

# Supporting Information

## Skeletal torsion tunneling and methyl internal rotation: The coupled large amplitude motions in phenyl acetate

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**Table S1.** Fourier expansion of the potential energy curve of phenyl acetate calculated at the MP2/6-311++G(d,p) level of theory given in Figure 3. The data were obtained by rotating phenyl ring about the O<sub>12</sub>–C<sub>13</sub> bond by varying the dihedral angle  $\alpha = \angle(\text{C}_{13}\text{-O}_{12}\text{-C}_3\text{-C}_2)$  in a grid of 10°, while all other molecular parameters were optimized. The potential is expanded as:

$$V(\beta) = b_0 + \sum_{n=1}^7 b_n \cos(n\beta);$$

Fourier expansion of the potential energy curves given in Figure 4 calculated at the MP2/6-311++G(d,p) level of theory, obtained by rotating the methyl group of phenyl acetate about the C<sub>13</sub>–C<sub>14</sub> bond (variation of  $\gamma = \angle(\text{O}_{15}\text{-C}_{13}\text{-C}_{14}\text{-H}_{16})$ ). The potential is expanded as

$$V(\alpha) = a_0 + \sum_{n=1}^3 a_n \cos(n\alpha).$$

	Hartree	cm <sup>-1</sup>
b <sub>0</sub>	–448.9579885	
b <sub>2</sub>	0.0017257	378.75
b <sub>4</sub>	0.0006207	136.23
b <sub>6</sub>	0.0000659	14.46
b <sub>8</sub>	0.0000508	11.15
b <sub>10</sub>	0.0000167	3.67
a <sub>0</sub>	–448.9579885	
a <sub>3</sub>	–0.0002567	–56.34
a <sub>6</sub>	0.0000301	6.61
a <sub>9</sub>	–0.0000011	–0.24

**Table S2.** Nuclear coordinates in the principal inertial axes of conformer  $I_b$  of phenyl acetate calculated at the MP2/6-311++G(d,p) level of theory. The atoms are numbered according to Figure 2.

	$I_b$		
	$a / \text{\AA}$	$b / \text{\AA}$	$c / \text{\AA}$
<b>C<sub>1</sub></b>	2.129450	-1.241971	-0.259741
<b>C<sub>2</sub></b>	0.771955	-1.042572	-0.530908
<b>C<sub>3</sub></b>	0.224578	0.225051	-0.333328
<b>C<sub>4</sub></b>	0.999498	1.295734	0.109160
<b>C<sub>5</sub></b>	2.357977	1.086871	0.373650
<b>C<sub>6</sub></b>	2.924949	-0.179501	0.187634
<b>H<sub>7</sub></b>	2.566113	-2.225941	-0.406045
<b>H<sub>8</sub></b>	0.140800	-1.855184	-0.877385
<b>H<sub>9</sub></b>	0.536384	2.268731	0.243770
<b>H<sub>10</sub></b>	2.971502	1.914671	0.718058
<b>H<sub>11</sub></b>	3.979207	-0.339289	0.394552
<b>O<sub>12</sub></b>	-1.114437	0.469936	-0.653461
<b>C<sub>13</sub></b>	-2.048428	-0.090306	0.185998
<b>C<sub>14</sub></b>	-3.430315	0.246504	-0.304588
<b>O<sub>15</sub></b>	-1.765125	-0.742914	1.159689
<b>H<sub>16</sub></b>	-3.549137	1.331532	-0.349219
<b>H<sub>17</sub></b>	-3.565594	-0.146130	-1.315149
<b>H<sub>18</sub></b>	-4.168358	-0.185816	0.369378

**Table S3.** The Fourier coefficients of the two-dimensional potential energy surface calculated at the MP2/6-311++G(d,p) level of theory by varying  $\alpha$  and  $\gamma$  in a grid of  $10^\circ$ , while all other parameters were optimized (Figure 5).

N°	Fourier term	Coefficient / Hartree	Coefficient / $\text{cm}^{-1}$
1	1	-458.9564929	/
2	$\cos(2\alpha)$	0.0017806	390.80
3	$\cos(4\alpha)$	0.0006556	143.89
4	$\cos(6\alpha)$	0.0000692	15.19
5	$\cos(3\gamma)$	-0.0002707	-59.41
6	$\cos(6\gamma)$	0.0000358	7.86
7	$\cos(2\alpha) \cdot \cos(3\gamma)$	-0.0000171	-3.75
8	$\cos(2\alpha) \cdot \cos(6\gamma)$	0.0000098	2.15
9	$\sin(2\alpha) \cdot \sin(3\gamma)$	-0.0000606	-13.30
10	$\cos(4\alpha) \cdot \cos(3\gamma)$	-0.0000125	-2.74
11	$\sin(4\alpha) \cdot \sin(3\gamma)$	-0.0000554	-12.16
12	$\sin(6\alpha) \cdot \sin(3\gamma)$	-0.0000249	-5.46

