4	86	-84
-5	75	76
-7	40	1
H# 11 K# 3		
1	106	-100
-1	110	-109
2	91	93
-2	50	-45
4	67	-65
-5	37	-37
-6	47	-45
-7	101	105
H# 11 K# 4		
1	55	-55
-2	66	-72
-3	62	77
-6	75	67
H# 11 K# 5		
1	37	31
-1	50	47
-4	48	39
H# 12 K# 0		
-4	58	-53
H# 12 K# 1		
0	43	-46
1	35	25
-1	95	84
3	82	87
-4	37	-16
-5	90	-90
H# 12 K# 2		
0	75	72
1	91	94
-2	76	63
-4	112	-118
-5	50	-45
H# 12 K# 3		
-1	37	40
-3	63	-70

Table 5 (*cont.*)

(*b*) Form II

0,0,L		
1	325	-307
2	503	-562
3	176	-167
4	119	-106
5	24	27
6	88	-84
7	125	117
0,1,L		
1	117	-106
2	110	114
3	258	250
4	240	-228
5	34	30
6	36	-61
7	167	175
0,2,L		
0	0*	-12
1	506	-510
2	410	402
3	86	67
4	416	-403
5	43	39
6	221	216
7	64	66
0,3,L		
1	93	-95
2	263	-239
3	415	391
4	65	-59
5	567	560
6	276	-274
7	201	-303
0,4,L		
0	503	-515
1	177	170
2	374	341
3	79	79
4	332	-303
5	10*	-20
6	150	-154
7	173	191
0,5,L		
1	1379	-1467
2	302	289
3	434	-411
4	230	-218
5	88	85
6	469	462
7	49	-49
0,6,L		
0	641	-662
1	183	-168
2	85	91
3	38	-42
4	74	-83
5	29	27
6	69	-54
7	21*	3
0,7,L		
1	60	-22
2	860	-847
3	224	201
4	184	181
5	72	-81
6	101	106
7	26*	-35
0,8,L		
0	390	401
1	731	-690
2	636	-580
3	304	-343
4	123	-122
5	343	343
6	423	-421
0,9,L		
1	7*	9
2	474	-444
3	297	-288
4	134	140
5	251	-250
6	195	199
0,10,L		
0	39	-52
1	0*	-26
2	593	547
3	141	137
4	21*	-13
5	49	37
6	119	-125
0,11,L		
1	293	270
2	109	96
3	119	121
4	270	-284
5	0*	7
6	57	63
0,12,L		
0	233	221
1	454	-419
2	313	303
3	205	193
5	38	-43
4	105	-103
6	10*	14
0,13,L		
1	186	179
2	165	-147
3	234	-238
4	92	82
5	185	190
6	45	39
0,14,L		
0	78	78
1	345	343
2	257	-258
3	98	-97
4	185	190
5	101	116
0,15,L		
1	41	-41
2	0*	-6
3	192	196
4	154	163
5	130	-127
0,16,L		
0	129	117
1	117	105
2	386	317
3	198	-196
4	27*	15
5	20*	23
0,17,L		
1	170	-179
2	138	136
3	53	52
4	34	34
0,18,L		
0	344	-354
1	362	-356
2	67	-67
3	109	110
4	98	106
0,19,L		
1	150	157
2	130	-120
3	98	94
0,20,L		
0	0*	-4
1	107	104
2	21*	-35
3	66	70
0,21,L		
1	92	101
2	172	-171
0,22,L		
0	201	-201
1,1,L		
-7	196	192
-6	78	93
-5	8*	-12
-4	140	-114
-3	101	97
-2	1250	-1313
-1	32	-33
0	0*	-40
1	267	249
2	363	349
3	269	259
4	102	81
5	28	-29
6	112	124
7	99	93
1,2,L		
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-6	40	-42
-5	177	-160
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-3	1161	1173
-2	107	104
-1	509	-489
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1	473	-453
2	530	509
3	560	-526
4	147	133
5	139	143
6	181	194
7	59	52
1,3,L		
-7	169	-170
-6	23*	23
-5	20	26
-4	553	-550
-3	476	-471
-2	452	420
-1	201	186
0	647	659
1	532	501
2	545	-507
3	283	-265
4	123	-117
5	66	-53
6	364	-372
7	6*	-1
1,4,L		
-7	152	161
-6	52	-63
-5	27	23
-4	79	80
-3	615	591
-2	437	400
-1	1072	1093
0	432	423
1	240	-225
2	172	-157
3	55	-62
4	270	270
5	44	-41
6	121	125
7	135	-136
1,5,L		
-7	154	150
-6	120	115
-5	227	214
-4	104	13
-3	535	-522
-2	544	522
-1	98	95
0	730	741
1	515	-483
2	764	736
3	304	-350
4	25	14
5	66	-75
6	113	109
7	222	227
1,6,L		
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-6	256	279
-5	37	-20
-4	239	-244
-3	743	-726
-2	634	604
-1	631	603
0	127	112
1	76	-69
2	39	38
3	372	340
4	371	-373
5	36	-42
6	228	231
1,7,L		
-7	67	-60
-6	59	-60
-5	319	-315
-4	240	235
-3	620	595
-2	21	12
-1	712	-697
0	251	-216
1	660	631
2	801	739
3	435	-431
4	306	-290
5	178	-174
6	214	-210
1,8,L		
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-6	27*	25
-5	349	-353
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-3	81	68
-2	335	-311
-1	144	-136
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1	112	107
2	858	-809
3	257	255
4	109	-120
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6	0*	-17
1,9,L		
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-5	120	112
-4	56	54
-3	84	99
-2	350	-341
-1	304	286
0	77	39
1	75	71
2	102	-105
3	231	227
4	130	-130
5	43	41
6	12*	2
1,10,L		
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-5	71	-72
-4	326	-339
-3	218	230
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-1	463	430
0	472	-449
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2	30	-31
3	241	-244
4	70	-76
5	30	-22
6	85	80
1,11,L		
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-5	135	137
-4	56	-51
-3	209	-276
-2	0*	10
-1	157	146
0	112	110
1	552	-520
2	435	-415
3	83	94
4	411	410
5	250	257
6	77	82
1,12,L		
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-5	135	-140
-4	147	-156
-3	46	43
-2	435	-405
-1	90	74
0	119	108
1	14*	21
2	363	-340
3	227	-224
4	37	46
5	14*	-1
6	56	-59
1,13,L		
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-5	137	-151
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-2	287	260
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0	137	-135
1	402	-400
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3	167	158
4	181	-186
5	85	-77
1,14,L		
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-1	201	192
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2	157	-147
3	89	87
4	197	-199
5	93	-97
1,15,L		
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-2	192	187
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1	219	224
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4	32	-25
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1,16,L		
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-1	210	-207
0	143	-138
1	122	121
2	55	-56
3	137	142
4	54	-54
1,17,L		
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-3	100	98
-2	101	-104
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0	155	156
1	138	-145
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3	20*	-22
4	98	-108
1,18,L		
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-3	6*	6
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-1	215	220
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1	240	-240
2	93	95
3	71	72
4	150	172
1,19,L		
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-2	31	-26
