

SUPPORTING INFORMATION for CC-COM-10-2014-008434

## Unprecedented directed lateral lithiations of tertiary carbons on NHC platforms

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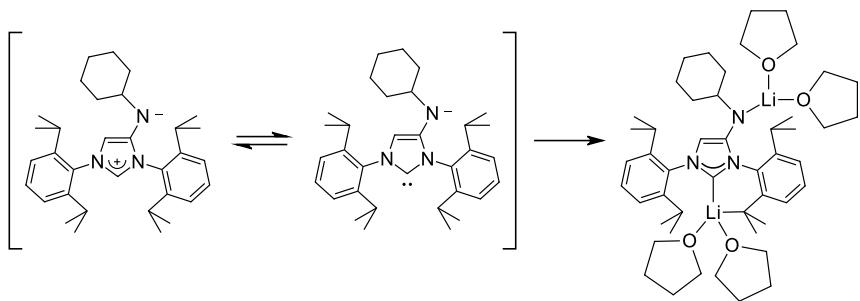
## Synthesis and characterization

### 1.1 General methods

Elemental analyses were carried out by the microanalytical laboratory of London Metropolitan University. All manipulations involving organometallics were performed under nitrogen or argon in a Braun glove-box or using standard Schlenk techniques as specified below. Solvents (THF, ether) were dried using standard methods and distilled under nitrogen prior use or passed through columns of activated alumina and subsequently purged with nitrogen or argon (toluene, pentane). The solvents used for the synthesis of the Li salts, after drying were stored over K mirror in the glove box until use. The starting materials were prepared according to literature procedures: 4-(4-*tert*.butyl-phenylamido)-1,3-(bis-diisopropylphenyl)-imidazolium,<sup>1</sup> and [4-(cyclohexylamido)-1,3-(bis-diisopropylphenyl)-imidazolium]-[4-(cyclohexylamino)-1,3-(bis-diisopropylphenyl)-imidazol-2-ylidene] equilibrium mixture.<sup>1</sup>

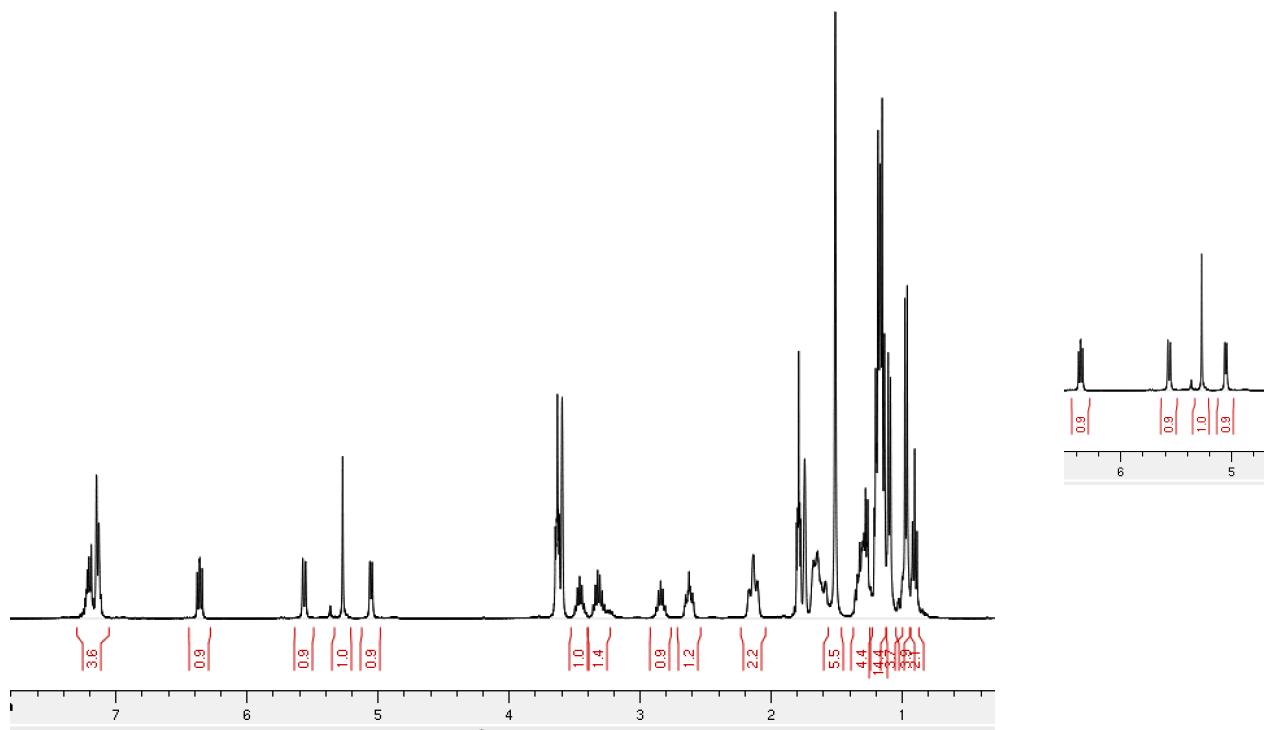
Solid Me<sub>3</sub>SiCH<sub>2</sub>Li was obtained from commercial (Aldrich) solutions by evaporation of the pentane under vacuum.

## 1.2. Synthesis of complex $3^{Cy}$



To a stirred solution of the equilibrium mixture of (4-(cyclohexylamido)-1,3-(bis-diisopropylphenyl)-imidazolium) and (4-(cyclohexylamino)-1,3-(bis-diisopropylphenyl)-imidazol-2-ylidene) (0.25 g, 0.50 mmol) in THF (20 ml) was added at room temperature solid  $\text{Me}_3\text{SiCH}_2\text{Li}$  (0.10 g, 1.0 mmol). The solution turned orange after 10 min and was stirred at room temperature for 12 h. After evaporation of the volatiles under reduced pressure, the solid residue was washed with pentane and re-dissolved in a small volume of THF (*ca.* 2 ml). The solution was slowly evaporated at -40 °C to give dark yellow-orange extremely air sensitive crystals. Yield: 0.33 g, (*ca.* 83%). Reproducible elemental analysis data could not be obtained, possibly due to the solvent dependency of the structure of  $3^{Cy}$ .

$^1\text{H-NMR}$ ,  $d^8\text{-THF}$ :  $\delta$ , 7.30 - 7.10 (m, 3H, non-lithiated DiPP), 6.36 (d of d,  $J = 8.3$  Hz and  $J = 6.8$  Hz, 1H, lithiated DiPP), 5.56 (d,  $J = 8.3$  Hz, 1H, lithiated DiPP), 5.27 (s, 1H, imidazol backbone), 5.05 (d, 1H,  $J = 6.8$  Hz, lithiated DiPP), 3.63 (m, THF) 3.46 (sept., 1H,  $J = 7.1$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 3.32 (sept., 1H,  $J = 7.1$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 2.84 (sept., 1H,  $J = 7.1$  Hz,  $\text{CH}(\text{CH}_3)_2$ ), 2.63 (m, 1H, Cy), 2.14 (br. t,  $J = 11.7$  Hz, 2H, cyclohexyl), 1.78 (m, THF), 1.67 (m, 4H, Cy), 1.51 (br. s, 6H,  $\text{LiCMe}_2$ ), 1.31 (m, 4H, Cy), 1.19 - 1.12 (four superimposed doublets, 12H,  $\text{CH}(\text{CH}_3)_2$ ), 1.10, (d,  $J = 7.1$  Hz, 3H,  $\text{CH}(\text{CH}_3)_2$ ) 0.97 (d, 3H,  $J = 7.1$  Hz,  $\text{CH}(\text{CH}_3)_2$ ).

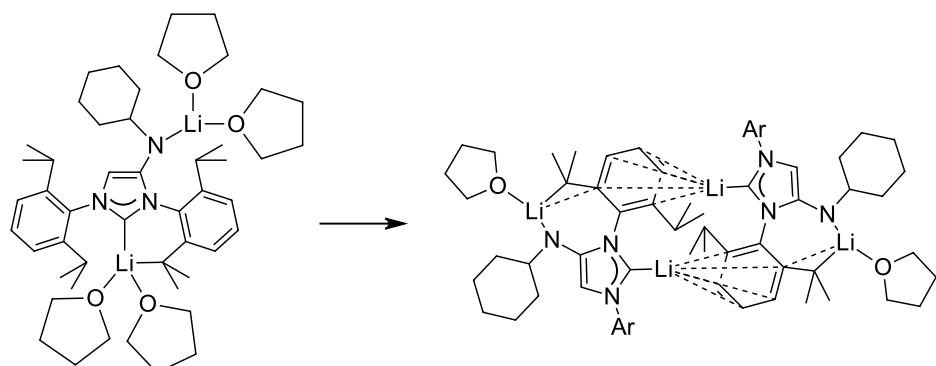


**Figure S1.**  $^1\text{H}$ -NMR of  $\mathbf{3}^{\text{Cy}}$ ; inset shows the  $\delta$  5.0-6.5 region where signals assignable to the C-H of the metalated ‘dearomatised’ ring were observed.

$^{13}\text{C}$ -NMR,  $d^8$ -THF:  $\delta$ , 157.10, 147.25, 147.18, 146.78, 141.55, 141.12, 127.97, 127.05, 123.06, 116.54, 110.77, 93.24, 90.94, 60.56, 55.15, 36.22, 36.05, 27.91, 27.82, 27.73, 27.63, 26.96, 25.86, 24.09, 23.37, 22.67, 22.02.

$^7\text{Li}$  (155.5 MHz),  $d^8$ -THF (293 K):  $\delta$ , 0.29 (1 Li, br), -0.21 (1 Li).

### 1.3 Synthesis of complex $\mathbf{4}^{\text{Cy}}$



Crystals of **3<sup>Cy</sup>** (0.10 g, 0.125 mmol) were stirred in pentane (*ca.* 5 ml) at room temperature for 12 h. The yellow-orange solution was filtered and cooled at -40 °C for 2 days to give orange crystals of **4<sup>Cy</sup>**. Yield 0.045 g (*ca.* 64 %).

Alternatively, **3<sup>Cy</sup>** (0.12 g, 0.15 mmol) was dissolved in ether and a solution of Me<sub>3</sub>SiCl (0.5 ml of 0.35 M solution in pentane, 0.15 mmol) was added at room temperature. After stirring for 8 h, the volatiles were removed under reduced pressure and the orange solid residue was crystallised from pentane at -40 °C. Yield 0.032 g (*ca.* 74%). It is plausible that the Me<sub>3</sub>SiCl and/or the large excess ether facilitates dissociation of coordinated THF from the Li centers of **3<sup>Cy</sup>**.

The solubility of **4<sup>Cy</sup>** in d<sup>8</sup>-toluene is limited but sufficient to record meaningful NMR spectra.

<sup>1</sup>H-NMR (400 MHz), (d<sup>8</sup>-toluene, 293 K): δ, 7.27 (t, *J* = 8Hz, 1H, *p*-C-H of non-metallated DiPP), 7.17 (d, *J* = 8 Hz, 2H, *m*-C-H of non-metallated DiPP), 5.66 (s, 1H, imidazole backbone), 5.40 - 5.25 (m, 2H, metallated DiPP), 4.75 (br d, *J* = 5.7 Hz, metallated DiPP), 3.42 (4H, m, THF), 3.28 ((sept, *J* = 7.1 Hz, 1H, CHCMe<sub>2</sub>), 2.86 (m, 1H, cyclohexyl), 2.67 (sept, *J* = 6.7 Hz, 1H, CHCMe<sub>2</sub>), 2.32 (br d, *J* = 12.3 Hz 1H, cyclohexyl) 2.18 (br d, *J* = 12.3 Hz 1H, cyclohexyl), 1.78 and 1.65 ((s, 3H each, CLi(CH<sub>3</sub>)<sub>2</sub>)), 1.47 (d, *J* = 7.1 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.40 (d, *J* = 7.0 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.34 – 1.16 (overlapping multiplets and doublets, 21H CH(CH<sub>3</sub>)<sub>2</sub> and cyclohexyl)).

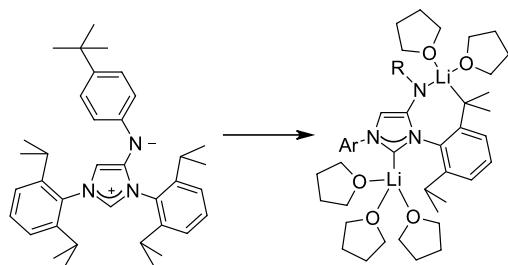
<sup>1</sup>H-NMR (600 MHz), d<sup>8</sup>-toluene (353 K): δ, 7.27 (t, *J* = 7.8Hz, 1H, *p*-C-H of non-metallated DiPP), 7.17 (d, *J* = 7.88 Hz, 2H, *m*-C-H of non-metallated DiPP), 5.58 (s, 1H, imidazole backbone), 5.35 (d of d, *J* = 9.1 Hz and *J* = 6.7 Hz, 1H, metallated DiPP), 5.28 (d, *J* = 9.1 Hz, 1H, metallated DiPP), 4.69 (d, *J* = 6.7 Hz, 1H, metallated DiPP), 3.47 (4H, m, THF), 3.39 (sept, *J* = 7.1 Hz, 1H, CHCMe<sub>2</sub>), 3.25 (sept, *J* = 7.1 Hz, 1H, CHCMe<sub>2</sub>), 2.82 (m, 1H, cyclohexyl), 2.64 (sept, *J* = 6.7 Hz, 1H, CHCMe<sub>2</sub>), 2.23 (d, br, *J* = 12.9 Hz, 1H, cyclohexyl), 2.11 (d, br, *J* = 12.9 Hz, 2H, cyclohexyl), 1.71 and 1.60 (s, 3H each, CLi(CH<sub>3</sub>)<sub>2</sub>), 1.44 (d, *J* = 7.1 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.40 (m, 7H, cyclohexyl), 1.37 (d, *J* = 7.0 Hz, CH(CH<sub>3</sub>)<sub>2</sub>), 1.27 – 1.20 (overlapping doublets, 12H, CH(CH<sub>3</sub>)<sub>2</sub>).