**Table S4:** Fitted molecular parameters of the A0 and A1 state lines of phenyl acetate using the program *spfit*. The experimental accuracy of the microwave (MW) lines is 2 kHz; that of the millimeterwave (mm) lines is 50 kHz; Observed frequencies ( $\nu_{\text{obs.}}$ , in MHz) of 80 rotational transitions of the A0 species (Fit A0 in Table S-4a), those of 20 A1 species transitions (Fit A0/A1 MW in Table S-4a), as well as those measured in the millimeterwave range (Fit A0/A1 mmw in Table S-4a) of phenyl acetate.  $\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$  values (in MHz) are obtained after a fit with the program *spfit*.

Par. <sup>a</sup>	Unit	Fit A0		Fit A0/A1 MW		Fit A0/A1 MW+mmw	
<i>A</i>	MHz	3636.711(15)	3637.77426(26)	3640.91673(57)	3637.78574(22)	3640.89497(27)	
<i>B</i>	MHz	802.815(15)	803.889579(74)	803.38861(17)	803.889288(63)	803.39054(16)	
<i>C</i>	MHz	749.905(15)	750.979441(79)	749.94790(38)	750.978551(62)	749.94787(31)	
<i>D<sub>J</sub></i>	kHz	0.1279(56)	0.2379(32)	−0.0696(48)	−0.2265(12)	0.0480(24)	
<i>D<sub>JK</sub></i>	kHz	---	---	6.245(45)	−1.445(13)	−3.829(16)	
<i>D<sub>K</sub></i>	kHz	2.64(27)	---	0.01132(52)	−0.924 (15)	1.350(22)	
<i>d<sub>1</sub></i>	kHz		---	−0.0550(19)	---	0.0394(12)	
<i>d<sub>2</sub></i>	kHz	−0.0784(42)	−0.1698(30)	---	0.16096(97)	−0.0134(16)	
<i>E</i>	GHz	36.5593(97)	36.40827(69)		36.40880(24)		
<i>E<sub>J</sub></i>	MHz	1.075(15)	---		---		
<i>F<sub>bc</sub></i>	MHz	28.295(13)	28.0573(55)		28.0652(19)		
<i>F<sub>bcJ</sub></i>	kHz	---	0.1607(61)		0.1890(45)		
<i>F<sub>ab</sub></i>	MHz	79.079(12)	78.9150(21)		78.7240(22)		
<i>F<sub>abJ</sub></i>	kHz	---	0.991(32)		1.0105(91)		
<i>F<sub>abJK</sub></i>	Hz	---	---		1.253(67)		
<i>N<sub>A0</sub>/N<sub>A1</sub></i> <sup>b</sup>		80	80	20	80/20	21/19/26	
rms <sup>c</sup>	kHz	1.3		3.6		40.0	

  

								$\nu_{\text{Obs.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$
<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	$\nu$	<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	$\nu$	MHz	Fit A1	Fit A0/A1 MW	Fit A0/A1 MW+mm
2	0	2	0	1	0	1	0	3108.4942	−0.6	0.2	0.8
4	0	4	0	3	0	3	0	6209.5879	−0.9	0.1	0.7
5	0	5	0	4	0	4	0	7755.0607	−0.6	0.0	0.4
6	0	6	0	5	0	5	0	9295.9683	0.2	0.4	0.2