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0	279	280
1	58	-61
2	102	-106
3	59	72
1,20,L		
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-2	122	-125
-1	0*	15
0	0*	26
1	251	258
2	157	157
1,21,L		
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-1	384	-392
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1	94	91
2	65	72
2,0,L		
-7	105	-107
-6	193	-202
-5	66	65
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-3	305	-306
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2	415	395
3	370	-334
4	141	-134
5	331	-329
6	25*	-29
7	111	-117
2,1,L		
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-1	258	-253
0	387	-375
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2	356	-338
3	689	-647
4	134	149
5	42	-45
6	59	-54
7	12*	-1
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0	1141	-1257
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2	259	-238
3	283	259
4	57	-51
5	10*	-21
6	240	-257
2,3,L		
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-3	552	-522
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0	151	-140
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3	243	234
4	30	-3
5	170	-177
6	302	-312
2,4,L		
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-4	202	-182
-3	208	-208
-2	250	-236
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0	740	-724
1	1409	1442
2	152	144
3	218	-199
4	23*	23
5	93	-95
6	140	147
2,5,L		
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-2	861	-825
-1	85	-81
0	367	-346
1	1276	1269
2	210	-189
3	335	-315
4	52	-50
5	145	158
6	90	90
2,6,L		
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-6	176	180
-5	157	154
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-2	165	149
-1	526	-504
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1	1272	1261
2	423	-398
3	430	411
4	257	242
5	181	-182
6	337	338
2,7,L		
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-6	25*	24
-5	41	48
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-2	69	-63
-1	157	-145
0	596	571
1	433	-420
2	235	219
3	86	-86
4	59	-58
5	282	-303
6	150	-144
2,8,L		
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-5	30	-27
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-3	224	-219
-2	10*	1
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0	153	154
1	466	-434
2	203	-181
3	200	196
4	169	160
5	80	-78
6	170	169
2,9,L		
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-1	756	752
0	403	-373
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2	406	-465
3	10*	10
4	99	109
5	37	24
6	170	186
2,10,L		
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-1	234	215
0	589	553
1	376	337
2	79	73
3	52	-55
4	117	-127
5	78	80
6	33	-33
2,11,L		
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-5	301	-307
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-2	156	-148
-1	132	123
0	409	382
1	115	103
2	142	-153
3	256	-261
4	181	-187
5	36	-32
6	15*	-16
2,12,L		
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-5	126	-128
-4	26	12
-3	179	184
-2	403	-386
-1	334	334
0	71	-66
1	200	-183
2	182	-178
3	198	-195
4	17*	2
5	201	-218
2,13,L		
-6	37	-28
-5	156	-150
-4	422	443
-3	92	-97
-2	0*	2
-1	131	134
0	0*	-5
1	130	120
2	36	-35
3	105	-114
4	247	246
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2,14,L		
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-4	74	-82
-3	148	-153
-2	250	253
-1	119	103
0	459	-462
1	23*	22
2	188	-189
3	132	141
4	154	-156
5	162	167
2,15,L		
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-4	168	-181
-3	37	43
-2	23*	17
-1	121	113
0	89	-97
1	175	180
2	131	131
3	53	58
4	10*	-11
2,16,L		
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-4	0*	7
-3	139	149
-2	172	170
-1	152	150
0	73	-98
1	190	-180
2	24*	27
3	35	35
4	69	-77
2,17,L		
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-3	12*	-3
-2	107	104
-1	373	380
0	320	-321
1	0*	8
2	0*	-10
3	108	127
4	118	-138
2,18,L		
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-3	115	-119
-2	304	-307
-1	428	-434
0	81	77
1	138	-134
2	0*	-9
3	154	160
2,19,L		
-3	23*	-27
-2	66	-76
-1	15*	-36
0	30	-50
1	116	120
2	10*	1
2,19,L		
3	15*	-12
2,20,L		
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-2	64	-63
-1	66	73
0	349	365
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2	6*	-24
2,21,L		
-2	153	-167
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0	197	-218
1	17*	-10
3,1,L		
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-2	966	-956
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0	226	-212
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3	453	423
4	29	23
5	37	-28
6	26*	18
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-6	11*	12
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-4	14*	-18
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-2	1232	-1252
-1	1118	-1191
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1	140	143
2	517	-488
3	446	-423
4	391	389
5	84	-86
6	75	-67
3,3,L		
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-5	141	139
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-2	891	871
-1	671	-653
0	407	-410
1	257	232
2	42	-43
3	64	80
4	100	-100
5	27	-40
6	57	-61
3,4,L		
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-3	253	-230
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-1	222	199
0	772	-745
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2	77	60
3	418	-405
4	134	-120
5	104	109
6	195	-203
3,5,L		
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-2	89	94
-1	326	-313
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2	281	-265
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6	281	288
3,6,L		
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-6	54	58
-5	274	-272
-4	179	-179
-3	400	-367
-2	165	146
-1	567	-537
0	282	-269
1	91	95
2	141	123
3	152	-137
4	161	-151
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6	22*	22
3,7,L		