<sup>13</sup>C{<sup>1</sup>H}-NMR (150.9 MHz), d<sup>8</sup>-toluene (353 K): δ, 181.26, 157.48, 151.84, 148, 147.61, 140.47, 123.54, 123.32, 113.37, 107.25, 93.08, 85.91, 68.28, 60.31, 37.30, 36.65, 34.65, 28.62, 28.25, 28.18, 27.88, 27.02, 26.20, 25.87, 25.76, 25.68, 24.77, 24.16, 23.81, 23.48, 22.77, 14.17.

<sup>7</sup>Li (233 MHz), d<sup>8</sup>-toluene (293 K): δ, 1.00 (1 Li), -2.25 (1 Li).

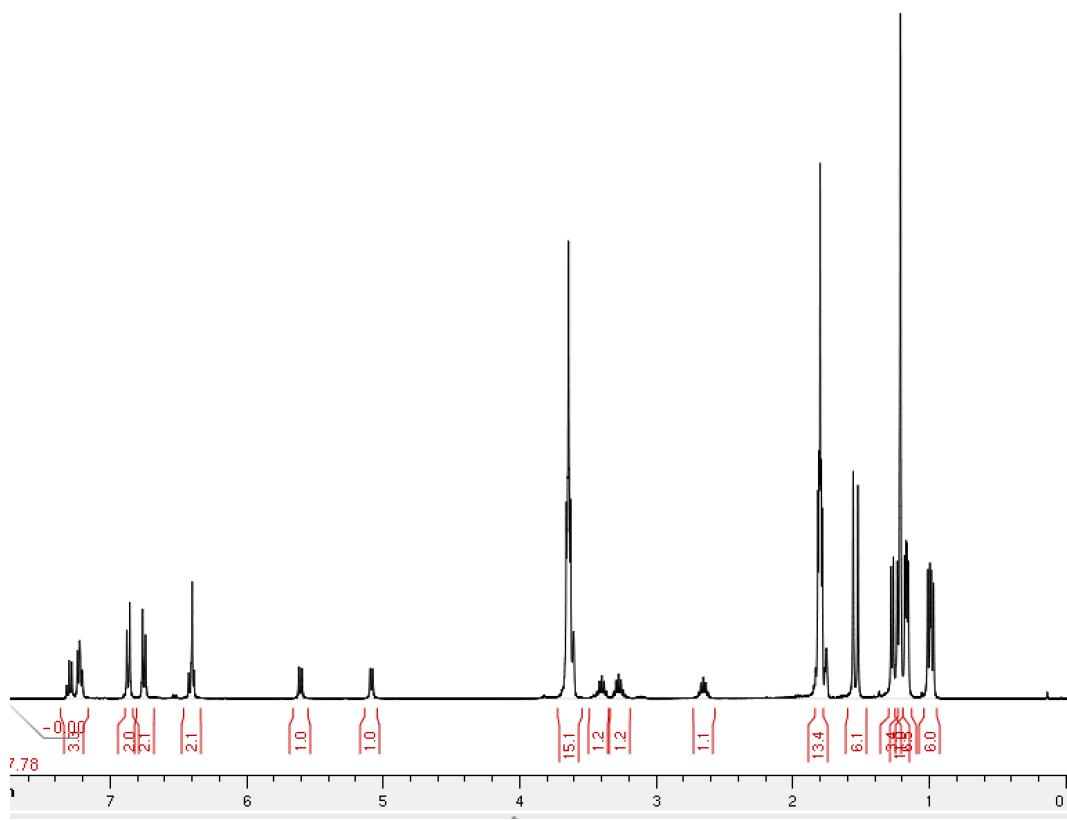
The d<sup>8</sup>-toluene solvent from the previous sample was removed under reduced pressure and the solid residue was redissolved in d<sup>8</sup>-THF and the <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>H}-NMR were recorded. The chemical shifts and integration of the peaks corresponding to the organolithium species in solution (except the integration of peaks corresponding to THF) were identical to those obtained for **3<sup>Cy</sup>** in d<sup>8</sup>-THF, supporting conversion of **4<sup>Cy</sup>** to **3<sup>Cy</sup>** on dissolution in THF.

#### 1.4. Synthesis of complex **5<sup>tBu-Ph</sup>**



To a stirred solution of 4-(4-*tert*.butyl-phenylamido)-1,3-(bis-diisopropylphenyl)-imidazolium (0.19 g, 0.50 mmol) in THF (20 ml) was added at room temperature solid Me<sub>3</sub>SiCH<sub>2</sub>Li (0.10 g, 1.00 mmol). The solution turned orange after 5 min and was stirred at room temperature for 12 h. Concentration to *ca.* 2 ml and slow cooling to -40 °C gave orange extremely air sensitive crystals suitable for crystallography. Additional amount of **5<sup>tBu-Ph</sup>** was obtained by concentration of the mother liquor, addition of pentane and isolation of the precipitated solid. Combined yield: 0.35 g, (77%). Reproducible elemental analysis data could not be obtained.

<sup>1</sup>H-NMR, (400 MHz, 293 K), d<sup>8</sup>-THF: δ, 7.30 and 7.22 (two multiplets, 3H, non-lithiated DiPP), 6.87 (virtual d, *J* = 9.0 Hz, 2H, 4-*t*-Bu-Ph), 6.75 (virtual d, *J* = 8.0 Hz, 2H, 4-*t*-Bu-Ph), 6.40 (d of d overlapping with one singlet, 2H in total, lithiated DiPP and imidazol-backbone), 5.60 (d, *J* = 8.0 Hz, 1H, lithiated DiPP), 5.08 (d, 1H, *J* = 7.0 Hz, lithiated DiPP), 3.64 (m, THF), 3.40 (sept, *J* = 7.0 Hz, 1H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.28 and 2.66 (two sept., *J* = 7.0 Hz, 1H each, CH(CH<sub>3</sub>)<sub>2</sub>), 1.80 (m, THF), 1.56 and 1.52 (two s, 3H each, LiCMe<sub>2</sub>), 1.27 (d, *J* = 7.0 Hz, 3H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.23 (d, *J* = 7.0 Hz, 3H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.21 (s, 9H, *t*-Bu), 1.17 and 1.16 (two d, 3H each, CH(CH<sub>3</sub>)<sub>2</sub>), 1.00 and 0.98 (two d, *J* = 7.0 Hz, 3H each, CH(CH<sub>3</sub>)<sub>2</sub>).



**Figure S2.**  $^1\text{H}$ -NMR of  $\mathbf{5}^{t\text{Bu-Ph}}$ .

$^{13}\text{C}\{^1\text{H}\}$ -NMR,  $d^8$ -THF (75.48 MHz, 298 K):  $\delta$ , 190.80, 154.02, 150.75, 146.88, 146.15, 140.81, 140.32, 132.11, 127.63, 127.24, 124.10, 122.78, 122.73, 116.49, 116.41, 110.92, 99.97, 92.92, 53.31, 33.01, 31.28, 27.61, 27.41, 27.24, 25.32, 23.41, 23.32, 23.19, 21.25.

$^7\text{Li}$  (155.5 MHz),  $d^8$ -THF (293 K):  $\delta$ , 0.44 (1 Li, br), -0.28 (1 Li).

## 2.1. X-ray crystallography - General methods

Summary of the crystal data, data collection and refinement for compounds **3<sup>Cy</sup>**, **4<sup>Cy</sup>** and **5<sup>tBu-Ph</sup>** are given in Table S1. The crystals were mounted on a glass fiber with grease, from Fomblin vacuum oil. Data sets were collected on a Bruker APEX II DUO Kappa-CCD diffractometer equipped with an Oxford Cryosystem liquid N<sub>2</sub> device, using Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) unless otherwise stated (see specific comments for each data set given below). The cell parameters were determined (APEX2 software)<sup>2</sup> from reflections taken from three sets of 12 frames, each at 10 s exposure. The structures were solved by direct methods using the program SHELXS-97.<sup>3</sup> The refinement and all further calculations were carried out using SHELXL-97.<sup>3</sup> The H-atoms were included in calculated positions and treated as riding atoms using SHELXL default parameters unless stated otherwise. The non-H atoms were refined anisotropically, using weighted full-matrix least-squares on  $F^2$ .

The following specific comments apply for the structures:

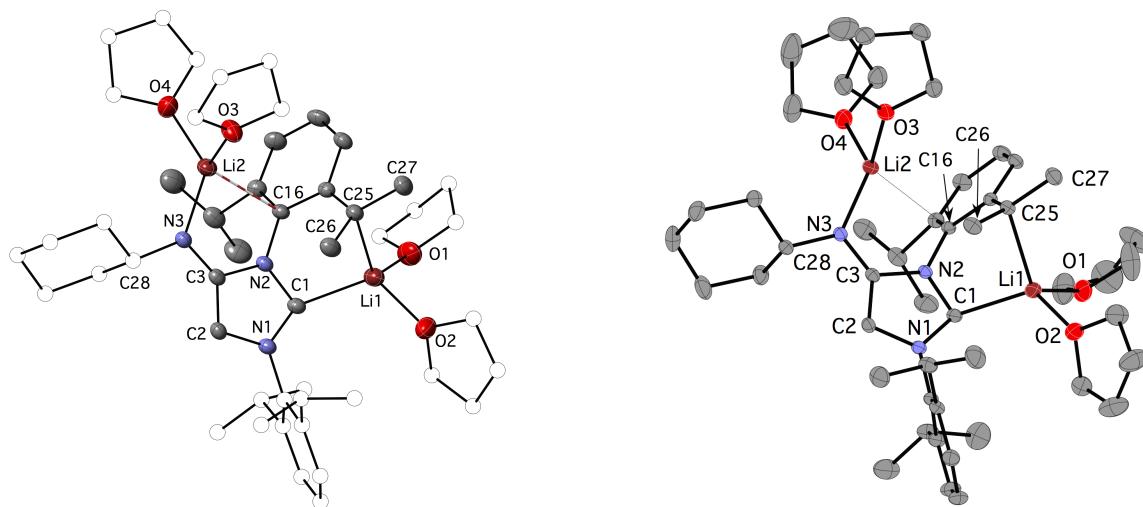
**Complex 4<sup>Cy</sup>:** SQUEEZE<sup>4</sup> was applied, the residual electron density being assigned to one molecule of THF. The crystal did not diffract far enough, so the ratio of observed to unique reflections is low (Alert B).

**Complex 5<sup>tBu-Ph</sup>:** There is one molecule of THF in the asymmetric unit. The methyls C35, C36, C37 are disordered over two positions. The carbons C48, C51 and C56 are also disordered over two positions.