7	0	7	0	6	0	6	0	10831.4987	0.3	0.1	-0.7
8	0	8	0	7	0	7	0	12360.9594	1.3	1.0	-0.4
9	0	9	0	8	0	8	0	13883.8276	0.2	0.7	-0.9
10	0	10	0	9	0	9	0	15399.8166	-2.6	0.2	-1.1
3	1	3	0	2	1	2	0	4581.6224	-1.3	-1.2	-0.3
4	1	4	0	3	1	3	0	6107.1090	-0.5	-0.7	0.3
5	1	5	0	4	1	4	0	7631.1655	-0.1	-0.7	0.3
6	1	6	0	5	1	5	0	9153.4918	0.9	-0.4	0.7
7	1	7	0	6	1	6	0	10673.8209	0.7	-1.1	0.0
8	1	8	0	7	1	7	0	12191.9296	1.3	-0.6	0.8
9	1	9	0	8	1	8	0	13707.6340	0.0	-1.2	0.9
10	1	10	0	9	1	9	0	15220.8007	-1.3	-0.2	3.1
3	1	2	0	2	1	1	0	4740.8490	-0.6	-0.5	1.1
4	1	3	0	3	1	2	0	6319.2761	-0.6	-0.9	0.9
5	1	4	0	4	1	3	0	7896.0503	-0.3	-1.0	0.7
6	1	5	0	5	1	4	0	9470.6769	-0.5	-1.7	-0.5
7	1	6	0	6	1	5	0	11042.6067	0.4	-1.2	-0.7
8	1	7	0	7	1	6	0	12611.2144	-0.6	-2.4	-2.6
9	1	8	0	8	1	7	0	14175.7923	-1.4	-2.8	-3.6
10	1	9	0	9	1	8	0	15735.5306	0.8	0.8	-0.1
4	2	2	0	3	2	1	0	6215.6765	0.1	-0.2	0.4
5	2	3	0	4	2	2	0	7773.6888	1.2	0.6	1.4
4	2	3	0	3	2	2	0	6204.7701	-0.8	-0.7	-0.5
5	2	4	0	4	2	3	0	7751.8940	0.3	0.3	0.6
7	0	7	0	6	1	5	0	7386.0268	0.0	-3.5	-1.7
8	0	8	0	7	1	6	0	8704.3787	0.1	-2.1	-2.1
9	0	9	0	8	1	7	0	9976.9920	1.0	1.2	-0.4
10	0	10	0	9	1	8	0	11201.0169	0.3	4.8	2.7
2	1	1	0	1	0	1	0	6048.1584	-1.1	7.7	1.1
3	1	2	0	2	0	2	0	7680.5136	-0.7	7.4	1.8
4	1	3	0	3	0	3	0	9339.3629	1.1	7.9	3.4
5	1	4	0	4	0	4	0	11025.8248	1.2	6.4	2.8

<sup>a</sup> All parameters refer to the principal axis system. Watson's S reduction in  $I^r$  representation was used.

<sup>b</sup> Number of lines. For the A0/A1 MW+mmw fit, the numbers of A0/A1 MW as well as A0/A1/A01 mm transitions are given. The A01 lines are interstate transitions ( $v_t = 0 \leftarrow 1$  or  $1 \leftarrow 0$ ).

<sup>c</sup> Root-mean-squares deviation of the fit.

**Table S5:** Fitted molecular parameters of the E0 and E1 states of phenyl acetate using the program *spfit*; Observed frequencies ( $\nu_{\text{obs.}}$ ) of 69 rotational transitions of the E0 species of phenylacetate (Fit E0 in Table S-5a) as well as those of 17 E1 species transitions (Fit E0/E1 in Table S-5a).  $\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$  values (in kHz) are obtained after a fit with the program *spfit*. Observed frequencies  $\nu_{\text{Obs.}}$  are given in MHz.

Par. <sup>a</sup>	Unit	Fit E0				Fit E0/E1				
$A$	MHz	3621.088(38)				3623.0028(17)				3629.3566(42)
$B$	MHz	801.872(38)				803.69612(14)				804.83313(50)
$C$	MHz	748.998(38)				751.02010(13)				749.74731(71)
$D_J$	kHz	---				8.92044(85)				24.610(31)
$D_{JK}$	kHz	13.33(25)				−77.728(83)				376.39(35)
$D_K$	kHz	−9.53(19)				32.29(31)				−47.39(98)
$d_I$	kHz	---				−0.26530(44)				−27.107(14)
$d_2$	MHz	---				−9.0950(10)				---
$E$	GHz	35.6076(68)				22.26975(30)				
$E_J$	MHz	1.930(38)				---				
$F_{bc}$	MHz	−28.4735(61)				4.4038(23)				
$F_{bcI}$	kHz	0.566(37)				---				
$F_{ab}$	MHz	76.811(39)				66.9364(73)				
$F_{abI}$	kHz	−3.973(73)				---				
$D_a$	MHz	401.87237(77)				402.01555(90)				380.72713(62)
$D_c$	MHz	33.6480(40)				20.0845(39)				21.441(75)
$D_{aK}$	MHz	−0.14046(17)				−0.15446(21)				---
$D_{cK}$	MHz	−0.7417(96)				25.1754(79)				−31.016(47)
$D_{cKK}$	MHz	0.1483(16)				−5.5413(12)				
$N_{\text{E0}}/N_{\text{E1}}^{\text{b}}$		69				60				17
rms <sup>c</sup>	kHz	10.6				358.8				
								$\nu_{\text{Obs.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$
$J$	$K_a$	$K_c$	$\nu$	$J$	$K_a$	$K_c$	$\nu$	MHz	Fit E0	Fit E0/E1
5	0	5	0	4	0	4	0	7751.4642	3.3	56.4
6	0	6	0	5	0	5	0	9291.0819	3.4	87.7
7	0	7	0	6	0	6	0	10824.9537	3.6	102.6