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-6	111	118
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1	186	174
2	368	-335
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4	226	-219
5	340	-348
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3,8,L		
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-3	77	-80
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1	38	-39
2	153	151
3	173	176
4	49	-64
5	155	-152
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3,9,L		
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2	465	-450
3	107	-108
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6	60	-52
3,10,L		
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-3	112	-111
-2	117	98
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1	525	497
2	0*	-18
3	143	140
4	41	43
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3,11,L		
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2	99	94
3	257	266
4	83	60
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3,12,L		
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-1	151	140
0	156	-155
1	123	-122
2	101	105
3	106	-110
4	130	135
5	86	85
3,13,L		
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-5	138	-144
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-2	79	90
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1	92	84
2	227	223
3	150	-149
4	252	-252
5	136	-143
3,14,L		
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1	36	31
2	121	-130
3	119	-125
4	0*	-7
3,15,L		
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-3	164	-151
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-1	247	-247
0	107	100
1	173	167
2	37	-27
3	10	-14
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3,16,L		
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-4	31	34
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0	176	179
1	100	-109
2	80	-84
3	21*	-10
4	84	-97
3,17,L		
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-3	78	81
-2	12*	-11
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0	222	-215
1	69	68
2	22	-8
3	219	-235
3,18,L		
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1	138	149
2	62	66
3	22*	-12
3,19,L		
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-1	260	266
0	19*	-23
1	188	-195
2	101	-117
3,20,L		
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-1	35	-47
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1	31	27
3,21,L		
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4,0,L		
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-1	1880	1898
0	298	299
1	81	89
2	589	-552
3	69	-61
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5	121	120
6	87	73
4,1,L		
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-6	52	-55
-5	120	-122
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-3	79	71
-2	113	-115
-1	109	-106
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1	489	-473
2	537	-492
3	112	-92
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5	128	-128
6	37	39
4,2,L		
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-6	18*	23
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1	129	120
2	491	461
3	17*	0
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6	44	-35
4,3,L		
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-6	79	-89
-5	220	-231
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-2	122	113
-1	112	-105
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1	121	130
2	31	24
3	233	-250
4	94	94
5	64	-62
6	106	106
4,4,L		
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-2	110	101
-1	101	-96
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1	131	-109
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3	36	45
4	37	-43
5	70	-77
6	29*	-14
4,5,L		
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-6	207	213
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1	240	-227
2	44	-50
3	280	290
4	84	-85
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6	74	-87
4,6,L		
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-5	55	-56
-4	11*	-17
-3	266	-254
-2	514	-510
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3	47	55
4	119	-124
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6	116	-126
4,7,L		
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-6	136	-136
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-2	315	-307
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3	176	-181
4	262	-254
5	150	-160
4,8,L		
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-2	104	-100
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0	378	-351
1	326	-314
2	216	213
3	78	-56
4	143	143
5	17*	22
4,9,L		
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-5	14*	-18
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-3	119	114
-2	185	-173
-1	356	-349
0	246	-215
1	34	-13
2	146	143
3	290	288
4	231	234
5	354	368
4,10,L		
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-3	37	30
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0	405	383
1	169	-180
2	19*	20
3	60	-69
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5	100	109
4,11,L		
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-4	72	-67
-3	185	-177
-2	0*	14
-1	73	-83
0	87	-94
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2	72	63
3	350	-360
4	196	-200
5	13*	-5
4,12,L		
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-2	66	68
-1	79	79
0	491	-490
1	246	259
2	49	-41
3	160	-160
4	83	-77
4,13,L		
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-4	101	-103
-3	62	-59
-2	29	43
-1	93	-89
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1	102	-105
2	65	74
3	92	88
4	60	65
4,14,L		
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-3	29	-32
-2	43	57
-1	161	-152
0	255	268
1	184	177
2	20*	-25
3	37	-33
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4,15,L		
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-4	291	304