**2.2. Table S1.** Summary of crystal data

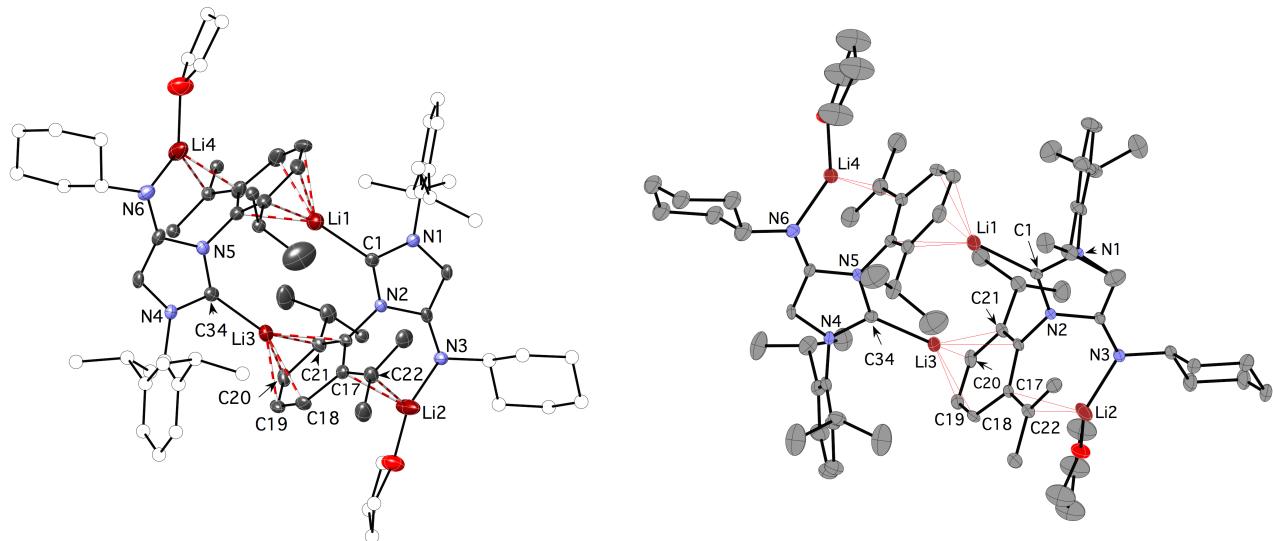
	<b>3<sup>Cy</sup></b>	<b>4<sup>Cy</sup></b>	<b>5<sup>tBu-Ph</sup>.THF</b>
Chemical formula	C <sub>49</sub> H <sub>77</sub> Li <sub>2</sub> N <sub>3</sub> O <sub>4</sub>	C <sub>37</sub> H <sub>53</sub> Li <sub>2</sub> N <sub>3</sub> O	C <sub>61</sub> H <sub>95</sub> Li <sub>2</sub> N <sub>3</sub> O <sub>6</sub>
CCDC Number	1020248	1020257	1020254
Formula Mass	786.02	569.70	980.28
Crystal system	Triclinic	Monoclinic	Triclinic
<i>a</i> (Å)	11.3020(5)	31.4483(16)	10.8651(6)
<i>b</i> (Å)	12.6719(6)	18.8909(10)	14.5756(9)
<i>c</i> (Å)	17.2731(8)	26.5581(13)	20.5112(13)
<i>α</i> (°)	91.2700(10)	90	102.510(2)
<i>β</i> (°)	103.5970(10)	94.3840(10)	100.7460(10)
<i>γ</i> (°)	99.0700(10)	90	106.6530(10)
Unit cell volume/Å <sup>3</sup>	2369.89(19)	15731.6(14)	2928.9(3)
Temperature/K	173(2) K	173(2)	173(2)
Space group	<i>P</i> -1	<i>C</i> 2/c	<i>P</i> -1
Formula units / cell, <i>Z</i>	2	8	2
Absorption coef. μ/mm <sup>-1</sup>	0.068	0.056	0.070
No. of reflections measured	41380	57744	39956
No. of independent reflections	11426	18986	14095
<i>R</i> <sub>int</sub>	0.0427	0.0950	0.0612
Final <i>R</i> <sub>f</sub> values ( <i>I</i> > 2σ( <i>I</i> ))	0.0633	0.0985	0.0744
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values ( <i>I</i> > 2σ( <i>I</i> ))	0.1578	0.2484	0.1796
Final <i>R</i> <sub>f</sub> values (all data)	0.1103	0.2398	0.1664
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values (all data)	0.1879	0.2983	0.2164
Goodness of fit on <i>F</i> <sup>2</sup>	1.021	0.900	1.023

### 2.3. The structure of $3^{\text{Cy}}$



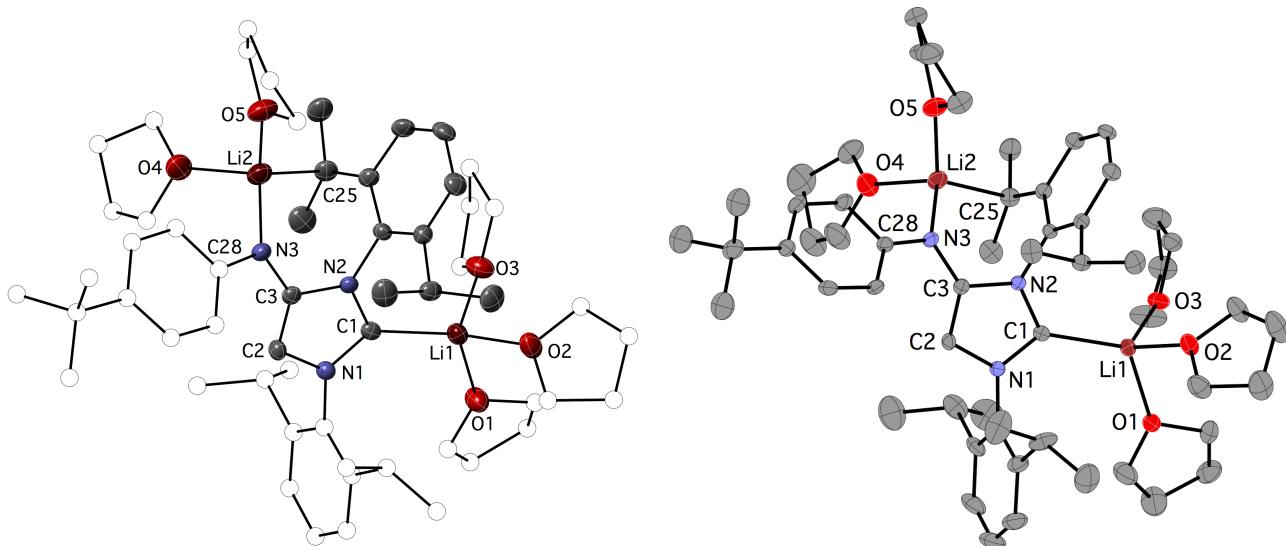
**Figure S3.** The structure of  $3^{\text{Cy}}$ . On the left the C atoms of the coordinated THF molecules, the Cy substituent and the distal DiPP are shown as hollow spheres; ellipsoids are at 40% probability. On the right all non-hydrogen atoms are depicted with ellipsoids at 20% probability level. Important bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ): C1-N1=1.352(2), C1-N2=1.375(2), C1-Li1=2.121(4), C2-C3=1.383(3), C2-N1=1.410(2), C3-N3=1.343(2), C3-N2=1.411(2), C4-N1=1.434(2), N3-Li2=1.948(4), C25-Li1=2.364(4), O1-Li1=1.982(4), O2-Li1=1.956(4), O3-Li2=1.970(4), O4-Li2=2.000(4), C16-Li2=2.563(4), N1-C1-N2=102.51(15), N1-C1-Li1=142.09(18), N2-C1-Li1=106.65(15), C3-C2-N1=106.67(15).

## 2.4. The structure of $4^{\text{Cy}}$

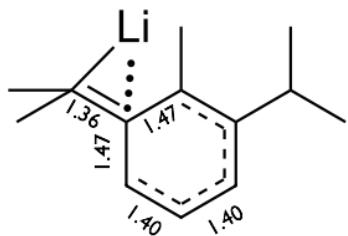


**Figure S4.** The structure of  $4^{\text{Cy}}$ . On the left the C atoms of the coordinated THF molecules, the Cy substituent and the distal DiPP are shown as hollow spheres; ellipsoids are at 40% probability. On the right all non-hydrogen atoms are depicted with ellipsoids at 20% probability level. Important bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ): C1-N1=1.349(4), C1-N2=1.367(4), C1-Li1=2.043(8), C2-C3=1.379(4), C2-N1= 1.394(4), C3-N3=1.343(4), C3-N2=1.415(4), C4-N1=1.436(4), N3-Li2=1.903(7), Li2-O1=1.882(9), C17-C22-C24=119.7(3), C23-C22-C24=112.3(3), C17-C22-Li2=69.8(3), C23-C22-Li2=103.9(3), C24-C22-Li2=110.9(3), N1-C1-N2=102.8(3), N1-C1-Li1=121.8(3), N2-C1-Li1=135.3(3), C3-N3-C28 =112.1(2), C3-N3-Li2=118.6(3), C28-N3-Li2=125.1(3).

## 2.5. The structure of $5^{t\text{Bu-Ph}}$



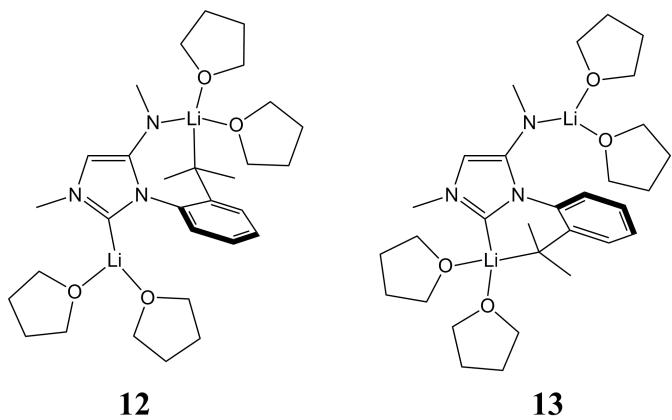
**Figure S5.** The structure of  $5^{t\text{Bu-Ph}}$ . On the left the C atoms of the coordinated THF molecules, the BuPh substituent and the distal DiPP are shown as hollow spheres; ellipsoids are at 30% probability. On the right all non-hydrogen atoms are depicted with ellipsoids at 20% probability level, with 30% probability ellipsoids; only one disordered  $t\text{Bu}$  and disordered THF ligands containing atoms O3 and O5 are shown. Important bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ): C1-N1=1.360(3), C1-N2=1.372(3), C1-Li1=2.179(5), C2-C3=1.357(3), C2-N1=1.393(3), C3-N3=1.368(3), C3-N2=1.409(3), C25-C26=1.498(4), C25-C27=1.520(3), C25-Li2=2.264(5), Li2-N3=1.994(4), N1-C1-N2=101.94(19), N1-C1-Li1=132.04(19), N2-C1-Li1=126.01(19), C3-N3-C28=117.95(18), C3-N3-Li2=114.37(19), C28-N3-Li2=123.0(2), C21-C25-C26=125.6(2), C21-C25-C27=117.1(2), C26-C25-C27=113.5(2), C21-C25-Li2=85.02(19), C26-C25-Li2=99.6(2), C27-C25-Li2=105.9(2).



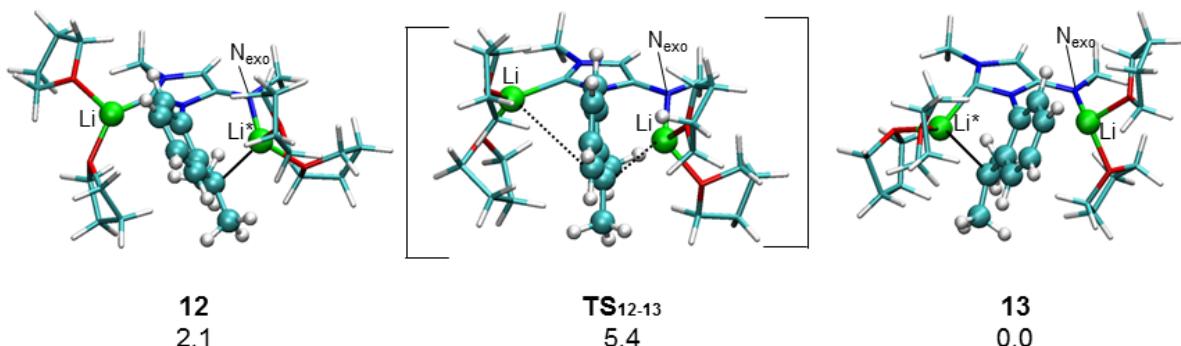
**Figure S6.** Schematic representation of the dearomatised DiPP structure in the dilithiated species  $3^{\text{Cy}}$ ,  $4^{\text{Cy}}$  and  $5^{t\text{Bu-Ph}}$ . See main text for the accurate bond distances in individual cases and discussion.

### 3. Computational Studies

Density functional theory (DFT) calculations are carried out with the M06-2X<sup>5</sup> density functional as implemented in Gaussian09,<sup>6</sup> combined with the 6-31++G(d,p) basis set.<sup>7-9</sup> Solvent effects are accounted for by means of single point calculations with the integral equation formalism version of the polarizable continuum model (IEFPCM) for THF.<sup>10</sup> Electronic energies relative to the most stable unlithiated tautomer (**1<sup>R</sup>** for Ph substituted systems and **2<sup>R</sup>** for Cy substituted systems) are given in kcal/mol. Despite of the size of the studied molecules, full substitution patterns, except the para-*t*-Bu group in (**1<sup>t-Bu-Ph</sup>** ⊕ **2<sup>t-Bu-Ph</sup>**) and related species (i.e the *t*-Bu-Ph group has been modelled by Ph group), have been included in the calculations of the lithiation process. Calculations of transition states could not be achieved at the used high-level method for these substituted molecules. Therefore, the simplified model depicted in Figure S7 has been used for the calculation of **TS<sub>12-13</sub>** (Figure S8). Frequency calculations were carried out for complexes **12**, **13** and **TS<sub>12-13</sub>** in order to ensuring their stationary character.