8	0	8	0	7	0	7	0	12352.2719	-0.5	62.1
9	0	9	0	8	0	8	0	13872.3882	-13.4	-93.7
5	1	4	0	4	1	3	0	7846.2794	-1.3	104.3
6	1	5	0	5	1	4	0	9431.3367	0.3	78.3
7	1	6	0	6	1	5	0	11012.5809	0.4	28.9
8	1	7	0	7	1	6	0	12588.1826	2.5	-10.9
9	1	8	0	8	1	7	0	14157.5752	2.2	-0.3
6	1	6	0	5	1	5	0	9193.8192	6.9	-39.8
7	1	7	0	6	1	6	0	10705.5461	0.2	2.3
8	1	8	0	7	1	7	0	12217.7159	-16.6	102.3
6	2	4	0	5	2	3	0	9313.8829	4.3	51.0
7	2	5	0	6	2	4	0	10866.8120	3.8	-170.3
8	2	6	0	7	2	5	0	12421.1218	-5.4	-334.2
2	1	1	0	1	0	1	0	6363.7671	6.3	-126.1
3	1	2	0	2	0	2	0	7939.8172	7.0	-52.9
4	1	3	0	3	0	3	0	9542.8732	2.7	37.4
5	1	4	0	4	0	4	0	11182.1519	-0.2	116.4
6	1	5	0	5	0	5	0	12862.0247	-3.0	138.5
7	1	6	0	6	0	6	0	14583.5246	-5.0	80.7
8	1	7	0	7	0	7	0	16346.7536	-6.0	-32.7
9	1	8	0	8	0	8	0	18152.0549	-5.4	-97.1
10	1	9	0	9	0	9	0	20000.1015	6.7	127.1
2	2	0	0	1	1	0	0	12044.4987	1.5	-296.8
2	2	1	0	2	1	2	0	8143.1451	-13.1	-366.2
3	2	2	0	3	1	3	0	8161.3736	-1.7	-128.1
4	2	3	0	4	1	4	0	8206.3684	7.8	118.0
5	2	4	0	5	1	5	0	8287.3646	9.6	295.0
6	2	5	0	6	1	6	0	8408.2908	3.8	333.4
7	2	6	0	7	1	7	0	8568.9705	-7.2	212.8
8	2	7	0	8	1	8	0	8767.0855	-13.0	13.1
9	2	8	0	9	1	9	0	8998.7679	13.3	-24.9
2	2	1	0	1	1	1	0	11244.5069	-7.9	-332.4
3	2	2	0	2	1	2	0	12800.5087	4.2	-111.8
3	2	1	0	2	1	1	0	13586.6575	-2.8	13.7

<sup>a</sup> All parameters refer to the principal axis system. Watson's S reduction in I<sup>r</sup> representation was used.

<sup>b</sup> Number of lines.

<sup>c</sup> Root-mean-squares deviation of the fit.



**Table S6:** Fitted molecular parameters of the A0 and E0 states of phenyl acetate using the program *XIAM*; Observed frequencies ( $\nu_{\text{obs.}}$ ) of 80 rotational transitions of the A0 species and 69 transitions of the E0 species of phenyl acetate.  $\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$  values (in MHz) are obtained after a fit with the program *XIAM*. Observed frequencies  $\nu_{\text{Obs.}}$  are given in MHz.

Par. <sup>a</sup>	Unit	Fit A0/E0	Calc. <sup>b</sup>
<i>A</i>	MHz	3632.65(48)	3592.4
<i>B</i>	MHz	804.71(15)	813.9
<i>C</i>	MHz	750.19(17)	744.3
<i>D<sub>J</sub></i>	kHz	8.17(98)	
<i>D<sub>JK</sub></i>	MHz	0.4312(86)	
<i>d<sub>1</sub></i>	kHz	−8.52(43)	
<i>d<sub>2</sub></i>	kHz	−37.74(30)	
<i>V<sub>3</sub></i>	cm <sup>−1</sup>	136.44(37)	113.2
$\angle(i,a)$	°	24.61(75)	23.2
$\angle(i,b)$	°	76.37(40)	77.1
$\angle(i,c)$	°	69.92(60)	71.0
<i>N<sub>A0</sub>/N<sub>E0</sub></i> <sup>c</sup>		80/69	
rms <sup>d</sup>	kHz	6872.0	

  