-3	13*	16
-2	60	-71
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0	360	366
1	240	-247
2	156	154
3	32	-34
4	161	-164
4,16,L		
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-3	252	252
-2	144	143
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0	113	-111
1	323	325
2	62	-66
3	16*	-6
4,17,L		
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-2	116	122
-1	176	-175
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1	109	-109
2	110	-117
3	120	-137
4,18,L		
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-2	120	-137
-1	114	113
0	87	-76
1	46	-54
2	135	140
4,19,L		
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-2	97	-87
-1	22*	-23
0	232	243
1	22*	10
4,20,L		
-2	95	93
-1	267	283
0	57	63
5,1,L		
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-6	89	84
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-4	128	-127
-3	206	202
-2	87	-91
-1	150	144
0	202	168
1	77	79
2	0*	-6
3	75	-66
4	92	101
5	39	-37
5,2,L		
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-6	137	-136
-5	28	25
-4	310	-315
-3	35	33
-2	265	-241
-1	95	-92
0	89	-77
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2	101	-105
3	292	292
4	76	69
5	21*	6
5,3,L		
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-6	110	111
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-4	17*	-17
-3	182	167
-2	4*	6
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0	211	210
1	99	-94
2	56	67
3	268	-262
4	249	256
5	140	-150
5,4,L		
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-6	10*	-1
-5	16*	11
-4	261	265
-3	428	395
-2	249	244
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0	40	58
1	145	-142
2	159	-160
3	301	306
4	141	149
5	43	36
5,5,L		
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-6	66	64
-5	96	97
-4	191	-191
-3	171	152
-2	141	-138
-1	297	-277
0	170	-174
1	177	-175
2	44	51
3	101	109
4	64	54
5	129	130
5,6,L		
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-6	15*	10
-5	99	-101
-4	14*	16
-3	52	-53
-2	499	-453
-1	214	204
0	56	-56
1	237	-229
2	100	100
3	0*	1
4	118	108
5	116	120
5,7,L		
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-3	456	439
-2	54	-56
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0	167	-159
1	140	-144
2	278	287
3	122	-128
4	222	225
5	92	-94
5,8,L		
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-5	97	-99
-4	32	29
-3	119	124
-2	52	-37
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0	59	49
1	221	-215
2	190	193
3	140	-151
4	80	-93
5	99	-96
5,9,L		
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-2	137	128
-1	156	150
0	42	-42
1	316	-313
2	159	168
3	60	-64
4	190	202
5	19*	3
5,10,L		
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-2	17*	-20
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1	61	55
2	148	157
3	266	-276
4	288	-315
5,11,L		
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-5	31	31
-4	25*	-15
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-2	86	-87
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0	82	-86
1	78	69
2	263	257
3	145	152
4	75	76
5,12,L		
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-4	173	-183
-3	223	219
-2	232	-238
-1	111	108
0	96	-94
1	20*	34
2	38	22
3	19*	-15
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5,13,L		
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-3	76	74
-2	15*	7
-1	63	-68
0	88	93
1	58	51
2	0*	-3
3	99	-97
4	39	-38
5,14,L		
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-4	194	193
-3	49	48
-2	166	-168
-1	40	41
0	66	68
1	106	105
2	88	-84
3	20*	-2
5,15,L		
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-3	65	59
-2	17*	12
5,15,L		
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1	158	-158
2	120	138
3	10*	-25
5,16,L		
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-3	181	-180
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-1	46	41
0	230	228
1	172	175
2	191	200
3	82	-80
5,17,L		
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-2	29	-32
-1	37	-37
0	75	77
1	42	-33
2	195	-212
5,18,L		
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-2	30	-30
-1	37	46
0	37	-40
1	0*	-4
5,19,L		
-2	47	48
-1	40	49
0	55	63
6,0,L		
-7	73	70
-6	0*	-8
-5	125	-130
-4	87	85
-3	113	-120
-2	0*	4
-1	216	-203
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1	382	-370
2	156	-157
3	139	139
4	74	-60
5	58	66
6,1,L		
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-6	29	44
-5	64	65
-4	0*	-4
-3	141	144
-2	233	-221
-1	84	73
0	0*	29
1	620	-597
2	122	-104
3	124	126
4	0*	-14
5	196	-203
6,2,L		
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1	132	-141
2	94	87
3	41	-39
4	87	106
5	160	-174
6,3,L		
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-6	47	-41
-5	176	-170
-4	216	219
-3	204	-8
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-1	103	100
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2	27	17
3	30	29
4	130	128
5	83	-86
6,4,L		
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0	160	164
1	70	69
2	117	-110
3	39	-26
4	16*	-19
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6,5,L		
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1	184	177
2	53	59
3	201	-203
4	26*	-11
5	95	93
6,6,L		
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0	39	-47
1	246	250
2	133	126
3	55	-58
4	69	72
6,7,L		
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0	175	-174
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2	427	-426
3	118	-106
4	241	-257
6,8,L		
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-3	47	45
-2	29	25
-1	123	-122
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1	212	207
2	18*	-21
3	207	220
4	26*	24
6,9,L		
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-5	11*	3
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-3	203	-196
-2	109	-88
-1	18	-10
0	0*	7
1	54	-49
2	196	201
3	617	632
4	200	205
6,10,L		
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-2	92	80