**Figure S7.** Isomers **12** and **13**, which are simplified models of **10<sup>R</sup>** and **3<sup>R</sup>**, respectively



**Figure S8.** Optimized structures of **12**, **TS<sub>12-13</sub>** and **13**. Relative energies in kcal/mol.

#### 4. Cartesian coordinates of the optimized geometries

**1<sup>Cy</sup>**

6	2.158860	3.182001	-0.359680
6	2.198499	1.998748	-1.342095
6	3.526543	2.005519	-2.100649
6	3.774557	3.337603	-2.811879
6	3.714775	4.512244	-1.831075
6	2.388674	4.520214	-1.066039
7	2.032831	0.727814	-0.667528
6	0.809838	0.435826	-0.351718
7	0.513015	-0.785058	0.331130
6	-0.814818	-0.898848	0.538079
7	-1.406808	0.171063	0.037546
6	-0.469958	1.029506	-0.515651
6	1.462191	-1.803453	0.666069
6	2.304251	-1.594700	1.767301
6	3.197872	-2.616604	2.093530
6	3.240663	-3.791342	1.347813
6	2.406500	-3.960911	0.247814
6	1.504416	-2.961578	-0.126197
6	-2.823249	0.392309	0.054518
6	-3.370558	1.114152	1.122125
6	-4.755360	1.302459	1.119283
6	-5.542310	0.794322	0.090842
6	-4.962247	0.089823	-0.960835
6	-3.582581	-0.122731	-1.005435
6	2.209823	-0.306378	2.568388
6	3.499774	0.031841	3.316857
6	0.666805	-3.074344	-1.390772
6	1.353997	-2.304273	-2.530125
6	-2.512296	1.645174	2.257360
6	-2.695578	3.155765	2.440858
6	-2.940748	-0.914572	-2.132829
6	-3.416111	-0.443246	-3.511128
6	0.377100	-4.516826	-1.808503
6	1.027712	-0.360437	3.547986
6	-3.204059	-2.416185	-1.953004
6	-2.815218	0.890566	3.558359
1	-0.769633	1.966418	-0.952285
1	-0.055905	-5.099209	-0.988781
1	1.283675	-5.026703	-2.150862
1	-0.329726	-4.522803	-2.643875
1	1.571453	-1.270330	-2.242836
1	0.720763	-2.305140	-3.424596
1	2.305195	-2.787007	-2.781959
1	2.466571	-4.876765	-0.330855
1	3.938488	-4.577548	1.620332
1	3.871165	-2.495231	2.935596
1	2.036144	0.499068	1.846117
1	0.942303	0.586117	4.092902
1	0.078500	-0.537954	3.031475
1	1.171327	-1.164088	4.279395
1	3.415419	1.029204	3.758622
1	4.361130	0.029208	2.642739
1	3.693665	-0.671434	4.134581
1	-4.277001	-2.630724	-2.013186
1	-2.696900	-2.987262	-2.737822
1	-2.843838	-2.775154	-0.983118
1	-1.857921	-0.750319	-2.087382
1	-3.252698	0.630370	-3.639441
1	-4.481086	-0.648327	-3.661825
1	-2.865033	-0.970367	-4.295602
1	-5.590825	-0.299501	-1.756398
1	-6.616862	0.948731	0.107520
1	-5.222325	1.848532	1.934250

1	-1.461135	1.471390	2.001708
1	-3.851487	1.055699	3.873575
1	-2.156127	1.235639	4.361167
1	-2.668219	-0.187199	3.434382
1	-2.474821	3.694036	1.514563
1	-3.719698	3.400535	2.742042
1	-2.021748	3.523387	3.220585
1	-1.313223	-1.721392	1.027484
1	1.392157	2.160028	-2.090761
1	4.327218	1.808252	-1.373928
1	3.533522	1.171431	-2.811507
1	4.742625	3.319579	-3.325524
1	3.008995	3.482427	-3.587966
1	4.540577	4.420805	-1.111165
1	3.857296	5.461670	-2.360144
1	2.370481	5.343266	-0.342020
1	1.566987	4.704181	-1.773860
1	2.948084	3.014624	0.387614
1	1.204043	3.186032	0.182067
1	-0.301401	-2.592781	-1.206462

### **1<sup>Ph</sup>**

6	1.965500	-2.297969	-1.096844
6	1.753347	-1.604305	0.104134
6	2.546183	-1.777303	1.246111
6	3.574360	-2.718837	1.173301
6	3.794268	-3.444814	0.006429
6	3.002449	-3.234194	-1.117678
7	0.671456	-0.663708	0.159196
6	0.799676	0.748999	0.015020
6	-0.539235	1.195113	0.014678
7	-1.355121	0.086274	0.175830
6	-0.623081	-1.012002	0.256519
7	2.004686	1.257820	-0.019844
6	2.203193	2.598507	-0.304166
6	1.347890	3.404345	-1.084525
6	1.662555	4.736426	-1.350333
6	2.828062	5.311259	-0.850113
6	3.693844	4.519274	-0.089744
6	3.392445	3.190276	0.171096
6	-2.790482	0.103910	0.163614
6	-3.433874	-0.010197	-1.076894
6	-4.830448	-0.006917	-1.069938
6	-5.537891	0.112972	0.122969
6	-4.864817	0.234230	1.334622
6	-3.468125	0.236411	1.381814
6	-2.654239	-0.176582	-2.371077
6	-3.135115	0.789726	-3.458736
6	-2.725815	0.329250	2.703734
6	-2.823717	-1.002735	3.460248
6	2.266097	-0.973388	2.504406
6	3.502075	-0.793586	3.387097
6	1.153883	-1.974978	-2.342371
6	1.729860	-0.724536	-3.026399
6	-2.730517	-1.629756	-2.859818
6	-3.233499	1.487462	3.568769
6	1.123844	-1.609291	3.310702
6	1.063239	-3.139110	-3.330854
1	-0.961194	2.183036	-0.037040
1	-5.370360	-0.101295	-2.007679
1	-6.623435	0.112314	0.107573
1	-5.430736	0.326448	2.257129
1	-1.603003	0.058786	-2.169323
1	-2.495257	0.705211	-4.342100
1	-3.102084	1.825418	-3.109168
1	-4.160751	0.566471	-3.770388
1	-2.357813	-2.328431	-2.103095

1	-2.130002	-1.757333	-3.766711
1	-3.764610	-1.906509	-3.093194
1	-1.668537	0.519249	2.487269
1	-3.865665	-1.226275	3.714877
1	-2.245584	-0.959374	4.388584
1	-2.440091	-1.832612	2.857582
1	-4.268017	1.326074	3.889140
1	-3.187261	2.436209	3.027062
1	-2.619573	1.575949	4.469835
1	4.215718	-2.881629	2.032919
1	4.598572	-4.173481	-0.031367
1	3.200395	-3.797330	-2.023511
1	1.956046	0.024688	2.176647
1	3.276420	-0.092771	4.196103
1	4.342338	-0.392129	2.813225
1	3.814164	-1.736739	3.849649
1	0.202078	-1.677959	2.723334
1	0.908843	-1.013031	4.204034
1	1.397013	-2.620949	3.631605
1	1.808390	0.117591	-2.331850
1	1.100293	-0.431621	-3.874126
1	2.736390	-0.937116	-3.403942
1	2.031820	-3.345675	-3.797730
1	0.366077	-2.885915	-4.135356
1	0.711828	-4.056698	-2.848255
1	4.065277	2.566380	0.752325
1	4.615179	4.943686	0.300011
1	3.063778	6.350527	-1.055091
1	0.987398	5.328543	-1.962949
1	0.453921	2.973050	-1.524619
1	-1.005330	-2.016091	0.358955
1	0.128726	-1.737319	-2.031270

## **2<sup>Cy</sup>**

6	-2.419837	-2.752359	-0.571425
6	-2.280577	-1.684834	-1.665141
6	-3.572151	-1.571142	-2.473062
6	-3.979489	-2.922623	-3.065630
6	-4.104660	-3.994835	-1.980107
6	-2.812183	-4.106688	-1.167607
7	-1.919432	-0.368334	-1.146390
6	-0.657646	-0.206598	-0.603016
7	-0.368440	0.831305	0.281243
6	0.955848	0.867941	0.663867
7	1.462637	-0.180877	-0.022497
6	0.515445	-0.867712	-0.797604
6	-1.364331	1.736887	0.770181
6	-2.263017	1.271577	1.744221
6	-3.253989	2.152513	2.186984
6	-3.328468	3.447355	1.684134
6	-2.413778	3.887781	0.731877
6	-1.413438	3.039980	0.249402
6	2.843076	-0.559561	-0.001762
6	3.282855	-1.457141	0.979805
6	4.631107	-1.826865	0.961363
6	5.495865	-1.320660	-0.003164
6	5.032248	-0.425980	-0.964062
6	3.694455	-0.025686	-0.981797
6	-2.103804	-0.117038	2.344850
6	-3.418935	-0.719605	2.843146
6	-0.422518	3.483885	-0.814028
6	-0.850107	2.966564	-2.196045
6	2.349834	-1.947045	2.073663
6	2.515516	-3.439610	2.373722
6	3.187262	1.013814	-1.967611
6	3.828961	0.897493	-3.352440
6	-0.215501	4.998506	-0.855575

6	-1.059261	-0.074525	3.470316
6	3.400060	2.419682	-1.384886
6	2.561812	-1.103619	3.338960
1	0.769413	-1.729170	-1.393943
1	0.032872	5.399262	0.131789
1	-1.104804	5.519839	-1.227465
1	0.607707	5.235838	-1.536189
1	-0.966862	1.879079	-2.207224
1	-0.103703	3.242168	-2.949308
1	-1.808977	3.412201	-2.486208
1	-2.480419	4.905312	0.361143
1	-4.100776	4.121529	2.042219
1	-3.968049	1.828800	2.937533
1	-1.714363	-0.784119	1.566835
1	-0.899907	-1.077919	3.881025
1	-0.103023	0.309506	3.102111
1	-1.403976	0.578357	4.280190
1	-3.262816	-1.766675	3.120215
1	-4.199372	-0.681226	2.075100
1	-3.791045	-0.200249	3.732480
1	4.470986	2.621049	-1.265788
1	2.981297	3.178526	-2.056026
1	2.921104	2.510935	-0.405330
1	2.108096	0.863382	-2.087441
1	3.738436	-0.116285	-3.754273
1	4.891184	1.162724	-3.330108
1	3.338533	1.587193	-4.046314
1	5.722555	-0.032284	-1.703746
1	6.539649	-1.620526	-0.003870
1	5.009894	-2.515004	1.711471
1	1.319430	-1.786023	1.734725
1	3.586466	-1.224549	3.709169
1	1.872558	-1.417144	4.130620
1	2.394374	-0.043473	3.126448
1	2.419904	-4.043033	1.465817
1	3.489692	-3.655967	2.824619
1	1.749676	-3.763628	3.085495
1	-1.474755	-1.984404	-2.352276
1	-4.370141	-1.209875	-1.805781
1	-3.442466	-0.818127	-3.256980
1	-4.922006	-2.820661	-3.613613
1	-3.221801	-3.237098	-3.796987
1	-4.931502	-3.730367	-1.306097
1	-4.357903	-4.961332	-2.429087
1	-2.922362	-4.851256	-0.372259
1	-2.002992	-4.461667	-1.821569
1	-3.199863	-2.420220	0.131148
1	-1.485182	-2.829366	-0.003424
1	-2.651635	0.067556	-0.591898
1	0.539592	3.024632	-0.562609

## 2<sup>Ph</sup>

6	-2.116379	-0.890283	2.095692
6	-1.680281	-1.347788	0.841057
6	-2.325202	-2.377833	0.137221
6	-3.462923	-2.945504	0.718465
6	-3.923263	-2.504594	1.955000
6	-3.252806	-1.494411	2.639019
7	-0.545703	-0.713917	0.237130
6	-0.666665	0.276976	-0.740180
6	0.603017	0.665495	-1.034160
7	1.429128	-0.105671	-0.209955
6	0.757955	-0.972359	0.587757
7	-1.911572	0.638909	-1.215173
6	-2.298780	1.901206	-1.673885
6	-1.470496	3.027082	-1.599812
6	-1.930393	4.257330	-2.068065

6	-3.205043	4.390227	-2.610475
6	-4.031316	3.266944	-2.675945
6	-3.585546	2.034755	-2.218234
6	2.835864	0.145229	-0.099123
6	3.258662	1.109944	0.826878
6	4.630490	1.357287	0.921471
6	5.534708	0.670799	0.117577
6	5.085377	-0.280639	-0.793816
6	3.722966	-0.562650	-0.921456
6	2.270821	1.811833	1.744621
6	2.541190	3.314251	1.867984
6	3.216366	-1.648476	-1.854334
6	3.208958	-2.995279	-1.115321
6	-1.748118	-2.897644	-1.170451
6	-2.799398	-3.497101	-2.106080
6	-1.379666	0.228945	2.814268
6	-1.812207	1.602170	2.278152
6	2.272122	1.136739	3.123232
6	4.015280	-1.747696	-3.156134
6	-0.640158	-3.918736	-0.868284
6	-1.544807	0.180192	4.334152
1	-2.660675	-0.004393	-0.993802
1	0.993876	1.377174	-1.742570
1	4.997136	2.090730	1.633827
1	6.597642	0.875696	0.203596
1	5.804788	-0.810739	-1.410225
1	1.267861	1.693868	1.317987
1	1.745567	3.788817	2.451041
1	2.580176	3.793965	0.885055
1	3.487322	3.515141	2.381174
1	2.051364	0.068740	3.031710
1	1.520798	1.598040	3.775000
1	3.252161	1.247036	3.601543
1	2.179154	-1.406013	-2.113769
1	4.230727	-3.274993	-0.833911
1	2.802354	-3.783032	-1.758906
1	2.604512	-2.936778	-0.205348
1	5.027027	-2.127982	-2.980150
1	4.097212	-0.776893	-3.654374
1	3.523485	-2.445411	-3.840632
1	-3.991130	-3.742985	0.205960
1	-4.807676	-2.956899	2.393539
1	-3.620584	-1.175387	3.608657
1	-1.281939	-2.055371	-1.696204
1	-2.342615	-3.728213	-3.072639
1	-3.631110	-2.806008	-2.278398
1	-3.207946	-4.431921	-1.708481
1	0.136494	-3.479617	-0.234953
1	-0.179582	-4.267801	-1.798744
1	-1.061276	-4.785324	-0.346135
1	-1.649789	1.693689	1.200239
1	-1.243637	2.396751	2.774607
1	-2.877493	1.770698	2.474068
1	-2.565195	0.435201	4.640926
1	-0.875388	0.910836	4.798168
1	-1.299618	-0.808259	4.733796
1	-4.229726	1.161196	-2.279597
1	-5.030665	3.349227	-3.092207
1	-3.552055	5.350774	-2.975339
1	-1.276834	5.121849	-1.999755
1	-0.485267	2.952231	-1.154993
1	-0.314399	0.098620	2.595475