							$\nu_{\text{Obs.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$
<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>	<i>J</i>	<i>K<sub>a</sub></i>	<i>K<sub>c</sub></i>		MHz	Fit A0/E0
2	0	2	1	0	1	A1	3108.4942	−0.46
4	0	4	3	0	3	A1	6209.5879	−0.73
5	0	5	4	0	4	A1	7755.0607	−0.87
6	0	6	5	0	5	A1	9295.9683	−1.12
7	0	7	6	0	6	A1	10831.4987	−1.49
8	0	8	7	0	7	A1	12360.9594	−1.81
9	0	9	8	0	8	A1	13883.8276	−1.61
10	0	10	9	0	9	A1	15399.8166	0.06
3	1	3	2	1	2	A1	4581.6224	1.43
4	1	4	3	1	3	A1	6107.1090	1.16
5	1	5	4	1	4	A1	7631.1655	0.44
6	1	6	5	1	5	A1	9153.9180	−0.16
7	1	7	6	1	6	A1	10673.8209	−1.60
8	1	8	7	1	7	A1	12191.9296	−2.03
9	1	9	8	1	8	A1	13707.6340	−0.99

10	1	10	9	1	9	A1	15220.8007	2.79
3	1	2	2	1	1	A1	4740.8490	-1.04
4	1	3	3	1	2	A1	6319.2761	-0.62
5	1	4	4	1	3	A1	7896.0503	0.19
6	1	5	5	1	4	A1	9470.6769	1.20
7	1	6	6	1	5	A1	11042.6067	2.05
8	1	7	7	1	6	A1	12611.2144	2.21
9	1	8	8	1	7	A1	14175.7923	1.08
10	1	9	9	1	8	A1	15735.5306	-2.06
4	2	2	3	2	1	A1	6215.6765	3.12
5	2	3	4	2	2	A1	7773.6888	3.60
4	2	3	3	2	2	A1	6204.7701	2.75
5	2	4	4	2	3	A1	7751.8940	3.08
7	0	7	6	1	5	A1	7386.0268	0.21
8	0	8	7	1	6	A1	8704.3787	-3.65
9	0	9	8	1	7	A1	9976.9920	-7.47
10	0	10	9	1	8	A1	11201.0169	-8.48
2	1	1	1	0	1	A1	6048.1584	-5.22
3	1	2	2	0	2	A1	7680.5136	-5.80
4	1	3	3	0	3	A1	9339.3629	-5.80
5	1	4	4	0	4	A1	11025.8248	-4.88
6	1	5	5	0	5	A1	12741.4407	-2.81

<sup>a</sup> All parameters refer to the principal axis system. Watson's S reduction in I<sup>r</sup> representation was used.

<sup>b</sup> Values of the equilibrium structure calculated at the MP2/6-311++G(d,p) level of theory.

<sup>c</sup> Number of lines.

<sup>d</sup> Root-mean-squares deviation of the fit.

**Table S7.** Observed frequencies ( $\nu_{\text{Obs.}}$ ) of 240 rotational transitions of phenyl acetate belonging to the four sub-states A0, A1, E0, and E1.  $\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$  values (in kHz) are obtained after a fit with the program *spfit*. Observed frequencies  $\nu_{\text{Obs.}}$  are given in MHz.

$J$	$K_a$	$K_c$	$\nu$	$J$	$K_a$	$K_c$	$\nu$	$\nu_{\text{Obs.}}$	$\nu_{\text{Obs.}} - \nu_{\text{Calc.}}$
10	10	0	0	9	9	0	0	69860.27	55.7
10	10	0	1	9	9	0	1	69973.31	-31.7
11	10	1	0	10	9	1	0	71367.20	62.0
11	10	1	1	10	9	1	1	71539.35	-71.5
12	10	2	0	11	9	2	0	72882.86	52.3
12	10	2	1	11	9	2	1	73103.17	-46.2
9	9	0	0	8	8	0	0	62463.90	39.6
9	9	0	1	8	8	0	1	62690.04	-4.6
10	9	1	0	9	8	1	0	63899.06	20.7
10	9	1	1	9	8	1	1	64294.65	22.1
11	9	2	0	10	8	2	0	65370.52	-15.8
11	9	2	1	10	8	2	1	65889.22	-35.3
13	9	4	0	12	8	4	0	68381.99	-8.9
13	9	4	1	12	8	4	1	69051.58	12.2
14	9	5	0	13	8	5	0	69910.62	-15.5
14	9	5	1	13	8	5	1	70620.86	7.3
15	9	6	0	14	8	6	0	71449.86	-81.7
15	9	6	1	14	8	6	1	72183.24	19.9
16	9	7	0	15	8	7	0	72997.60	-90.4
16	9	7	1	15	8	7	1	73739.29	-23.5
11	8	3	1	10	7	3	1	60427.38	94.5
12	8	4	0	11	7	4	0	60400.58	-54.6
12	8	4	1	11	7	4	1	62031.47	91.9
13	8	5	0	12	7	5	0	61964.70	-13.4
13	8	5	1	12	7	5	1	63616.43	97.5
14	8	6	1	13	7	6	1	65186.53	65.5
15	8	7	1	14	7	7	1	66744.70	21.4
16	8	8	1	15	7	8	1	68293.01	34.4
17	8	9	1	16	7	9	1	69832.76	17.0
18	8	10	1	17	7	10	1	71364.89	-39.3
19	8	11	1	18	7	11	1	72890.09	-64.8
17	7	10	0	16	6	10	0	59624.34	-27.9
18	7	11	0	17	6	11	0	61010.03	-133.8
18	7	12	0	17	6	12	0	61010.49	-143.7
19	7	12	0	18	6	12	0	62386.59	-53.2
19	7	13	0	18	6	13	0	62387.42	-148.5
20	7	13	0	19	6	13	0	63751.88	45.4
20	7	14	0	19	6	14	0	63753.51	-76.4
21	7	14	0	20	6	14	0	65104.52	186.2