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0	121	-124
1	91	-89
2	32	-36
3	13*	7
4	56	62
6,11,L		
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-4	11*	18
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-2	61	-56
-1	126	-128
0	125	129
1	290	300
2	514	-520
3	223	-225
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6,12,L		
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-2	87	-93
-1	65	-73
0	60	-62
1	442	-445
2	15*	-8
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6,13,L		
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-4	67	71
-3	51	50
-2	49	-51
-1	17*	-10
0	0*	5
1	234	239
2	17*	26
3	84	85
6,14,L		
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-3	49	60
-2	10*	2
-1	43	39
0	160	156
1	255	-270
2	89	87
3	100	-102
6,15,L		
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-2	57	46
-1	40	61
0	129	-127
1	160	157
2	6*	7
6,16,L		
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-2	12*	2
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0	125	122
1	27*	-15
2	97	-102
6,17,L		
-3	170	-171
-2	115	110
-1	27*	34
0	339	-368
1	74	-76
6,18,L		
-2	24*	22
-1	139	146
0	19*	-13
7,1,L		
-6	75	-77
-5	151	155
-4	123	130
-3	40	-50
-2	284	276
-1	101	-97
0	267	-245
1	16*	-25
2	57	53
3	186	214
4	154	-181
7,2,L		
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-5	59	-62
-4	25*	32
-3	399	-390
-2	465	-454
-1	187	190
0	315	302
1	128	119
2	207	-202
3	39	41
4	64	-62
7,3,L		
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-5	25*	32
-4	135	137
-3	189	198
-2	277	-275
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0	15*	9
1	83	69
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3	57	56
4	55	-65
7,4,L		
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-2	172	169
-1	430	-426
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1	110	110
2	72	85
3	68	-68
4	49	59
7,5,L		
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-2	162	-159
-1	10*	7
0	68	80
1	14*	7
2	113	121
3	43	-51
4	100	129
7,6,L		
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0	104	-107
1	79	85
2	247	258
3	29	22
4	54	-69
7,7,L		
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-3	47	-51
-2	190	194
-1	185	-181
0	202	-206
1	80	78
2	166	166
3	86	-96
4	92	-86
7,8,L		
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-5	76	86
-4	126	116
-3	22*	20
-2	121	109
-1	30	22
0	106	-100
1	100	110
2	60	-72
3	53	-52
7,9,L		
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-4	43	-44
-3	21*	-11
-2	109	104
-1	32	-30
0	151	144
1	294	-299
2	224	-214
3	160	171
7,10,L		
-5	159	165
-4	80	77
-3	51	-59
-2	85	85
-1	9*	16
0	224	231
1	114	-17
2	294	-309
3	46	-48
7,11,L		
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-4	34	-28
-3	79	-76
-2	148	148
-1	26*	19
0	115	119
1	145	159
2	171	-198
3	58	-39
7,12,L		
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-4	79	-86
-3	73	71
-2	22*	20
-1	225	-218
0	0*	3
1	166	174
2	38	49
7,13,L		
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-3	66	70
-2	44	40
-1	93	91
0	37	-42
1	104	108
2	99	112
7,14,L		
-4	113	137
-3	20*	17
-2	36	-24
-1	68	60
0	55	59
1	76	-65
2	135	144
7,15,L		
-3	208	211
-2	76	-81
-1	65	-63
0	78	80
1	58	57
7,16,L		
-2	82	-91
-1	115	-122
0	88	100
8,0,L		
-6	16*	-12
-5	77	85
-4	140	130
-3	239	-237
-2	31	25
-1	297	280
0	254	-253
1	269	-277
2	39	41
3	128	140
8,1,L		
-6	75	71
-5	125	128
-4	124	123
-3	64	59
-2	29	-18
-1	107	-94
0	227	-217
1	20*	26
2	121	124
3	165	-175
8,2,L		
-6	14*	39
-5	88	-91
-4	250	233
-3	60	59
-2	75	66
-1	71	74
0	179	-179
1	264	265
2	40	-45
3	36	34
8,3,L		
-6	77	76
-5	216	222
-4	35	-36
-3	40	44
-2	125	112
-1	102	-86
0	188	188
1	37	30
2	33	-45
3	29	23
8,4,L		
-6	101	-93
-5	55	-54
-4	294	301
-3	58	53
-2	55	-56
-1	240	-247
0	61	-54
1	46	-38
2	79	86
3	57	46
8,5,L		
-5	131	142
-4	115	-125
-3	48	-49
-2	74	-73
-1	45	45
0	95	-89
1	133	134
2	47	54
3	66	-66
8,6,L		
-5	244	-257
-4	81	-75
-3	22*	13
-2	213	214
-1	25*	29
0	71	65
1	86	-94
2	211	-220
3	20*	7
8,7,L		
-5	110	117
-4	186	192
-3	106	-112
-2	49	62
-1	58	55
0	152	-157
1	107	-99
2	115	-110
3	64	11
8,8,L		
-5	64	60
-4	114	-112
-3	0*	10
-2	45	-40
-1	249	252
0	26*	-6
1	32	-47
2	161	-163
8,9,L		
-5	142	-154
-4	43	-53
-3	37	36
-2	101	-110
-1	73	-74
0	31	34
1	220	226
2	590	623
8,10,L		
-4	41	-45
-3	27*	-21
-2	15*	-6
-1	53	51
0	78	80
1	151	146
2	162	-165
8,11,L		
-4	46	44
-3	15*	1
-2	117	-120
-1	0*	0
0	92	85
1	362	-382
2	39	43
8,12,L		
-4	58	63
-3	70	85
-2	56	59
-1	214	-240
0	54	-56
1	204	215
8,13,L		
-3	68	73
-2	106	109
-1	26*	-31
0	30	36
1	107	111
8,14,L		
-2	151	161
-1	165	183
0	0*	-10
9,1,L		
-5	16*	-12
-4	87	86
-3	23*	-26
-2	94	91
-1	160	162
0	107	122
1	85	-95
2	19*	18
9,2,L		
-5	91	-111
-4	158	154
-3	180	-181
-2	11*	12
-1	103	107
0	16*	3
1	19*	-7
2	34	43
9,3,L		
-5	63	-63
-4	72	-73
-3	191	197
-2	42	37
-1	151	151
0	37	30
1	60	-64
2	102	-106
9,4,L		
-5	79	74
-4	213	222
-3	61	62
-2	10*	-16
-1	49	-43
0	42	39
1	52	-54
2	42	32
9,5,L		
-5	61	54
-4	129	-134
-3	84	83
-2	74	69
-1	46	44
0	263	-268
1	101	-98
2	29*	-25
9,6,L		
-4	116	-110
-3	17*	19
-2	32	32
-1	69	-69
0	90	103
1	107	101
2	84	75
9,7,L		
-4	129	139
-3	51	-43
-2	164	-151
-1	40	-43
0	225	228
1	263	274
9,8,L		
-4	122	140
-3	21*	15
-2	143	-146
-1	14*	-17
0	113	-112
1	147	-159
9,9,L		
-4	74	-60
-3	10*	-9
-2	71	71
-1	24*	-17
0	68	-72
1	63	-71
9,10,L		
-3	71	75
-2	111	-111
-1	16*	-19
0	166	-165
9,11,L		
-3	45	-35
-2	83	89
-1	111	122
0	19*	30
10,0,L		
-4	441	-468
-3	306	314
-2	63	66
-1	85	-94
0	182	-181
1	60	76
10,1,L		
-4	79	84
-3	28*	14
-2	43	-44
-1	45	-47
0	52	47
1	83	-87
10,2,L		
-4	74	-73
-3	116	115
-2	14*	-9
-1	107	112
0	75	75
1	85	-90
10,3,L		
-4	45	-41
-3	130	126
-2	22*	14
-1	0*	-3
0	40	-42
10,4,L		
-3	96	102
-2	111	-106
-1	31	31
0	180	191
10,5,L		
-3	91	85
-2	159	-167
-1	16*	-20
0	126	129
10,6,L		
-3	60	67
-2	142	155
-1	54	-55
0	0*	5
10,7,L		
-2	89	93
-1	120	-136