### 3<sup>Cy</sup>

6	-1.378012	0.286874	0.424751
6	-0.464930	2.362553	0.064464
1	-0.503579	3.428136	-0.089193

6	0.596567	1.470894	0.105086
6	-2.954713	2.124014	0.144093
6	-3.456360	2.521493	-1.107021
6	-4.767569	3.002635	-1.165152
1	-5.178913	3.314254	-2.122522
6	-5.559415	3.071007	-0.023610
1	-6.580701	3.434412	-0.090802
6	-5.036884	2.683335	1.206472
1	-5.656447	2.750887	2.096520
6	-3.721994	2.222985	1.318738
6	-2.630579	2.425140	-2.379500
1	-1.643042	2.039033	-2.113546
6	-2.432250	3.804807	-3.018357
1	-1.786593	3.725647	-3.898817
1	-1.966748	4.499855	-2.313089
1	-3.386656	4.237365	-3.339445
6	-3.262350	1.442131	-3.371672
1	-3.364511	0.455948	-2.909307
1	-2.632342	1.342424	-4.262358
1	-4.255625	1.779513	-3.693517
6	-3.157429	1.824915	2.671356
1	-2.067840	1.787330	2.570724
6	-3.645023	0.425400	3.070008
1	-4.739357	0.408514	3.148067
1	-3.229844	0.139539	4.043753
1	-3.333418	-0.316832	2.327829
6	-3.488668	2.845322	3.765562
1	-4.557904	2.855237	4.003721
1	-3.196035	3.856662	3.468525
1	-2.951951	2.587452	4.684186
6	0.685602	-1.005483	0.636900
6	1.318241	-1.150007	1.884428
6	1.839535	-2.394339	2.265473
1	2.352667	-2.512382	3.212786
6	1.663308	-3.490009	1.410346
1	2.061069	-4.462299	1.698537
6	1.004992	-3.373221	0.203122
1	0.907751	-4.254374	-0.423730
6	0.460390	-2.119424	-0.272636
6	1.311606	0.003044	2.880137
1	1.329868	0.941082	2.319679
6	2.523237	0.015119	3.814605
1	2.531121	0.942837	4.396230
1	3.454479	-0.046152	3.242822
1	2.498708	-0.817140	4.526743
6	0.005058	-0.051294	3.687348
1	-0.863534	-0.055603	3.020356
1	-0.074126	0.812233	4.358614
1	-0.026729	-0.964917	4.294382
6	-0.244538	-2.046640	-1.487092
6	-0.324564	-0.763098	-2.302030
1	0.521402	-0.087112	-2.108053
1	-1.236157	-0.164501	-2.142604
1	-0.301198	-1.010093	-3.373035
6	-0.452245	-3.321978	-2.274711
1	0.476328	-3.739072	-2.718157
1	-1.138676	-3.148284	-3.110956
1	-0.886586	-4.134290	-1.674836
6	2.415973	2.900616	-0.232261
1	1.699601	3.516807	-0.814412
6	2.624347	3.594842	1.125884
1	1.669949	3.624526	1.665566
1	3.303328	2.961732	1.718194
6	3.219692	4.997230	0.982218
1	2.511852	5.641266	0.440314
1	3.369395	5.453463	1.967569
6	4.540041	4.948244	0.209595

1	5.271713	4.365595	0.789330
1	4.957791	5.954684	0.091787
6	4.344697	4.288591	-1.157656
1	5.298747	4.230762	-1.695196
1	3.679596	4.918860	-1.764773
6	3.725161	2.895893	-1.023508
1	3.535553	2.463670	-2.012182
1	4.432789	2.223146	-0.511353
6	-1.857922	-2.940196	2.338090
1	-0.893459	-2.466465	2.139297
1	-2.350515	-2.420118	3.165655
6	-1.717085	-4.448246	2.574828
1	-2.434336	-4.795900	3.325866
1	-0.709019	-4.701986	2.911004
6	-2.052007	-5.045024	1.203068
1	-2.412811	-6.075249	1.254129
1	-1.173202	-5.001718	0.553126
6	-3.109966	-4.073626	0.698166
1	-3.192650	-4.026746	-0.392867
1	-4.099080	-4.298316	1.123871
6	-4.034897	-2.071628	-2.516099
1	-4.093724	-3.162552	-2.397534
1	-3.252298	-1.841048	-3.244571
6	-5.413146	-1.467933	-2.864571
1	-5.367546	-0.863800	-3.773855
1	-6.147888	-2.260363	-3.027298
6	-5.773779	-0.607406	-1.634344
1	-6.822242	-0.704124	-1.343330
1	-5.565581	0.448874	-1.822266
6	-4.824749	-1.123915	-0.557102
1	-4.538480	-0.377472	0.189160
1	-5.224041	-2.015432	-0.049515
6	4.135363	-0.252462	-2.688264
1	4.858267	0.323764	-2.103832
1	3.458884	0.445087	-3.198698
6	4.774844	-1.250259	-3.678793
1	5.858342	-1.313883	-3.549730
1	4.583382	-0.942256	-4.709508
6	4.080760	-2.589933	-3.347949
1	3.792861	-3.152412	-4.238698
1	4.734163	-3.223753	-2.740281
6	2.877107	-2.153989	-2.517305
1	2.039084	-1.823539	-3.147520
1	2.512805	-2.896051	-1.804858
6	5.498823	0.202157	1.337646
1	5.718530	-0.019384	2.392317
1	5.248928	1.260453	1.242562
6	6.634841	-0.281900	0.422979
1	7.596951	-0.277546	0.940302
1	6.724493	0.367711	-0.452455
6	6.181037	-1.707736	0.012457
1	6.017576	-1.765729	-1.067472
1	6.907898	-2.475904	0.286556
6	4.850265	-1.890492	0.754185
1	4.091206	-2.454597	0.207879
1	4.992048	-2.349577	1.742773
7	-1.633116	1.594105	0.228549
7	-0.011151	0.229067	0.384658
7	1.922961	1.549431	-0.076914
8	-2.676671	-2.790987	1.154605
8	-3.643546	-1.480680	-1.278378
8	3.376507	-1.041164	-1.772148
8	4.365619	-0.560048	0.937423
3	-2.060536	-1.579861	-0.213661
3	2.796412	-0.146481	-0.104624

6	-2.846513	-4.139162	-0.814726
8	-2.563915	-3.092219	0.119364
6	-1.785213	-3.608176	1.226056
6	-1.640768	-5.109150	0.974857
6	-1.793232	-5.206435	-0.546939
3	-1.931243	-1.457264	-0.655043
8	-3.419886	-0.922857	-1.744309
6	-3.656845	-1.116105	-3.139350
6	-5.065691	-0.549061	-3.421785
6	-5.583861	-0.114354	-2.035279
6	-4.683143	-0.883874	-1.075329
6	-1.316853	0.070142	0.630201
7	-1.624151	1.369539	0.825257
6	-0.489519	2.179471	0.970803
6	0.603253	1.348728	0.842057
7	0.046820	0.068500	0.669683
7	1.950729	1.476059	0.895092
6	2.528044	2.724143	0.768061
6	-2.963686	1.861436	0.814373
6	-3.396710	2.641347	-0.271748
6	-4.721799	3.085994	-0.270784
6	-5.592403	2.746879	0.759777
6	-5.138217	1.978323	1.827104
6	-3.813044	1.537527	1.887522
6	0.783651	-1.159328	0.509451
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6	1.877713	-3.026702	1.616436
6	1.819569	-3.733272	0.407405
6	1.255547	-3.189041	-0.728330
6	0.652657	-1.872907	-0.752988
6	-2.476364	3.006119	-1.425395
6	-2.173275	4.509710	-1.428244
6	-3.329566	0.717714	3.071758
6	-3.792058	-0.739955	2.943379
6	1.227823	-1.012610	3.004463
6	2.417464	-1.266303	3.933432
6	-0.033932	-1.416088	-1.894180
6	-0.178724	0.056517	-2.250596
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6	-3.776311	1.311095	4.412503
6	-0.093540	-1.420450	3.674069
6	-0.130084	-2.337760	-3.091450
3	2.951061	-0.104224	0.379149
8	3.541166	0.023904	-1.484549
6	3.596379	1.342293	-2.043363
6	4.422534	1.172463	-3.321925
6	4.171488	-0.301142	-3.728783
6	3.291839	-0.846652	-2.592902
8	4.665098	-0.742587	1.053926
6	5.819021	0.091778	0.849476
6	6.912941	-0.836837	0.332950
6	6.094463	-1.859077	-0.459715
6	4.870914	-2.027320	0.432520
1	-0.564161	3.236738	1.161338
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1	-5.821152	1.727735	2.634043
1	-1.530900	2.475699	-1.284944
1	-1.479889	4.757392	-2.238763
1	-1.720331	4.822867	-0.482301
1	-3.088448	5.095274	-1.573294
1	-3.256531	1.481968	-2.753426
1	-2.341837	2.760802	-3.576452
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1	-2.235033	0.727339	3.052892
1	-4.887778	-0.794676	2.929730
1	-3.432739	-1.330517	3.794342

1	-3.406997	-1.187077	2.021462
1	-4.858511	1.221641	4.556634
1	-3.507736	2.368668	4.489538
1	-3.292182	0.772576	5.233299
1	2.324648	-3.473618	2.496547
1	2.249420	-4.732429	0.350369
1	1.261832	-3.775194	-1.641139
1	1.196141	0.062775	2.815747
1	2.337966	-0.625242	4.817238
1	3.362866	-1.042719	3.427953
1	2.449207	-2.303616	4.284283
1	-0.941238	-1.224960	3.007692
1	-0.245927	-0.862937	4.605605
1	-0.085610	-2.491959	3.910081
1	0.447412	0.711806	-1.635096
1	-1.208112	0.445241	-2.178056
1	0.133250	0.215256	-3.295905
1	0.832399	-2.475379	-3.627393
1	-0.833496	-1.934927	-3.829141
1	-0.481215	-3.346863	-2.837042
1	-0.814900	-3.103687	1.222838
1	-2.312691	-3.370291	2.154353
1	-2.438797	-5.668825	1.474672
1	-0.676901	-5.480025	1.331037
1	-2.098549	-6.196648	-0.893362
1	-0.852941	-4.927066	-1.032361
1	-2.797349	-3.713081	-1.822754
1	-3.862130	-4.519403	-0.634984
1	-3.599678	-2.187273	-3.375703
1	-2.855995	-0.599037	-3.675403
1	-5.028884	0.291830	-4.118542
1	-5.705569	-1.318076	-3.861890
1	-6.641420	-0.343946	-1.886862
1	-5.440257	0.958484	-1.882769
1	-4.527217	-0.394497	-0.110268
1	-5.040875	-1.911790	-0.910533
1	4.035567	2.013524	-1.301945
1	2.572770	1.681476	-2.255134
1	5.482399	1.339170	-3.110547
1	4.119850	1.883336	-4.093776
1	3.664113	-0.388271	-4.692224
1	5.113464	-0.851675	-3.799419
1	2.226474	-0.798953	-2.844963
1	3.526185	-1.867783	-2.280300
1	6.061548	0.574956	1.799445
1	5.569372	0.864490	0.110868
1	7.428179	-1.324972	1.167052
1	7.653757	-0.307129	-0.269979
1	5.797483	-1.433631	-1.424703
1	6.618150	-2.801941	-0.632293
1	3.959116	-2.303265	-0.107371
1	5.035399	-2.769105	1.223396
6	3.812916	2.914568	1.326380
6	4.529479	4.088675	1.130914
6	3.989775	5.136951	0.381583
6	2.711815	4.978118	-0.156534
6	1.986795	3.805421	0.033983
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1	5.514602	4.193660	1.579142
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1	1.010932	3.699335	-0.430418

