CHEMISTRY OF MATERIALS

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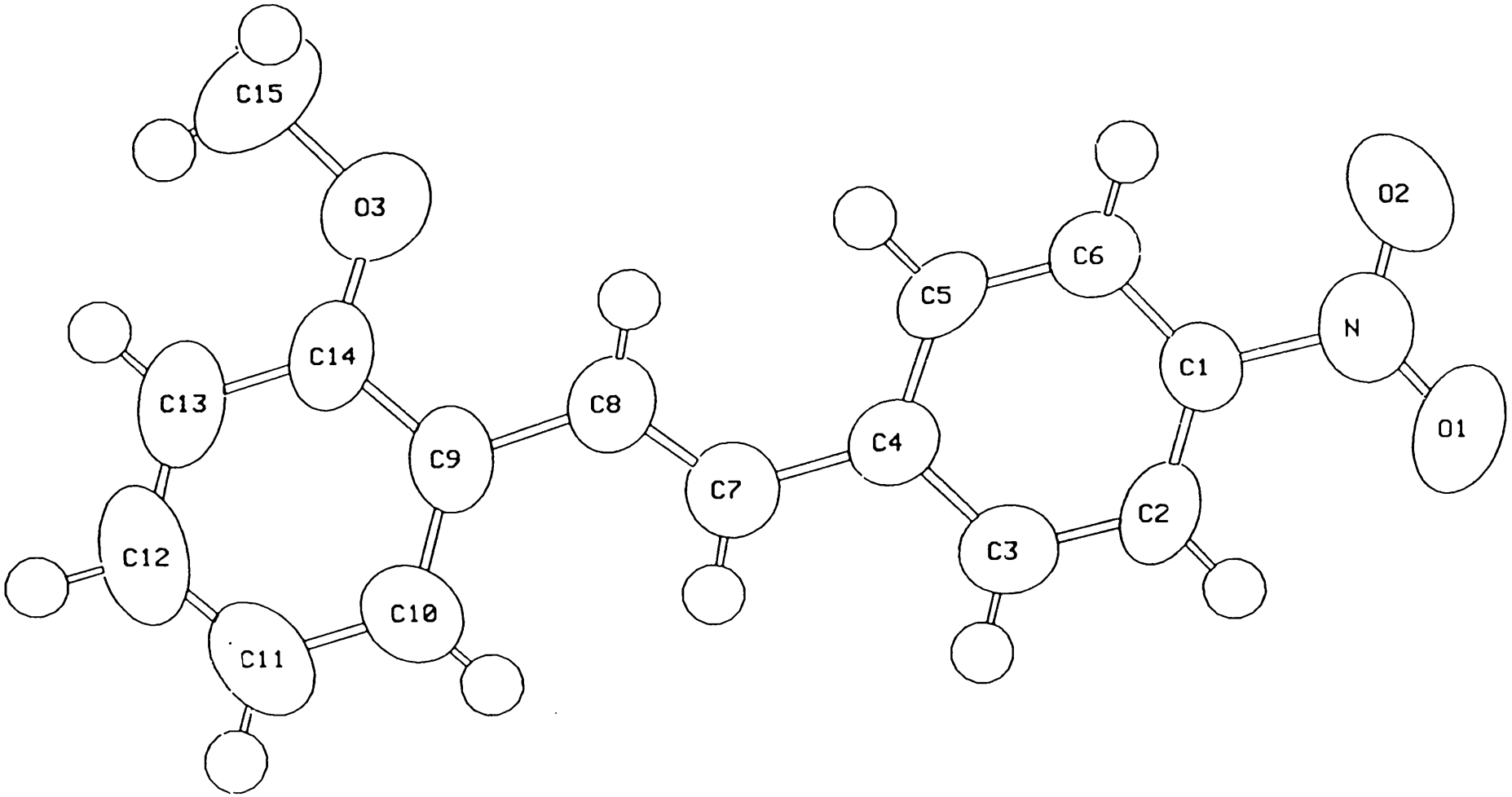
GRUBBS

3-4

The Structure of 2-Methoxy-4′-Nitrostilbene



50% thermal ellipsoids
H's given arbitrary, small B's.