21	7	15	0	20	6	15	0	65107.61	81.4
15	8	7	0	14	6	8	1	65121.42	15.3
16	8	8	0	15	6	10	1	66709.00	-48.0
17	8	9	0	16	6	11	1	68301.05	14.3
18	8	10	0	17	6	12	1	69896.57	-0.4
19	8	11	0	18	6	13	1	71495.17	32.0
20	8	12	0	19	6	14	1	73096.39	-35.2
14	7	7	1	13	7	6	0	60090.62	83.4
14	7	8	1	13	7	7	0	60090.62	83.3
15	7	8	1	14	7	7	0	61601.87	66.0
15	7	9	1	14	7	8	0	61601.87	65.7
16	7	9	1	15	7	8	0	63104.76	55.8
16	7	10	1	15	7	9	0	63104.76	55.1
17	7	10	1	16	7	9	0	64599.96	18.9
17	7	11	1	16	7	10	0	64599.96	17.2
18	7	11	1	17	7	10	0	66087.71	-27.7
18	7	12	1	17	7	11	0	66087.71	-31.9
19	7	12	1	18	7	11	0	67567.96	-21.3
19	7	13	1	18	7	12	0	67567.96	-30.9
20	7	13	1	19	7	12	0	69040.32	1.2
20	7	14	1	19	7	13	0	69040.32	-19.9
21	7	14	1	20	7	13	0	70504.25	17.8
21	7	15	1	20	7	14	0	70504.25	-27.0
22	7	15	1	21	7	14	0	71959.17	52.5
22	7	16	1	21	7	15	0	71959.17	-40.0
23	7	16	1	22	7	15	0	73404.44	58.1
23	7	17	1	22	7	16	0	73404.44	-127.0
2	0	2	0	1	0	1	0	3108.4942	0.7
4	0	4	0	3	0	3	0	6209.5879	0.6
5	0	5	0	4	0	4	0	7755.0607	0.4
6	0	6	0	5	0	5	0	9295.9683	0.3
7	0	7	0	6	0	6	0	10831.4987	-0.6
8	0	8	0	7	0	7	0	12360.9594	-0.3
9	0	9	0	8	0	8	0	13883.8276	-1.1
10	0	10	0	9	0	9	0	15399.8166	-2.0
3	1	3	0	2	1	2	0	4581.6224	-0.1
4	1	4	0	3	1	3	0	6107.1090	0.5
5	1	5	0	4	1	4	0	7631.1655	0.5
6	1	6	0	5	1	5	0	9153.4918	0.7
7	1	7	0	6	1	6	0	10673.8209	-0.1
8	1	8	0	7	1	7	0	12191.9296	0.3
9	1	9	0	8	1	8	0	13707.6340	-0.2
10	1	10	0	9	1	9	0	15220.8007	1.2
3	1	2	0	2	1	1	0	4740.8490	0.7
4	1	3	0	3	1	2	0	6319.2761	0.6
5	1	4	0	4	1	3	0	7896.0503	0.4