(L), the e.s.d.'s are less than 0·4° for H–H–H, 3° for H–H–L and 4° for L–H–L angles. The average C–C bond length of 1·388, C–N of 1·480 and N–O of 1·221 Å are in good agreement with those reported for other polynitroaromatic compounds (see references quoted by Cady, 1967). The interior angles of the benzene ring at the carbon atoms bearing the nitro-substitutents are significantly larger than the remaining angles; this is consistent with the hypothesis of Carter, McPhail & Sim (1966) concerning the effect of electron-withdrawing power on bond geometry.

The least-squares best plane through the benzene ring as determined by the method of Schomaker, Waser, Marsh & Bergman (1959) is

$$-1\cdot749x+7\cdot856y-2\cdot352z=-1\cdot559$$

and $\sigma_p=0\cdot027$ Å. The distances of selected atoms from this plane and angles of twist for the nitro groups are shown in Fig. 3. The *o*-nitro groups are rotated appreciably with respect to the plane through the carbon skeleton which is the result of intramolecular steric hindrance (the contact separations between oxygen atoms are 3·02–3·10 Å). The remaining *p*-nitro group rotation is caused by a near-neighbor contact with an adjacent symmetry-related molecule. The close contact separation of 2·83 Å involves a nitrogen and oxygen atom from each *p*-substituted nitro group. A feature not in common with other azobenzene compounds concerns the azo-nitrogen atom. In HNAB this nitrogen atom is located off the least-squares benzene plane (0·26 Å) towards the direction of the molecular center; the N–C bond forms an angle of 10·4° with the benzene plane. This is not the case in azobenzene and *p*-azotoluene. In those compounds in which no bulky *o*-substitution exists, the corresponding angle is smaller than 1·5°.

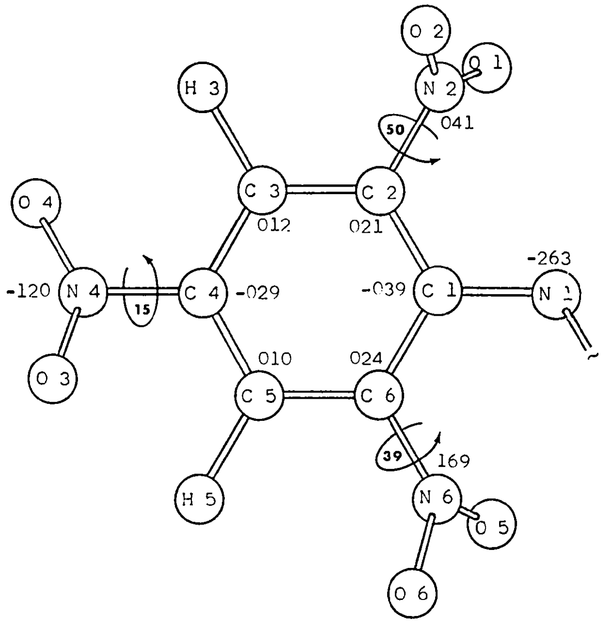

Fig. 3. Deviation of atoms from best plane of benzene ring (in 0·001 Å units) and angles of twist for HNAB, form I.