I-4-M1

I-4-M2

The Structure of 2-Methoxy-4′-Nitrostilbene

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Abstract.

The structure of 2-methoxy-4′-nitrostilbene, $C_{15}H_{13}NO_3$, has been determined. It crystallizes in the orthorhombic system, in space group $Pna2_1$, (#33), with $a = 14.422(6)$Å, $b = 7.329(2)$Å, $c = 12.237(7)$Å, , volume = 1293.4 (10)Å^3; $z = 4$.

Experimental.

A plate-like crystal was cut to size and glued to a glass fiber with epoxy cement. Preliminary cell dimensions and an orientation matrix were calculated from the setting angles of 25 reflections with $11° < 2\theta < 24°$. (Final cell dimensions came from data on 22 reflections with $20° < 2\theta < 23°$.) The reflections were broad; the three independent data sets were collected with omega scans for that reason. The data were reduced to structure factors, correcting for a minor decay, and the structure was solved by MULTAN. Least squares refinement was normal; hydrogen atoms were introduced at calculated positions (C-H = 0.95Å) or based on a difference map (C15). They were assigned thermal parameters 20% greater than the equivalent isotropic thermal parameter of the carbon atom they are bonded to. The difference map for C15 showed two orientations of the three hydrogen atoms, so six half-atoms were

used to model the disorder. The final difference map had several peaks of +0.4 eÅ^{-3}, one near the nitro group and two near C9; one hole of -0.4 eÅ^{-3} was at C3.

Calculations were done with programs of the CRYM Crystallographic Computing System and ORTEP. Scattering factors and corrections for anomalous scattering were taken from a standard reference (International Tables for X-ray Crystallography, Vol. IV, p. 71, p. 149; Birmingham, Kynoch Press, 1974). $R = \Sigma||F_o| - |F_c||/\Sigma F_o$, for only $F_o^2 > 0$, and goodness of fit $= [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{\frac{1}{2}}$ where n is the number of data and p the number of parameters refined. The function minimized in least squares was $\Sigma w(F_o^2 - F_c^2)^2$, where $w = 1/\sigma^2(F_o^2)$. Variances of the individual reflections were assigned based on counting statistics plus an additional term, $0.014I^2$. Variances of the merged reflections were determined by standard propagation of error plus another additional term, $0.014\langle I\rangle^2$.

Discussion.

The molecule displays the expected geometry. Carbon-carbon bonds in the benzene rings average 1.381 (15)Å; the external bonds are as expected, also. The C=C between the rings is 1.307(11)Å, short as is usual in this type of compound. All bond angles are within normal ranges.

The molecules stack in the cell parallel to the *a c* plane, with π-π interactions as short as 3.43Å (C6-C13) and 3.45Å (C3-O3). Most other interplanar interactions are in the 3.55-3.8Å range. The molecules themselves are all nearly parallel, but their axes meet at angles of about 100°. The *a c* plane is a polar plane and all the molecules do have a component of their N-O3 vector aligned approximately along *c*.

Acknowledgements.

We thank the NSF for Grant CHE-8219039 to purchase the diffractometer.

References.

International Tables for X-ray Crystallography, Vol. IV, p. 71, p. 149; Birmingham, Kynoch Press, 1974

I-4-M4

Table S I. Crystallographic Data for 2-Methoxy-4′-Nitrostilbene

Crystal Color: yellow	Crystal Habit: plates
$a = 14.422(6)$ Å	
$b = 7.329(2)$ Å	
$c = 12.237(7)$ Å	
T = 23°C	λ = 0.71073 Å
CAD-4	2θ range: 3° - 50°
ω	Octants of data collected: ±h,k,l; h,-k,l.
Graphite monochromator: yes	μ = 0.99 cm^{-1}
$\mu r_{max} = 0.035$	
Crystal Size: 0.12 × 0.46 × 0.52mm	
Total Number Reflections: 3941	
Total Independent Reflections: 1196	
GOF for Merging: 1.09	
Number of Reflections used in Refinement: 1196	
Number of Reflections with $F_o^2 > 0$: 848	
Number of Reflections with $F_o^2 > 3\sigma(F_o^2)$: 522	
(R for reflections with h $F_o^2 > 3\sigma(F_o^2)$: 0.046	