## 5<sup>Cy</sup>

6	4.658986	1.395884	1.262934
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6	6.103115	-0.124518	2.405763
6	5.299924	1.171513	2.626556
3	2.643700	-0.832548	0.316937
8	2.615450	-2.001800	1.875653
6	1.908051	-3.256314	2.009016
6	1.400888	-3.304359	3.448509
6	1.273409	-1.821021	3.805932
6	2.454939	-1.210190	3.062976
6	1.041499	0.459601	-0.150764
7	0.888346	1.754077	-0.495379
6	-0.438511	2.080783	-0.817114
6	-1.190689	0.923134	-0.663710
7	-0.222124	-0.045033	-0.284920
7	-2.476643	0.570097	-0.760788
6	-3.416315	1.559631	-1.260288
6	-3.591151	2.783008	-0.336386
6	-4.589890	3.805928	-0.885543
6	-4.219906	4.231641	-2.308064
6	-4.155209	3.010965	-3.228418
6	-3.140676	1.987709	-2.714021
6	1.898974	2.752464	-0.387907
6	1.822233	3.652236	0.686530
6	2.790753	4.657651	0.775639
6	3.804927	4.753583	-0.168446
6	3.876102	3.833035	-1.213121
6	2.931379	2.812031	-1.344561
6	-0.502930	-1.443068	-0.123025
6	-0.096338	-2.302913	-1.151332
6	-0.333250	-3.685482	-1.037353
6	-1.040072	-4.153353	0.078774
6	-1.486310	-3.306466	1.073837
6	-1.223462	-1.879862	1.063782
6	0.772173	3.512957	1.776229
6	1.429984	3.178275	3.120985
6	3.015257	1.773424	-2.455234
6	1.883000	1.932947	-3.481323
6	0.479872	-1.732663	-2.448241
6	-0.641968	-1.116386	-3.301302
6	-1.677094	-1.061015	2.112275
6	-2.398858	-1.732897	3.262865
6	-0.103708	4.765458	1.881383
6	4.367519	1.763318	-3.168014
6	1.234917	-2.755675	-3.297263
6	-1.163861	0.345326	2.395268
3	-3.239484	-0.698545	0.490870
8	-4.279051	-1.983098	-0.546355
6	-4.834554	-3.161189	0.056111
6	-4.549567	-4.312678	-0.912768
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6	-3.657818	-2.317313	-1.801677
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1	4.550245	5.539585	-0.089108
1	4.687243	3.914272	-1.929121
1	0.120604	2.677415	1.513574
1	0.481997	5.643847	2.175779
1	-0.887515	4.616186	2.631153
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1	2.028446	2.263500	3.042287
1	0.664263	3.013804	3.886198
1	2.086803	3.987015	3.462426
1	2.880828	0.797494	-1.972403

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1	4.520670	2.677357	-3.752953
1	0.897404	1.842202	-3.016764
1	1.968966	1.157689	-4.251710
1	1.950404	2.911090	-3.971772
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1	-1.238782	-5.220193	0.173414
1	-2.010840	-3.738501	1.919443
1	1.184552	-0.932803	-2.189072
1	1.999257	-3.280041	-2.719465
1	1.722152	-2.250327	-4.139360
1	0.555046	-3.504447	-3.718272
1	-0.220217	-0.601360	-4.172689
1	-1.248406	-0.409743	-2.729703
1	-1.305955	-1.911096	-3.666246
1	-0.078707	0.451867	2.251305
1	-1.361788	0.595458	3.445798
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1	-1.776872	-2.473174	3.805485
1	3.738349	1.980124	1.278902
1	5.362343	1.861463	0.556573
1	4.518967	1.022196	3.378619
1	5.922583	2.011820	2.941239
1	6.085016	-0.774013	3.283848
1	7.149162	0.099442	2.180468
1	6.110242	-0.878065	0.341131
1	4.979331	-1.761618	1.406376
1	2.608696	-4.066970	1.786661
1	1.091889	-3.265349	1.281815
1	2.128556	-3.800749	4.100628
1	0.448415	-3.835971	3.514919
1	2.285592	-0.171774	2.753612
1	3.384992	-1.264162	3.649457
1	-3.758901	1.073090	2.751004
1	-4.944326	0.040937	3.589814
1	-7.709731	1.339740	1.325412
1	-6.293296	1.821575	0.373497
1	-6.756689	-0.877702	1.725063
1	-6.160319	-0.570677	0.062220
1	-5.911382	-2.995096	0.189764
1	-4.373017	-3.310594	1.038033
1	-3.613491	-4.805884	-0.635683
1	-5.352399	-5.053979	-0.922156
1	-5.340729	-3.346365	-2.698281
1	-3.779701	-4.157189	-2.970366
1	-2.591202	-2.496917	-1.633361
1	-3.774811	-1.454761	-2.462468
1	1.313932	-1.628615	4.880895
1	0.336970	-1.426414	3.403667
1	-5.469953	2.716101	2.388198
1	-6.543116	1.725500	3.380833
1	-4.402369	1.055313	-1.277240
1	-2.130606	2.411542	-2.786402
1	-3.143939	1.089127	-3.342840
1	-3.902784	3.314236	-4.251296
1	-5.152739	2.548902	-3.274039
1	-3.238244	4.727861	-2.295573
1	-4.942253	4.963255	-2.688250
1	-4.643180	4.678286	-0.222577
1	-5.599394	3.369527	-0.911148
1	-2.623327	3.275864	-0.184406
1	-3.904231	2.418669	0.651139
8	3.500383	-2.029669	-0.954269
6	3.707318	-3.437106	-0.757500

6	4.596590	-3.890718	-1.914349
6	5.396034	-2.619633	-2.218044
6	4.349807	-1.531427	-1.994353
1	4.207977	-3.577748	0.209602
1	2.725721	-3.922834	-0.725607
1	3.991261	-4.173059	-2.781120
1	5.224000	-4.741898	-1.641099
1	5.812055	-2.597690	-3.227605
1	6.217569	-2.508184	-1.501755
1	3.741723	-1.359822	-2.893836
1	4.766619	-0.577049	-1.658074

### 5<sup>Ph</sup>

6	5.682560	0.360255	-2.415095
8	4.441218	0.796095	-1.878429
6	4.492914	2.225593	-1.801197
6	5.978557	2.588904	-1.586254
6	6.716283	1.238798	-1.714785
3	3.281893	-0.266142	-0.741723
8	4.479381	-1.577487	0.064871
6	5.133081	-2.714717	-0.518514
6	4.965974	-3.864523	0.476287
6	4.803822	-3.120334	1.805016
6	3.968797	-1.925503	1.373724
7	2.479779	0.851341	0.664994
6	3.273214	1.616077	1.490810
6	2.827810	2.526693	2.481966
6	3.728594	3.219982	3.287420
6	5.106005	3.057721	3.151989
6	5.566824	2.150213	2.193737
6	4.680458	1.446933	1.391641
6	1.145756	1.096604	0.578169
6	0.340584	2.206777	0.682106
7	-0.962665	1.792478	0.387967
6	-1.036959	0.471324	0.099843
7	0.253769	0.056584	0.233295
6	-2.074898	2.684637	0.457937
6	-2.226158	3.637963	-0.563838
6	-3.275081	4.556089	-0.454118
6	-4.145793	4.512813	0.629319
6	-3.999091	3.533470	1.607671
6	-2.967657	2.592011	1.543336
6	0.644444	-1.308006	0.015015
6	0.376919	-2.227423	1.033838
6	0.705977	-3.582329	0.850721
6	1.358319	-3.955052	-0.335661
6	1.682775	-3.043051	-1.316341
6	1.331796	-1.634481	-1.228339
6	-1.356780	3.576834	-1.810760
6	-1.954639	2.541060	-2.778175
6	-2.843452	1.482021	2.581155
6	-1.614354	1.652737	3.485420
6	-0.147732	-1.742784	2.385355
6	0.988216	-1.087957	3.190253
6	1.695996	-0.752500	-2.252680
6	2.559319	-1.264414	-3.386815
6	-1.181769	4.926982	-2.507549
6	-4.099116	1.323267	3.440058
6	-0.771949	-2.847422	3.239546
6	1.208067	0.669482	-2.473736
3	-2.610773	-0.881172	-0.325912
8	-2.730600	-1.982066	-1.947374
6	-1.709923	-2.988416	-2.173164
6	-1.042429	-2.639643	-3.511492
6	-1.525647	-1.210598	-3.783175
6	-2.909174	-1.236110	-3.156020
8	-4.435461	-0.092942	-0.519237

6	-5.482264	-1.026084	-0.784889
6	-6.211755	-0.486250	-2.027185
6	-5.805834	1.006737	-2.074020
6	-4.982196	1.198121	-0.796944
1	5.798221	3.611856	3.777009
1	0.566494	3.235380	0.910113
1	-3.417052	5.308874	-1.223087
1	-4.950838	5.237535	0.707477
1	-4.706288	3.503359	2.429330
1	-0.364272	3.218089	-1.519608
1	-2.115863	5.276033	-2.961142
1	-0.446243	4.831424	-3.311480
1	-0.830068	5.695046	-1.812086
1	-2.035239	1.563282	-2.290024
1	-1.320844	2.426509	-3.664461
1	-2.954809	2.857253	-3.102850
1	-2.704715	0.548544	2.020928
1	-4.000836	0.432738	4.068947
1	-5.004158	1.212718	2.831596
1	-4.240504	2.178533	4.110401
1	-0.681487	1.625370	2.917178
1	-1.582165	0.842034	4.222296
1	-1.666180	2.604799	4.026164
1	0.501817	-4.319500	1.617781
1	1.617594	-5.001430	-0.492106
1	2.167325	-3.405282	-2.217627
1	-0.921095	-0.985160	2.204596
1	-1.525690	-3.413176	2.687414
1	-1.245429	-2.408246	4.125509
1	-0.013329	-3.553284	3.594356
1	0.604722	-0.673893	4.129829
1	1.488133	-0.291490	2.633741
1	1.743366	-1.844370	3.439008
1	0.257295	0.897172	-1.989361
1	1.053806	0.833586	-3.550847
1	1.923881	1.443079	-2.147979
1	3.417634	-1.862534	-3.044873
1	2.975251	-0.419754	-3.947112
1	2.020770	-1.898774	-4.116889
1	1.765889	2.667474	2.646601
1	3.337744	3.902560	4.038314
1	6.635535	1.983604	2.072192
1	5.059663	0.728364	0.668380
1	-4.156982	1.903514	-0.892026
1	-5.614508	1.504758	0.048851
1	-5.191326	1.214896	-2.954670
1	-6.666090	1.678958	-2.103289
1	-5.884226	-1.009979	-2.928105
1	-7.292237	-0.620660	-1.938471
1	-6.157075	-1.056718	0.084213
1	-5.019857	-2.005137	-0.925254
1	-2.193282	-3.971927	-2.195863
1	-1.013876	-2.946418	-1.330590
1	-1.384764	-3.317192	-4.300810
1	0.044019	-2.704844	-3.435178
1	-3.307452	-0.254320	-2.882711
1	-3.634938	-1.754680	-3.801741
1	3.840887	2.525474	-0.977716
1	4.108708	2.638276	-2.743540
1	7.652504	1.314059	-2.273027
1	6.936188	0.824832	-0.725829
1	5.687646	0.520981	-3.504296
1	5.778882	-0.708389	-2.211165
1	6.191264	-2.458536	-0.662945
1	4.676565	-2.928417	-1.491085
1	4.050275	-4.419224	0.250607
1	5.814473	-4.552827	0.456908

1	5.775558	-2.794659	2.193019
1	4.299622	-3.715551	2.570248
1	2.912929	-2.195264	1.277057
1	4.063145	-1.041847	2.009316
1	-1.540198	-0.950417	-4.844594
1	-0.893576	-0.497085	-3.246253
1	6.135377	3.040479	-0.604655
1	6.316113	3.297097	-2.347742
8	-3.151665	-2.240385	0.954928
6	-3.200003	-3.649477	0.663478
6	-4.010164	-4.282269	1.794892
6	-4.914685	-3.125998	2.234002
6	-3.985622	-1.927041	2.077896
1	-3.695222	-3.776682	-0.307628
1	-2.170466	-4.017755	0.591129
1	-3.356928	-4.584315	2.618962
1	-4.565740	-5.160799	1.459752
1	-5.292181	-3.233110	3.253230
1	-5.770058	-3.033324	1.555538
1	-3.349076	-1.787097	2.962874
1	-4.502273	-0.987360	1.859772

### **6<sup>Cy</sup>**

6	-4.506892	-1.934334	0.626629
6	-3.848376	-1.977556	-0.764357
6	-4.477427	-0.922041	-1.693716
6	-6.000322	-1.061339	-1.767009
6	-6.628264	-0.996978	-0.372834
6	-6.029850	-2.067996	0.542932
7	-2.401016	-1.947330	-0.730919
6	-1.809041	-0.873206	-0.265479
6	-2.133498	0.385752	0.271390
7	-0.927407	1.050430	0.540137
6	0.159318	0.320595	0.249011
7	-0.377652	-0.843670	-0.241448
6	-0.868589	2.356612	1.109279
6	-0.671363	2.473503	2.493373
6	-0.586385	3.758786	3.037755
6	-0.717769	4.883980	2.231924
6	-0.937341	4.742946	0.863892
6	-1.016564	3.478829	0.273560
6	0.438398	-1.892182	-0.758902
6	1.035698	-1.726201	-2.022243
6	1.853134	-2.754705	-2.503383
6	2.050699	-3.914102	-1.759640
6	1.426916	-4.068422	-0.522966
6	0.610443	-3.062422	0.000777
6	-0.532430	1.245516	3.376468
6	-1.464431	1.302467	4.591753
6	-1.283474	3.326604	-1.215571
6	-0.579219	4.394110	-2.063235
6	0.707382	-0.507854	-2.868300
6	1.809195	-0.134223	-3.859877
6	-0.104433	-3.200357	1.335294
6	0.624870	-2.420032	2.438758
6	0.925163	1.065128	3.816762
6	-2.792484	3.369389	-1.503039
6	-0.631891	-0.732684	-3.586744
6	-0.312753	-4.652913	1.762327
3	2.198902	0.392612	0.326055
8	3.594779	-0.609983	1.119849
6	4.087749	-1.686926	0.294724
6	4.333230	-2.838436	1.256647
6	4.800843	-2.098778	2.513779
6	3.919217	-0.849540	2.504943
8	2.994241	1.423375	-1.022651
6	2.277097	2.576149	-1.504697