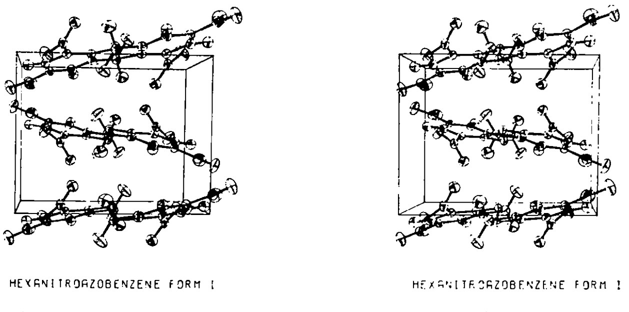

Fig. 4. Stereo pair illustrating the molecular packing in HNAB, form I.

As observed in the stereo molecular packing illustration of Fig. 4, the ring carbon atoms are nearly isotropic. The thermal parameters which might be more indicative of anisotropic motion are those for the nitrogen and oxygen atoms of the *p*-nitro substituents (the *o*-nitro substituents are sterically hindered). Although these atoms suggest some motional anisotropy, they are also involved in the 2·83 Å near-neighbor contact with an adjacent molecule involving N(4) and O(4'). There does not appear to be any other significant intermolecular interaction in the structure.

Form II

Covalent bond lengths found for the form II polymorph are given in Fig. 5 (no correction for thermal motion) and the bond angles and angles of twist in Fig. 6. Although the estimated standard deviations are the same as those given for form I, they appear to be underestimated. The average C–C bond length of 1·375, C–N of 1·482 and N–O of 1·211 Å are comparable to form I. However, the differences between these averages are probably not real as a consequence of neglect of thermal corrections. The N–O separations are consistently (though not significantly) smaller in form II; this probably results from the thermal motion of the oxygen atoms which is generally larger and more anisotropic in form II. Within the limits of error of the determination, the benzene rings are planar. The equations of the best plane through the rings are:

$$\text{ring C(1)–C(6)};\ -7\cdot156x+11\cdot90y-2\cdot599z=-0\cdot545\ (\sigma_p=0\cdot007\ \text{Å})$$

$$\text{ring C(11)–C(61)};\ 8\cdot817x+6\cdot961y-4\cdot768z=9\cdot152\ (\sigma_p=0\cdot011\ \text{Å})$$

where x, y and z are fractional coordinates of the monoclinic cell. The distances of selected atoms from the best planes are:

C(1) through C(6);	0·000, 0·009, −0·008, 0·000, 0·008, −0·008 Å
C(11) through C(61);	−0·013, 0·004, 0·010, −0·013, 0·002, 0·010 Å
N(1) through N(6);	0·105, 0·117, −0·020, −0·076 Å
N(11) through N(61);	−0·041, 0·052, −0·099, −0·034 Å.

As shown in Fig. 6 one nitro group, O(4)–N(4)–O(3), is twisted only 1° with respect to carbon ring C(1) → C(6) and is essentially coplanar with the ring. All other substitutent groups are substantially rotated out of the benzene planes. Although the two carbon rings of the molecule are not parallel to each other as in form I and are rotated to each other by an angle of 81°, the molecule possesses a *trans* configuration.

A comparison of the geometrical configurations of molecules found in the two polymorphic forms proves interesting. In form I, because of the center of symmetry, the two carbon rings of the molecule are parallel

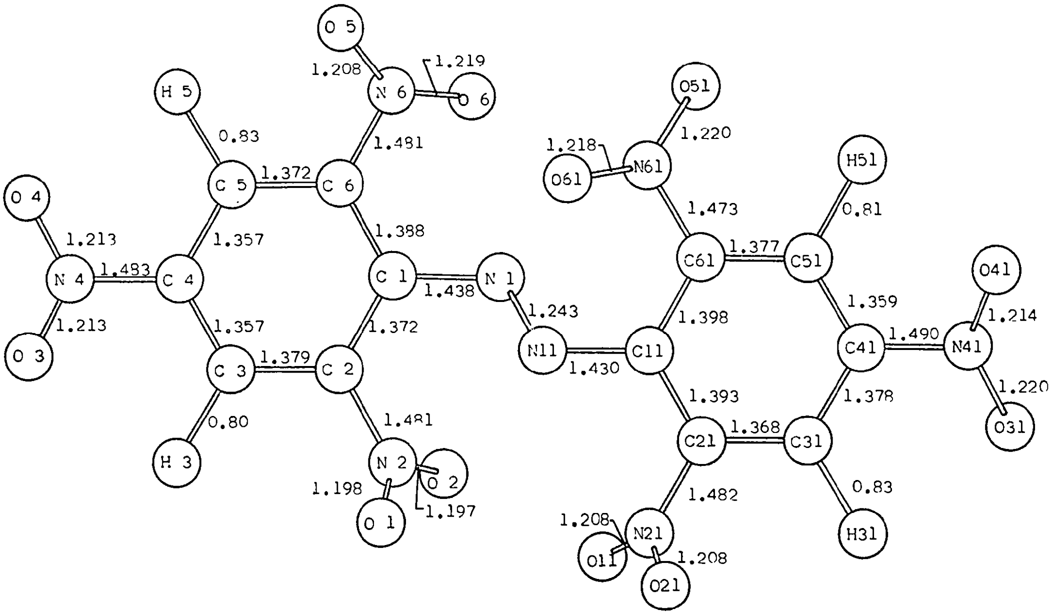

Fig. 5. Bond lengths (Å) in HNAB, form II.