Table S II. Final Heavy Atom Parameters for 2-Methoxy-4′-Nitrostilbene

x, y, z and U_{eq}[a] $\times 10^4$

Atom	x	y	z	U_{eq}
O1	5341(4)	1353(9)	14222	1168(21)
O2	4319(3)	1030(8)	12946(6)	1081(17)
N	5120(5)	1229(9)	13266(6)	820(19)
C1	5861(5)	1311(10)	12436(8)	593(18)
C2	6736(5)	1676(9)	12756(7)	701(19)
C3	7418(5)	1746(10)	11992(8)	760(23)
C4	7258(5)	1473(10)	10890(7)	600(19)
C5	6339(5)	1109(10)	10598(7)	652(19)
C6	5629(4)	1040(9)	11355(8)	637(20)
C7	8028(4)	1535(11)	10111(8)	726(22)
C8	7993(4)	1267(10)	9056(8)	660(20)
C9	8805(5)	1290(10)	8307(7)	655(21)
C10	9724(5)	1232(10)	8681(7)	813(21)
C11	10451(5)	1228(11)	7967(9)	975(26)
C12	10304(7)	1266(11)	6855(10)	1017(29)
C13	9400(7)	1362(10)	6478(8)	882(26)
C14	8561(6)	1364(11)	7180(7)	706(25)
O3	7742(4)	1436(8)	6852(6)	944(17)
C15	7556(6)	1393(13)	5701(8)	1107(30)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

Table S III. Assigned Hydrogen Parameters for 2-Methoxy-4′-Nitrostilbene

x, y and $z \times 10^4$

Atom	x	y	z	B
H2	6877	1882	13495	6.9
H3	8035	1989	12241	7.3
H5	6200	897	9837	6.5
H6	5009	775	11148	6.6
H7	8617	1801	10405	7.0
H8	7393	1004	8745	6.5
H10	9834	1235	9444	8.0
H11	11067	1168	8225	9.6
H12	10815	1210	6342	9.8
H13	9293	1457	5700	9.1
H15A	7229	2454	5526	10.4
H15B	7226	329	5552	10.4
H15C	8151	1381	5365	10.4
H15D	6922	1273	5598	10.4
H15E	7893	388	5425	10.4
H15F	7790	2503	5419	10.4

Table S IV. Anisotropic Displacement Parameters for 2-Methoxy-4′-Nitrostilbene

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	1375(54)	1465(52)	664(38)	−150(44)	204(39)	−27(49)
O2	766(32)	1270(44)	1208(44)	64(35)	200(40)	200(41)
N	919(49)	713(38)	827(51)	51(48)	153(50)	44(47)
C1	589(40)	575(40)	614(50)	57(43)	74(42)	23(39)
C2	875(50)	757(47)	472(40)	8(45)	77(51)	−79(40)
C3	721(53)	831(55)	728(57)	−34(41)	−81(50)	7(50)
C4	674(43)	542(47)	583(51)	39(45)	−55(44)	−31(38)
C5	853(50)	666(47)	437(36)	38(49)	−100(44)	−44(41)
C6	676(51)	628(47)	606(52)	−82(38)	−46(44)	12(46)
C7	715(54)	760(53)	704(53)	−46(44)	6(44)	−37(45)
C8	804(52)	559(44)	616(51)	−9(41)	50(40)	−38(44)
C9	798(52)	479(41)	689(56)	−3(46)	181(46)	−76(47)
C10	706(46)	790(50)	943(57)	−10(55)	44(53)	−53(57)
C11	736(52)	935(59)	1254(76)	−28(47)	223(61)	−210(69)
C12	1124(71)	786(61)	1142(78)	−13(61)	528(69)	−106(68)
C13	1228(74)	680(51)	737(58)	−48(61)	310(61)	69(53)
C14	995(66)	517(50)	606(57)	−92(60)	177(57)	−11(50)
O3	1085(43)	966(41)	782(37)	162(39)	−87(38)	−38(42)
C15	1686(95)	881(61)	754(55)	23(69)	−268(59)	−23(60)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