6	1	5	0	5	1	4	0	9470.6769	−0.5
7	1	6	0	6	1	5	0	11042.6067	−0.5
8	1	7	0	7	1	6	0	12611.2144	−2.1
9	1	8	0	8	1	7	0	14175.7923	−3.0
10	1	9	0	9	1	8	0	15735.5306	0.5
4	2	2	0	3	2	1	0	6215.6765	0.4
5	2	3	0	4	2	2	0	7773.6888	1.4
4	2	3	0	3	2	2	0	6204.7701	−0.3
5	2	4	0	4	2	3	0	7751.8940	0.7
7	0	7	0	6	1	5	0	7386.0268	−0.5
8	0	8	0	7	1	6	0	8704.3787	−1.1
9	0	9	0	8	1	7	0	9976.9920	0.0
10	0	10	0	9	1	8	0	11201.0169	1.6
2	1	1	0	1	0	1	0	6048.1584	0.9
3	1	2	0	2	0	2	0	7680.5136	1.3
4	1	3	0	3	0	3	0	9339.3629	2.7
5	1	4	0	4	0	4	0	11025.8248	2.0
6	1	5	0	5	0	5	0	12741.4407	0.8
7	1	6	0	6	0	6	0	14488.0778	−1.4
8	1	7	0	7	0	7	0	16267.7935	−2.9
9	1	8	0	8	0	8	0	18082.6308	−1.2
10	1	9	0	9	0	9	0	19934.3311	−2.4
11	1	10	0	10	0	10	0	21824.0082	3.7
2	2	0	0	1	1	0	0	11663.0142	0.6
3	2	1	0	2	1	1	0	13161.6347	0.9
4	2	2	0	3	1	2	0	14636.4606	−1.0
5	2	3	0	4	1	3	0	16090.8723	−1.2
6	2	4	0	5	1	4	0	17529.1857	−1.4
7	2	5	0	6	1	5	0	18956.6266	−2.0
8	2	6	0	7	1	6	0	20379.2607	−1.6
9	2	7	0	8	1	7	0	21803.8708	0.1
10	2	8	0	9	1	8	0	23237.7920	4.2
2	2	1	0	1	1	1	0	11715.0204	1.7
3	2	2	0	2	1	2	0	13315.4571	0.5
4	2	3	0	3	1	3	0	14938.6052	0.7
5	2	4	0	4	1	4	0	16583.3903	1.0
6	2	5	0	5	1	5	0	18248.5244	0.5
7	2	6	0	6	1	6	0	19932.4812	0.8
8	2	7	0	7	1	7	0	21633.4639	1.5
9	2	8	0	8	1	8	0	23349.3822	3.9
3	2	1	0	3	1	3	0	8739.2871	0.0
4	2	2	0	4	1	4	0	8847.8553	0.7
5	2	3	0	5	1	5	0	8990.3760	−1.1
6	2	4	0	6	1	6	0	9171.2491	−0.3
7	2	5	0	7	1	7	0	9395.5471	−0.4
8	2	6	0	8	1	8	0	9668.8574	−1.6

9	2	7	0	9	1	9	0	9997.0468	-3.0
10	2	8	0	10	1	10	0	10385.9660	3.4
3	2	2	0	3	1	2	0	8415.3275	-5.0
4	2	3	0	4	1	3	0	8300.8285	1.1
5	2	4	0	5	1	4	0	8156.6692	-1.7
6	2	5	0	6	1	5	0	7982.2909	-2.2
3	2	1	0	3	1	3	0	8739.2859	-1.2
4	2	2	0	4	1	4	0	8847.8556	1.0
5	2	3	0	5	1	5	0	8990.3760	-1.1
6	2	4	0	6	1	6	0	9171.2500	0.6
7	2	5	0	7	1	7	0	9395.5470	-0.5
8	2	6	0	8	1	8	0	9668.8569	-2.1
8	1	7	0	7	2	5	0	4697.1924	-2.7
9	1	8	0	8	2	6	0	6407.7480	-1.6
11	1	10	0	10	2	8	0	9787.2322	0.3
3	1	2	1	2	0	2	1	7690.4720	6.0
4	1	3	1	3	0	3	1	9358.0513	5.3
5	1	4	1	4	0	4	1	11057.8825	1.6
6	1	5	1	5	0	5	1	12792.5630	-3.2
7	1	6	1	6	0	6	1	14565.1298	-9.8
8	1	7	1	7	0	7	1	16378.9919	-9.9
9	1	8	1	8	0	8	1	18237.8357	11.4
2	2	0	1	1	1	0	1	11674.5391	-6.8
3	2	1	1	2	1	1	1	13187.6276	6.8
2	2	0	1	2	1	2	1	8672.1067	0.7
2	2	1	1	1	1	1	1	11727.2715	-2.9
3	2	2	1	2	1	2	1	13344.6781	-1.9
3	2	2	1	3	1	2	1	8440.7634	-6.5
4	2	3	1	4	1	3	1	8355.3119	-3.3
5	2	4	1	5	1	4	1	8261.1730	2.0
4	2	2	1	4	1	4	1	8896.1206	1.0
5	2	3	1	5	1	5	1	9078.6066	7.3
6	2	4	1	6	1	6	1	9317.2543	11.1
7	2	5	1	7	1	7	1	9616.5305	-8.0
8	0	8	1	7	1	6	1	8685.8878	2.5
5	0	5	2	4	0	4	2	7751.4642	1.1
6	0	6	2	5	0	5	2	9291.0819	-1.7
7	0	7	2	6	0	6	2	10824.9537	-1.4
8	0	8	2	7	0	7	2	12352.2719	0.4
9	0	9	2	8	0	8	2	13872.3882	2.6
5	1	5	2	4	1	4	2	7681.4597	-2.1
6	1	6	2	5	1	5	2	9193.8192	6.4
7	1	7	2	6	1	6	2	10705.5461	5.7
8	1	8	2	7	1	7	2	12217.7159	-14.9
5	1	4	2	4	1	3	2	7846.2794	2.1
6	1	5	2	5	1	4	2	9431.3367	1.7