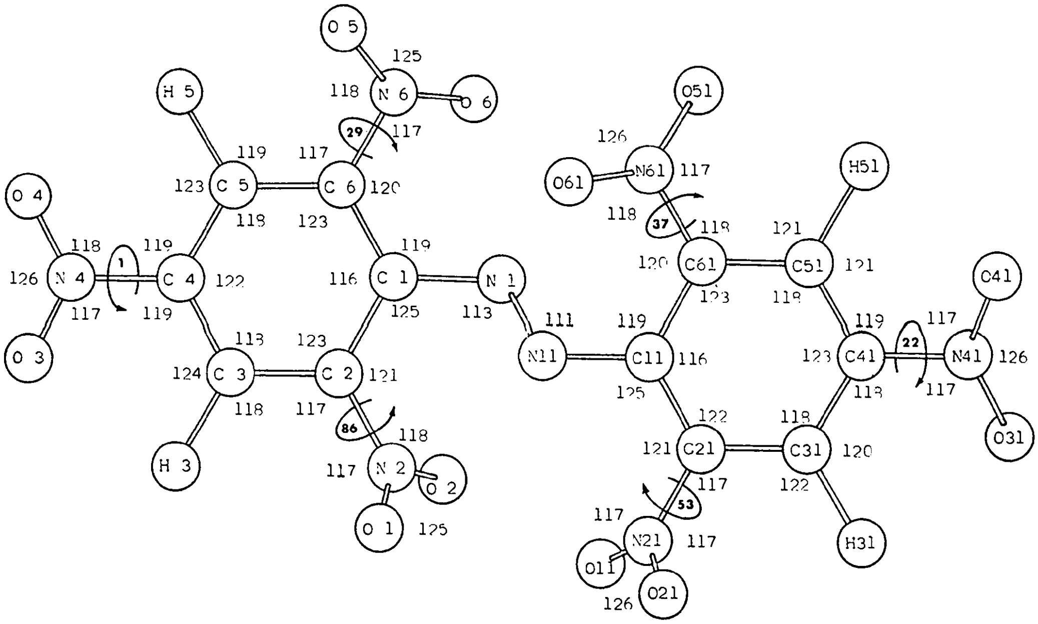

Fig. 6. Bond angles and angles of twist (°) in HNAB, form II.

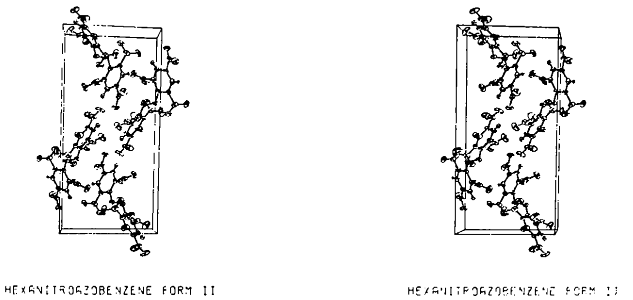

Fig. 7. Stereo pair illustrating the molecular packing in HNAB, form II.

whereas in form II they are rotated to each other by 81°. The center of symmetry in form I demands that the torsion angle about the azo linkage be 180°; this restriction is removed in form II and the angle becomes 177·5° which indicates a slight twist or strain in the double bond of the azo group. Furthermore, the angles between the carbon ring planes and the azo group (*i.e.*, plane through ring C(1) and C(1)–N=N in form II) are 49·4 and 50·9° for C(1) and C(11), respectively, compared with the single value of 43·2° in form I. These differences in the configurations and particularly the 81° twist of the planes result in less efficient molecular packing and is probably important in yielding the higher-energy less-stable form II polymorph with a lower (≈3%) density.

As seen in the stereo molecular packing illustrations of Fig. 7, the angle of rotation of the nitro groups seems to be dependent primarily upon steric effects. Even though the thermal motion for nitrogen and oxygen atoms is quite large, there appears to be no significant intermolecular interactions in the structure.

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The Crystal Structure of $BaCd_{4\cdot43}$

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$BaCd_{4\cdot43}$ has a hexagonal sub-cell, space group *P*6/*mmm*, with lattice constants $a=10\cdot740$ (3), $c=10\cdot200$ (3) Å, $\varrho_{obs}=7\cdot35$ g cm^{-3}. The true unit cell appears to be hexagonal with doubled *a* and *c* axes. A reasonable solution has been obtained for the sub-cell by the symbolic addition method using photographic data. The sub-cell contains 7 atoms of Ba and 31 of Cd, with one set of cadmium positions partially occupied.

In a previous paper (Bruzzone, 1972) a phase had been reported to exist in the Ba–Cd system with the approximate composition $BaCd_{4\cdot5}$ and a preliminary examination of a single crystal had shown hexagonal symmetry of Laue group 6/*mmm*. The purpose of the present work was the determination of the crystal structure of this phase.

Starting with Ba 99·5% pure supplied by Fluka (Switzerland) and Cd 99·999% pure produced by Koch-Light Co. (Great Britain), alloys of the composition $BaCd_{4\cdot5}$ were melted in iron crucibles under argon. After melting, some samples were quenched and some were annealed at 500°C.

Single-crystal techniques confirmed the Laue sym-