I-4-M7

Table S V. Complete Distances and Angles for 2-Methoxy-4'-Nitrostilbene

Distance(Å)			Angle(°)			
O1	-N	1.216(9)	O2	-N	-O1	124.1(6)
O2	-N	1.228(9)	C1	-N	-O1	118.0(7)
N	-C1	1.475(11)	C1	-N	-O2	117.8(7)
C1	-C2	1.347(11)	C2	-C1	-N	119.0(7)
C1	-C6	1.379(11)	C6	-C1	-N	118.6(7)
C2	-C3	1.359(11)	C6	-C1	-C2	122.4(7)
C2	-H2	0.939	C3	-C2	-C1	119.0(7)
C3	-C4	1.382(11)	H2	-C2	-C1	121.1
C3	-H3	0.957	H2	-C2	-C3	120.0
C4	-C5	1.398(11)	C4	-C3	-C2	123.0(7)
C4	-C7	1.464(11)	H3	-C3	-C2	117.4
C5	-C6	1.381(10)	H3	-C3	-C4	119.6
C5	-H5	0.966	C5	-C4	-C3	115.8(7)
C6	-H6	0.949	C7	-C4	-C3	120.2(7)
C7	-C8	1.307(11)	C7	-C4	-C5	123.9(7)
C7	-H7	0.943	C6	-C5	-C4	122.5(7)
C8	-C9	1.488(11)	H5	-C5	-C4	118.4
C8	-H8	0.964	H5	-C5	-C6	119.1
C9	-C10	1.403(11)	C5	-C6	-C1	117.2(7)
C9	-C14	1.396(11)	H6	-C6	-C1	120.9
C10	-C11	1.366(12)	H6	-C6	-C5	121.8
C10	-H10	0.946	C8	-C7	-C4	127.6(7)
C11	-C12	1.378(13)	H7	-C7	-C4	116.2
C11	-H11	0.943	H7	-C7	-C8	116.3
C12	-C13	1.385(14)	C9	-C8	-C7	125.2(7)
C12	-H12	0.968	H8	-C8	-C7	117.0
C13	-C14	1.369(13)	H8	-C8	-C9	117.8
C13	-H13	0.967	C10	-C9	-C8	122.9(7)
C14	-O3	1.385(11)	C14	-C9	-C8	119.4(7)
O3	-C15	1.435(11)	C14	-C9	-C10	117.7(7)
C15	-H15A	0.934	C11	-C10	-C9	121.1(7)
C15	-H15B	0.931	H10	-C10	-C9	118.7
C15	-H15C	0.952	H10	-C10	-C11	120.1
C15	-H15D	0.926	C12	-C11	-C10	120.9(8)
C15	-H15E	0.945	H11	-C11	-C10	120.6
C15	-H15F	0.946	H11	-C11	-C12	118.5
			C13	-C12	-C11	118.4(9)
			H12	-C12	-C11	121.5
			H12	-C12	-C13	120.2
			C14	-C13	-C12	121.6(9)
			H13	-C13	-C12	118.8
			H13	-C13	-C14	119.6
			C13	-C14	-C9	120.2(8)
			O3	-C14	-C9	115.5(7)
			O3	-C14	-C13	124.3(8)
			C15	-O3	-C14	117.6(7)
			H15A	-C15	-O3	107.5

Table S V. Complete Distances and Angles for 2-Methoxy-4'-Nitrostilbene *(CON'T.)*