6	3.356432	3.516640	-2.026547
6	4.388299	2.523229	-2.572304
6	4.338671	1.411206	-1.527528
1	-3.079244	0.839672	0.508348
1	-0.421574	3.880070	4.105189
1	-0.653034	5.875671	2.669909
1	-1.043464	5.630762	0.246930
1	-0.817232	0.372936	2.779647
1	-1.194566	2.118029	5.271416
1	-1.402003	0.366216	5.155507
1	-2.502900	1.446594	4.280648
1	1.584753	1.004607	2.943794
1	1.040921	0.145523	4.402140
1	1.255378	1.909519	4.433077
1	-0.914077	2.337533	-1.515164
1	-0.633304	4.121913	-3.122377
1	0.473671	4.517092	-1.790828
1	-1.063292	5.370769	-1.955877
1	-3.318581	2.574737	-0.971075
1	-2.978427	3.241027	-2.574648
1	-3.209024	4.335137	-1.193631
1	2.325615	-2.657252	-3.476106
1	2.678878	-4.708922	-2.151938
1	1.566838	-4.992469	0.029866
1	0.577305	0.335103	-2.181142
1	2.778498	-0.027124	-3.359059
1	1.564972	0.816571	-4.347215
1	1.915930	-0.880866	-4.654231
1	-0.938305	0.177042	-4.116227
1	-1.413250	-1.017628	-2.874323
1	-0.533018	-1.541944	-4.320154
1	1.585613	-2.896461	2.675242
1	0.025586	-2.405121	3.356609
1	0.813297	-1.383600	2.135904
1	-0.813955	-5.226148	0.976927
1	-0.937934	-4.686021	2.659828
1	0.634668	-5.149065	2.006714
1	1.683750	2.973617	-0.676294
1	1.597110	2.258503	-2.305189
1	2.975942	4.204381	-2.784751
1	3.783477	4.102999	-1.206089
1	5.388484	2.947451	-2.681222
1	4.063074	2.141605	-3.545860
1	4.542488	0.417065	-1.937463
1	5.023979	1.601122	-0.692499
1	5.021339	-1.359082	-0.182265
1	3.337270	-1.902384	-0.471119
1	5.067542	-3.549739	0.872396
1	3.395248	-3.370687	1.439612
1	2.983839	-1.010194	3.050119
1	4.417846	0.039978	2.900270
1	5.857547	-1.825716	2.425309
1	4.672321	-2.680093	3.429488
1	-4.118580	-2.956011	-1.195309
1	-4.222002	0.085372	-1.337434
1	-4.029368	-1.025285	-2.689281
1	-6.425959	-0.285074	-2.414485
1	-6.253681	-2.028401	-2.225709
1	-6.438396	-0.004445	0.062247
1	-7.716880	-1.112404	-0.437160
1	-6.476675	-2.008807	1.542826
1	-6.284101	-3.059759	0.140877
1	-4.252451	-0.990998	1.128621
1	-4.078221	-2.739156	1.236600
1	-1.095752	-2.758024	1.188282

**6<sup>Ph</sup>**

6	-4.722345	-0.428366	0.506617
6	-3.860161	0.475939	-0.131896
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6	-5.672575	1.887689	-0.778776
6	-6.557837	1.005863	-0.168134
6	-6.087632	-0.138395	0.470361
7	-2.453277	0.187268	-0.117782
6	-1.563125	0.572332	0.875756
6	-0.310505	0.061164	0.537632
7	-0.531904	-0.652890	-0.658605
6	-1.810587	-0.537314	-1.024492
7	0.939741	0.184194	0.995459
6	1.167710	0.509707	2.323181
6	2.451578	0.990551	2.673866
6	2.772207	1.306407	3.987543
6	1.836107	1.150622	5.013332
6	0.575148	0.656100	4.689483
6	0.239396	0.341061	3.374160
6	0.423314	-1.497881	-1.332473
6	1.367117	-0.887449	-2.243990
6	2.261478	-1.861499	-2.836752
6	2.219406	-3.201004	-2.524806
6	1.302986	-3.728163	-1.599678
6	0.393176	-2.859491	-0.994676
6	1.487497	0.480244	-2.546565
6	2.472386	0.871222	-3.631780
6	-0.547068	-3.376117	0.088794
6	-1.032928	-4.806104	-0.158662
6	-3.329479	2.589372	-1.461973
6	-3.565774	4.049465	-1.062188
6	-4.201254	-1.696768	1.162239
6	-4.356071	-2.889562	0.207739
6	0.392305	1.510269	-2.311080
6	0.129276	-3.268459	1.464872
6	-3.417615	2.417723	-2.984507
6	-4.883324	-1.987198	2.502736
3	2.298284	0.524006	-0.444658
8	3.833960	-0.502485	0.019606
6	4.955597	-0.705974	-0.853692
6	5.338525	-2.182209	-0.723169
6	4.788204	-2.544189	0.659553
6	3.498931	-1.737843	0.689611
8	2.661921	2.419981	-0.259648
6	3.642240	3.154611	-0.982690
6	3.992608	4.358805	-0.084422
6	2.828850	4.404994	0.936500
6	1.832589	3.387915	0.377060
1	4.822455	-2.766869	-1.490084
1	6.415228	-2.339809	-0.821304
1	5.468619	-2.210692	1.450939
1	4.606370	-3.614914	0.779164
1	3.141219	-1.478739	1.689180
1	2.699994	-2.239419	0.132178
1	4.662950	-0.437459	-1.874245
1	5.762839	-0.041966	-0.520838
1	3.209688	3.480430	-1.939338
1	4.478638	2.481503	-1.186162
1	4.061600	5.277061	-0.672470
1	4.950914	4.212500	0.418317
1	2.392003	5.400840	1.038617
1	3.165216	4.074807	1.923027
1	1.234807	2.871731	1.130450
1	1.169075	3.841127	-0.375908
1	-0.164122	0.503851	5.471580
1	3.191191	1.106016	1.884620
1	3.769165	1.675691	4.214841

1	2.088371	1.399708	6.038718
1	-0.739351	-0.080076	3.167844
1	-1.882872	1.199316	1.690341
1	0.733991	2.483147	-2.683221
1	0.123108	1.681227	-1.260157
1	-0.546826	1.286135	-2.849101
1	2.526191	1.960474	-3.727722
1	3.497974	0.527320	-3.439423
1	2.203583	0.477500	-4.629406
1	0.469266	-2.247349	1.666066
1	1.004930	-3.927704	1.501530
1	-0.562070	-3.572447	2.259633
1	-1.440763	-2.740645	0.113991
1	-1.775524	-5.082773	0.597424
1	-1.488867	-4.909515	-1.148216
1	-0.213872	-5.527973	-0.084865
1	1.300032	-4.787163	-1.372728
1	2.913659	-3.874527	-3.024306
1	2.975654	-1.526271	-3.580037
1	-2.689607	3.065333	-3.482861
1	-4.418342	2.680318	-3.345774
1	-3.210676	1.384479	-3.280980
1	-2.312535	2.324008	-1.153727
1	-2.795751	4.685465	-1.509002
1	-4.537127	4.412096	-1.414235
1	-6.791948	-0.815603	0.943790
1	-7.623550	1.212343	-0.187348
1	-6.054664	2.777660	-1.270235
1	-5.936992	-2.253680	2.370449
1	-4.391308	-2.832944	2.991771
1	-3.132278	-1.559872	1.363411
1	-5.414249	-3.069063	-0.012668
1	-3.838164	-2.716902	-0.741342
1	-3.939652	-3.795852	0.658798
1	-4.830158	-1.124231	3.172639
1	-3.528191	4.174886	0.023791
1	-2.248817	-0.980043	-1.905789

## 7<sup>Cy</sup>

6	-3.220408	-2.817016	-1.672694
8	-3.562493	-1.739772	-0.798524
6	-4.638555	-2.185167	0.019702
6	-4.259657	-3.619510	0.375884
6	-3.551910	-4.115875	-0.902780
3	-2.420047	-0.191105	-0.504557
8	-3.796741	0.762110	0.468148
6	-4.967063	1.218715	-0.228467
6	-5.201452	2.661677	0.226167
6	-4.488743	2.703927	1.582279
6	-3.286875	1.809368	1.315788
7	-0.909184	-0.420365	0.723321
6	0.323384	-0.158358	0.325829
6	1.614984	-0.656940	0.562710
7	2.500561	0.034277	-0.262503
6	1.826321	0.922223	-0.976935
7	0.535344	0.870912	-0.630591
6	3.896474	-0.274117	-0.390760
6	4.238971	-1.472354	-1.031393
6	5.596295	-1.804319	-1.092389
6	6.559022	-0.962081	-0.553971
6	6.188163	0.240502	0.045235
6	4.847512	0.616466	0.143729
6	-0.431549	1.854424	-1.038455
6	-0.346538	3.110524	-0.419041
6	-1.279109	4.097153	-0.749509
6	-2.292189	3.779793	-1.669208
6	-2.397867	2.535391	-2.249633

6	-1.455007	1.467107	-1.986969
6	3.199957	-2.383740	-1.663822
6	3.493318	-2.612386	-3.151446
6	4.429645	1.928438	0.799278
6	3.749290	1.691720	2.156750
6	0.662299	3.364295	0.697586
6	0.074729	2.910125	2.042897
6	-1.582355	0.209873	-2.599012
6	-2.702227	0.034021	-3.605405
6	-1.102028	-1.428264	1.754861
6	-0.689630	-2.845978	1.316500
6	-0.910246	-3.890043	2.415029
6	-0.213097	-3.480476	3.714733
6	-0.710886	-2.110332	4.178579
6	-0.472090	-1.045736	3.105542
6	3.108883	-3.716741	-0.910652
6	5.584094	2.918862	0.962275
6	1.140451	4.815452	0.779302
6	-0.421639	-0.763098	-2.757308
1	1.982799	-1.431409	1.212065
1	5.897887	-2.728684	-1.577489
1	7.608947	-1.232947	-0.610004
1	6.958927	0.893073	0.439271
1	2.223387	-1.895867	-1.593454
1	4.057052	-4.263184	-0.965389
1	2.327754	-4.346419	-1.348090
1	2.870281	-3.559206	0.145754
1	3.566737	-1.662421	-3.688919
1	2.687719	-3.198869	-3.603826
1	4.430239	-3.160343	-3.297568
1	3.694473	2.406166	0.140547
1	5.190503	3.876284	1.314930
1	6.109963	3.093481	0.018908
1	6.310137	2.570311	1.704911
1	2.853432	1.070612	2.069163
1	3.452933	2.650952	2.595305
1	4.446397	1.201505	2.845703
1	-1.232001	5.083116	-0.303115
1	-3.014955	4.546232	-1.944626
1	-3.187760	2.367157	-2.973449
1	1.552729	2.751903	0.520329
1	1.499962	5.175284	-0.189560
1	1.957704	4.895687	1.505004
1	0.342298	5.485115	1.114947
1	0.811925	3.025641	2.845991
1	-0.237503	1.861161	1.999059
1	-0.803572	3.517967	2.293432
1	0.498705	-0.284414	-3.130176
1	-0.687657	-1.520942	-3.502985
1	-0.142181	-1.314522	-1.845108
1	-3.698201	0.242321	-3.187066
1	-2.732163	-0.997851	-3.970074
1	-2.599880	0.682077	-4.495372
1	-2.164573	-2.701436	-1.929913
1	-3.818740	-2.732681	-2.588788
1	-5.123409	-4.229050	0.650985
1	-3.562877	-3.607716	1.218054
1	-5.575263	-2.148350	-0.558239
1	-4.705881	-1.502956	0.869518
1	-5.800448	0.560605	0.049050
1	-4.791817	1.137041	-1.306598
1	-4.714238	3.352091	-0.467755
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1	-4.193140	3.713969	1.876241
1	-2.497522	2.348445	0.781979
1	-2.859333	1.331433	2.201183