7	1	6	2	6	1	5	2	11012.5809	-1.6
8	1	7	2	7	1	6	2	12588.1826	-1.5
9	1	8	2	8	1	7	2	14157.5752	0.8
2	1	1	2	1	0	1	2	6363.7671	7.6
3	1	2	2	2	0	2	2	7939.8172	3.1
4	1	3	2	3	0	3	2	9542.8732	-2.2
5	1	4	2	4	0	4	2	11182.1519	-2.5
6	1	5	2	5	0	5	2	12862.0247	-1.5
7	1	6	2	6	0	6	2	14583.5246	-0.5
8	1	7	2	7	0	7	2	16346.7536	-0.6
9	1	8	2	8	0	8	2	18152.0549	-2.2
10	1	9	2	9	0	9	2	20000.1015	4.1
7	0	7	2	6	1	5	2	7254.0108	-1.6
8	0	8	2	7	1	6	2	8593.6998	-1.6
9	0	9	2	8	1	7	2	9877.9060	3.1
2	2	0	2	1	1	0	2	12044.4987	6.0
2	2	1	2	1	1	1	2	11244.5035	-0.8
3	2	1	2	3	1	3	2	9766.2308	-0.6
6	2	4	2	5	2	3	2	9313.8829	10.4
7	2	5	2	6	2	4	2	10866.8120	10.0
8	2	6	2	7	2	5	2	12421.1218	-9.7
4	2	2	2	4	1	4	2	9810.6165	-4.5
5	2	3	2	5	1	5	2	9890.6759	-3.8
6	2	4	2	6	1	6	2	10010.7377	-1.8
7	2	5	2	7	1	7	2	10172.0048	3.7
8	2	6	2	8	1	8	2	10375.4088	6.9
9	2	7	2	9	1	9	2	10623.4504	2.5
10	2	8	2	10	1	10	2	10921.0265	-14.5
11	2	9	2	11	1	11	2	11275.5630	6.1
2	2	1	2	2	1	2	2	8143.1451	4.6
3	2	2	2	3	1	3	2	8161.3736	-1.2
4	2	3	2	4	1	4	2	8206.3684	-1.8
5	2	4	2	5	1	5	2	8287.3646	-0.7
6	2	5	2	6	1	6	2	8408.2908	1.4
7	2	6	2	7	1	7	2	8568.9705	3.2
8	2	7	2	8	1	8	2	8767.0855	2.7
9	2	8	2	9	1	9	2	8998.7679	-3.4
2	2	1	2	1	1	1	2	11244.5069	2.7
3	2	2	2	2	1	2	2	12800.5087	-6.4
3	2	1	2	2	1	1	2	13586.6575	-2.3
2	2	0	2	2	1	1	2	8929.5822	11.1
3	2	1	2	3	1	2	2	8903.2291	1.0
4	2	2	2	4	1	3	2	8850.8349	-6.6
5	2	3	2	5	1	4	2	8766.0758	-8.8
6	2	4	2	6	1	5	2	8648.6208	-1.4
7	2	5	2	7	1	6	2	8502.8501	8.4

8	2	6	2	8	1	7	2	8335.7881	−1.0
4	1	4	2	3	0	3	2	8583.0909	−4.9
5	1	5	2	4	0	4	2	10057.5530	−6.3
6	1	6	2	5	0	5	2	11499.9080	−0.9
7	1	7	2	6	0	6	2	12914.3708	5.1
3	1	2	3	2	0	2	3	7930.9383	−0.1
4	1	3	3	3	0	3	3	9544.9891	−2.7
5	1	4	3	4	0	4	3	11200.7613	6.4
6	1	5	3	5	0	5	3	12903.0873	−4.5
7	1	6	3	6	0	6	3	14653.7840	1.0
2	2	0	3	1	1	0	3	12037.6303	−3.8
3	2	1	3	2	1	1	3	13595.6562	2.0
2	2	1	3	1	1	1	3	11279.2188	0.7
3	2	2	3	2	1	2	3	12851.6183	−0.1
2	2	1	3	2	1	2	3	8177.3047	−0.6
2	2	0	3	2	1	1	3	8921.3300	3.7
3	2	1	3	3	1	2	3	8907.7525	−1.9