			Angle(°)
H15B	-C15	-O3	107.8
H15C	-C15	-O3	104.8
H15D	-C15	-O3	108.7
H15E	-C15	-O3	105.7
H15F	-C15	-O3	105.8
H15B	-C15	-H15A	113.2
H15C	-C15	-H15A	111.4
H15C	-C15	-H15B	111.6
H15E	-C15	-H15D	112.7
H15F	-C15	-H15D	112.6
H15F	-C15	-H15E	110.9

Table S VI. Observed and Calculated Structure Factors for 2-Methoxy-4'-Nitrostilbene

I-4-M9

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

0 0 1

2	919	933	-17
4	254	262	-29
6	138	136	7
8	275	264	30
10	49	58	-24
12	39	56	-31
14	53	63	-15

0 1 1

1	141	149	-39
3	353	363	-32
5	431	434	-6
7	211	215	-16
9	63	64	0
11	-43	23	-62
13	-18	24	-19

0 2 1

0	347	347	0
2	145	139	28
4	126	125	3
6	88	87	6
8	10	25	-20
10	14	34	-21
12	-20	31	-43
14	11	4	2

0 3 1

1	169	163	26
3	127	130	-18
5	276	266	28
7	115	113	10
9	17	31	-21
11	51	42	24
13	-34	15	-29

0 4 1

0	1348	1322	22
2	286	270	48
4	130	130	2
6	36	51	-38
8	92	94	-9
10	19	30	-14
12	51	49	3

0 5 1

1	96	94	7
3	113	110	11
5	140	142	-8
7	54	61	-23
9	41	32	18
11	23	30	-7

0 6 1

0	121	126	-24
2	54	56	-7
4	35	53	-45
6	27	34	-12
8	-29	12	-21
10	18	32	-15

0 7 1

1	41	49	-16
3	-16	16	-16
5	42	45	-5
7	-22	7	-11

0 8 1

0	145	150	-16
2	26	35	-11
4	31	33	-3

1 1 1

0	109	108	2
1	309	310	-4
2	97	101	-24
3	73	78	-22
4	212	217	-21
5	171	177	-30
6	284	281	9
7	74	75	-4
8	52	54	-9
9	51	52	-3
10	42	45	-6
11	-13	33	-28
12	-21	20	-23
13	-38	14	-37
14	-14	20	-13

1 2 1

0	1840	1655	117
1	1740	1624	90
2	393	403	-36
3	155	156	-4
4	54	58	-18
5	143	141	12
6	274	280	-18
7	108	111	-17
8	97	90	30
9	42	42	1
10	24	41	-23
11	98	100	-5
12	19	38	-26
13	-27	20	-24
14	20	35	-18

1 3 1

0	85	85	0
1	174	171	13
2	142	146	-20
3	137	135	10
4	119	115	22
5	174	174	-1
6	187	184	11
7	79	79	0
8	-16	19	-21
9	5	37	-31
10	3	27	-15
11	57	62	-13
12	15	17	-1
13	-19	13	-13

1 4 1

0	308	306	5
1	63	50	51
2	136	136	-3
3	49	52	-11
4	81	81	2
5	39	40	-1
6	25	33	-15
7	-18	12	-15
8	10	23	-12
9	-25	10	-22
10	57	49	22
11	-24	14	-19
12	21	28	-6

1 5 1

0	34	34	0
1	109	110	-3
2	53	50	11
3	23	37	-30
4	60	59	4
5	43	50	-23
6	49	56	-19
7	-35	0	-44
8	-33	12	-30
9	32	26	11
10	40	26	19
11	25	19	6

1 6 1

0	209	207	8
1	241	245	-12
2	39	34	9
3	-13	26	-24
4	14	35	-29
5	18	38	-39
6	54	56	-6
7	-9	24	-13
8	25	19	5
9	19	13	3
10	-24	11	-18

1 7 1

0	57	55	4
1	44	43	2
2	22	25	-4
3	-27	21	-33
4	-7	31	-21
5	36	44	-11
6	21	36	-19
7	8	22	-8
8	-26	5	-18

1 8 1

0	66	59	20
1	11	13	0
2	22	21	0
3	13	19	-5
4	-22	15	-13
5	8	9	0

2 0 1

0	239	226	48
1	922	924	-2
2	881	938	-75
3	351	349	5
4	330	320	25
5	130	130	-1
6	418	435	-39
7	146	149	-11
8	99	104	-22
9	25	27	-2
10	192	187	17
11	122	126	-15
12	55	50	10
13	16	29	-9
14	-29	12	-16

2 1 1

0	-20	37	-78
1	318	319	-4
2	111	108	19
3	205	212	-30
4	103	101	7
5	59	61	-10
6	244	238	21
7	45	47	-9
8	5	27	-25
9	73	70	13
10	78	78	-1
11	108	110	-6
12	-31	15	-33
13	-23	18	-18
14	24	19	3

2 2 1

0	368	351	48
1	198	184	56
2	170	172	-5
3	117	114	13
4	53	54	-2
5	44	45	-4
6	31	27	9
7	-16	16	-16
8	-11	21	-15
9	22	22	0
10	44	37	9
11	13	14	0
12	-13	16	-13
13	-21	9	-10
14	-17	7	-6

2 3 1

0	-17	6	-11
1	222	214	27
2	233	220	44
3	-10	20	-16
4	-14	14	-13
5	17	33	-38
6	78	74	18
7	35	46	-30
8	-35	8	-36
9	47	45	4
10	51	44	17
11	37	49	-20
12	-10	16	-9
13	16	11	3

2 4 1

0	174	164	37
1	322	301	56
2	284	278	17
3	101	102	-2
4	71	74	-14
5	40	45	-16
6	154	156	-6
7	67	74	-26
8	29	37	-16
9	-19	21	-19
10	94	88	20
11	77	78	-3
12	-10	21	-11

2 5 1

0	59	55	16
1	104	104	0
2	11	20	-11
3	18	13	3
4	62	64	-7

5	30	41	-18
6	95	99	-18
7	-29	15	-31
8	-24	20	-27
9	23	24	-1
10	40	45	-9
11	52	50	3

2 6 1

0	130	130	-1
1	79	73	20
2	54	58	-11
3	59	61	-5
4	-31	20	-50
5	-26	19	-35
6	-32	5	-34
7	-25	7	-15
8	-31	13	-29
9	-20	13	-15
10	28	30	-1

2 7 1

0	-7	3	-1
1	43	43	0
2	44	59	-40
3	-25	3	-14
4	17	5	5
5	-18	10	-13
6	-24	7	-12
7	5	16	-5
8	-17	4	-5

2 8 1

0	4	37	-37
1	44	56	-19
2	33	46	-20
3	-25	11	-15
4	8	2	1
5	29	8	14

3 1 1

0	208	204	15
1	146	143	14
2	228	239	-48
3	256	260	-13
4	114	112	11
5	171	170	3
6	62	62	-1
7	8	20	-10
8	25	31	-12
9	45	53	-23
10	157	149	31
11	59	61	-4
12	26	37	-16
13	-31	11	-24
14	-12	10	-5

3 2 1

0	217	209	28
1	182	192	-43
2	152	153	-3
3	162	163	-5
4	157	158	-1
5	224	215	33
6	61	69	-37
7	175	177	-12
8	178	172	25
9	78	80	-7
10	243	233	36
11	-25	3	-14
12	56	64	-23
13	4	22	-11

3 3 1

0	128	128	-1
1	66	71	-27
2	170	165	19
3	79	79	0
4	111	105	29
5	115	117	-8
6	97	97	0
7	23	33	-16
8	38	43	-14
9	72	69	10
10	137	130	27
11	52	44	19
12	32	39	-13
13	-25	12	-16

3 4 1

0	131	126	25
1	120	122	-8
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13 3 1

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13 4 1

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14 1 1

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15 1 1

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15 2 1

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15 3 1

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16 0 1

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5	-20	3	-6

16 1 1

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16 2 1

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16 3 1

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17 1 1

0	35	17	18