1	-2.652508	-4.688732	-0.663741
1	-4.205889	-4.758037	-1.498103
1	-2.193090	-1.469584	1.929049
1	0.608899	-0.895100	2.981934
1	-0.884427	-0.079528	3.419486
1	-0.221202	-1.820055	5.115022
1	-1.787484	-2.178041	4.393026
1	0.872949	-3.433199	3.545983
1	-0.381170	-4.234412	4.491895
1	-0.558322	-4.872657	2.079248
1	-1.985504	-3.994462	2.619943
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6	5.798267	-1.617486	-0.915409
6	6.603654	-0.864402	-0.066605
6	6.046070	0.106643	0.760047
7	2.476150	-0.180053	-0.145104
6	1.547554	-0.762444	0.706975
6	0.307245	-0.178670	0.442863
7	0.576844	0.773417	-0.565623
6	1.868871	0.728716	-0.895201
7	-0.958167	-0.371333	0.832520
6	-1.233674	-1.010545	2.031395
6	-2.567504	-1.427568	2.260280
6	-2.939740	-2.065362	3.435519
6	-2.007945	-2.311001	4.447208
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6	-0.313385	-1.235414	3.080320
6	-0.363503	1.700012	-1.144554
6	-1.277880	1.195194	-2.147638
6	-2.222306	2.202781	-2.586851
6	-2.213748	3.489966	-2.100372
6	-1.304026	3.919534	-1.118510
6	-0.372237	3.002067	-0.626075
6	-1.321111	-0.116520	-2.641527
6	-2.393883	-0.468764	-3.650674
6	0.542043	3.382160	0.533371
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6	3.853511	-3.698180	-1.909402
6	4.059246	1.430335	1.628273
6	4.336696	2.817033	1.030671
6	-0.132905	-1.066991	-2.640855
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6	-5.018960	0.907792	-0.818992
6	-5.308008	2.364206	-0.452729
6	-4.702317	2.474060	0.949922
6	-3.459213	1.609514	0.811205
8	-2.798628	-2.306353	-0.795849
6	-4.088194	-2.900534	-0.853255
6	-4.099539	-3.923040	0.286354
6	-2.615324	-4.336414	0.416873
6	-1.863466	-3.341283	-0.488455
1	-4.776107	3.031025	-1.137084
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1	-4.221915	-3.384517	-1.831956
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1	0.039362	-2.021257	5.040781
1	-3.308517	-1.230048	1.489949
1	-3.974862	-2.372340	3.567284
1	-2.299617	-2.814555	5.362779
1	0.702791	-0.868086	2.998436
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1	-0.369535	-1.933079	-3.268308
1	0.150466	-1.480657	-1.661696
1	0.778530	-0.619387	-3.072074
1	-2.453290	-1.555702	-3.774238
1	-3.395846	-0.140316	-3.341824
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1	1.476106	2.813365	0.445880
1	1.676325	5.043390	1.327752
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1	2.494337	-2.081177	-1.592829
1	3.127542	-4.232575	-2.529233
1	4.847696	-3.900680	-2.321307
1	6.688049	0.687513	1.415742
1	7.675598	-1.035839	-0.049073
1	6.248999	-2.370721	-1.554602
1	5.621129	1.587731	3.150964
1	4.014455	2.081736	3.690519
1	2.973366	1.282503	1.648691
1	5.413535	3.017377	1.003565
1	3.952922	2.899484	0.008296
1	3.857809	3.594209	1.635240
1	4.391422	0.359407	3.500068
1	3.812112	-4.111122	-0.897395
1	2.341286	1.350973	-1.640110

## 8<sup>Cy</sup>

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6	5.666697	-1.845732	-1.218957
6	4.699340	-0.682523	-1.398019
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6	0.670646	-1.373399	2.081530
6	0.495220	-2.896134	1.944455
6	0.589733	-3.610031	3.295329
6	1.921141	-3.297069	3.982376
6	2.111087	-1.786467	4.143284
6	1.986306	-1.064684	2.799963

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6	-6.108434	0.843237	1.215414
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6	-4.972859	-3.491418	-1.344672
6	0.209492	1.020580	-1.464006
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6	1.999063	0.910335	-3.069204
6	2.278125	2.254934	-2.841996
6	1.509094	2.986898	-1.941030
6	0.466515	2.386717	-1.226387
6	0.580894	-1.179570	-2.676623
6	-0.719312	-1.250282	-3.494610
6	-0.392323	3.170601	-0.243993
6	-0.320836	4.683789	-0.449244
6	-4.150822	2.216289	3.061345
6	-4.482853	-1.541370	-2.873416
6	1.677682	-1.957387	-3.406674
6	-0.054584	2.822123	1.214461
8	3.540492	1.316032	0.866641
6	4.645705	0.785175	1.603132
6	5.840570	1.712062	1.291893
6	5.192956	2.919809	0.576641
6	3.708623	2.733624	0.878943
1	-2.237456	-1.403535	1.598780
1	-6.558008	1.594252	1.859166
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1	-6.999411	-1.824045	-0.684537
1	-2.808987	1.603094	1.517994
1	-3.424653	2.928701	3.466687
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1	-3.283720	3.996518	1.124198
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1	1.716724	4.043923	-1.804714
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1	1.428061	-3.023190	-3.420610
1	2.651595	-1.838449	-2.924217
1	1.771577	-1.631778	-4.449241
1	-1.543397	-0.738961	-2.992361
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1	-0.234781	-3.277251	3.942037
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1	1.979959	-3.794167	4.957392
1	3.082108	-1.569999	4.605622
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1	2.817982	-1.371997	2.144048
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1	6.345643	2.011687	2.213023
1	5.576449	3.879583	0.928694
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1	2.532649	-2.877551	-0.831659
1	3.585210	-2.694775	0.590404
1	4.429741	-3.269911	-2.287958
1	5.113159	-3.941773	-0.796445
1	6.165122	-1.782213	-0.244315
1	6.431215	-1.881399	-1.997950
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6	0.961472	0.546156	4.546923
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6	-0.050042	3.114788	-3.406644
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6	-0.034581	2.777445	-0.922538

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6	3.270212	3.709318	1.036561
6	4.395461	3.344414	0.062310
6	3.699498	2.318088	-0.823238
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1	3.107104	2.805273	-1.610744
1	4.365139	1.585184	-1.291439
1	4.427203	0.086305	1.531604
1	5.652630	0.420091	0.267646
1	5.241427	-2.200684	1.799172
1	6.768150	-1.305031	1.635204
1	6.926966	-1.823981	-0.724666
1	6.205111	-3.328779	-0.141476
1	4.970532	-1.544663	-2.013458
1	4.074834	-2.751445	-1.062240
1	2.822126	-1.625104	1.961409
1	3.775868	-1.314197	4.224690
1	2.577766	0.087919	5.908355
1	0.421177	1.153586	5.268796
1	-0.499990	0.886308	3.014785
1	-1.303822	1.772095	-2.314727

**9<sup>Cy</sup>**

6	-1.435089	-1.680220	-0.186636
7	-0.122413	-1.442241	0.245141
6	0.214849	-0.136783	0.196705
7	-0.920399	0.460303	-0.270086
6	-1.925128	-0.455054	-0.544576
6	0.777042	-2.456202	0.700165
6	1.064326	-2.530966	2.074351
6	1.987998	-3.492162	2.493416
6	2.580454	-4.363369	1.583925
6	2.260317	-4.282167	0.233245
6	1.362085	-3.320251	-0.238973
6	1.054873	-3.233104	-1.724416
6	2.327482	-2.995438	-2.544408
1	3.032744	-3.830269	-2.450674
1	2.823046	-2.080540	-2.207865
1	2.077100	-2.882466	-3.604387
1	0.402221	-2.370957	-1.887321
1	0.057658	-4.396354	-3.263660
1	0.938521	-5.381877	-2.083396
1	-0.608098	-4.645300	-1.638161
6	1.427721	-0.456231	3.433228
1	1.706994	0.113248	2.540398
1	0.980184	0.232084	4.159293
1	2.337113	-0.877311	3.879134
1	2.243304	-3.564878	3.546755
1	3.289865	-5.108827	1.930934
1	2.723922	-4.968738	-0.470962
6	0.439534	-1.577085	3.079028
1	-0.435101	-1.118371	2.605011
6	-0.041896	-2.293876	4.345062
1	0.795621	-2.670650	4.941748
1	-0.694656	-3.137813	4.103092
1	-0.601357	-1.594763	4.974524
8	3.370212	-0.082377	-0.803788
1	4.567412	0.129326	0.872394
6	4.025224	-0.658257	0.328230
1	5.833865	-1.888848	0.365104
1	4.432894	-2.635951	-0.418310
6	4.970698	-1.695017	-0.275667
1	3.251584	-1.079926	0.975792
6	5.360466	-1.075712	-1.636169
1	5.293536	-1.813161	-2.439735
1	6.381271	-0.686306	-1.626761
6	4.344769	0.069630	-1.835671
1	3.812661	0.034828	-2.790248
1	4.829003	1.050693	-1.737114
3	1.839517	1.026251	-0.426313
1	3.032879	4.608368	2.399672
6	1.689449	3.103919	1.591012
6	2.293984	4.503634	1.597333
6	2.975928	4.554086	0.226888
6	3.521854	3.135880	0.097385
1	4.511189	3.032286	0.563761
1	3.574346	2.789681	-0.940959
1	3.760197	5.311357	0.154420
1	2.227342	4.735738	-0.550667
8	2.594327	2.296369	0.803378
1	1.526997	5.271630	1.720450
1	1.412977	-0.246047	-2.845771
1	1.613421	2.646910	2.581897
1	0.704949	3.101842	1.111282
1	-0.304320	-0.104530	-2.463611
1	0.312431	0.552852	-3.966956
6	0.821627	1.788911	-2.265127
1	2.209118	3.448897	-2.643317

1	2.502601	1.993681	-3.596286
1	1.173001	3.069311	-4.024279
6	-0.120209	2.478025	-1.456148
6	-1.000039	1.883508	-0.473776
6	-1.777805	2.614016	0.435623
6	-1.796190	4.010847	0.356790
6	-1.006255	4.636781	-0.616529
6	-0.207598	3.916628	-1.481001
1	0.355832	4.456044	-2.234141
1	-1.031771	5.721002	-0.706905
1	-2.404581	4.599774	1.032985
1	-0.580029	1.270491	2.452959
1	-1.942962	1.222201	3.597992
1	-1.215397	2.778965	3.135618
6	-1.494548	1.783692	2.769377
1	-1.871494	-2.665574	-0.203052
7	-3.105338	-0.061937	-1.129966
6	-2.476326	1.909255	1.594321
1	-2.740355	0.891601	1.290680
6	-4.282821	-0.908715	-1.001991
1	-3.982591	-1.918701	-1.323133
6	-4.826555	-0.991695	0.431267
1	-4.042120	-1.347769	1.109518
1	-5.096287	0.025385	0.753660
6	-6.060799	-1.895057	0.499757
1	-5.774359	-2.921178	0.227904
1	-6.441956	-1.936396	1.525643
6	-7.149705	-1.405563	-0.458099
1	-8.016716	-2.074307	-0.426066
1	-7.497768	-0.416491	-0.128816
6	-6.614377	-1.299706	-1.888690
1	-6.360136	-2.305014	-2.253086
1	-7.386597	-0.908382	-2.559155
6	-5.367368	-0.414226	-1.957391
1	-4.964195	-0.377513	-2.974496
1	-5.634376	0.616264	-1.676779
6	-3.772830	2.589233	2.038672
1	-4.285014	1.966798	2.780219
1	-4.451036	2.747353	1.193229
1	-3.582670	3.561766	2.503499
6	0.543440	0.431053	-2.893875
6	1.710977	2.621413	-3.165540
6	0.315534	-4.488293	-2.203955
1	-3.270249	0.939077	-1.069752

### **$\mathbf{g}^{\text{Ph}}$**

6	-4.408078	-1.931063	-0.741825
6	-4.484378	-0.564409	-0.447455
6	-5.725164	0.084563	-0.542707
6	-6.860304	-0.619005	-0.920950
6	-6.789301	-1.984982	-1.201191
6	-5.558120	-2.626886	-1.111586
7	-3.375230	0.197279	-0.073633
6	-2.120627	-0.268137	0.244029
6	-1.631648	-1.460986	0.693099
7	-0.249415	-1.278589	0.802855
6	0.139934	-0.025805	0.474231
7	-1.031860	0.590030	0.153626
6	0.674064	-2.317713	1.140087
6	0.858113	-3.380944	0.239761
6	1.789701	-4.366205	0.578765
6	2.526123	-4.284334	1.755197
6	2.320926	-3.223034	2.631427
6	1.379845	-2.227635	2.353081
6	-1.082258	1.978565	-0.233471
6	-1.559422	2.891534	0.721499
6	-1.494348	4.260755	0.450789

6	-0.917201	4.680940	-0.757518
6	-0.403113	3.786565	-1.670823
6	-0.424931	2.358311	-1.465437
6	0.095740	-3.489244	-1.071334
6	1.049801	-3.528273	-2.269850
6	1.157831	-1.085140	3.330589
6	1.047648	-1.570195	4.780397
6	-2.002437	2.407533	2.098416
6	-0.772525	2.318620	3.016474
6	0.197663	1.474699	-2.376327
6	0.861522	2.082346	-3.596926
6	-0.838159	-4.706166	-1.065126
6	2.266853	-0.032197	3.194984
6	-3.088737	3.276668	2.735895
6	-0.317957	0.055731	-2.597314
3	1.601941	0.892704	-0.739390
8	2.801632	-0.456917	-1.370062
6	3.316401	-0.592819	-2.696125
6	4.308336	-1.776273	-2.652834
6	4.356110	-2.176811	-1.163053
6	3.782655	-0.952158	-0.457238
8	2.758085	2.188852	0.075008
6	3.591737	2.836540	-0.895528
6	3.114192	4.282531	-0.938138
6	2.720837	4.521928	0.522931
6	2.122544	3.174815	0.924364
1	-2.112641	-2.387078	0.958272
1	1.950777	-5.201257	-0.098584
1	3.255877	-5.052425	1.993656
1	2.892579	-3.173357	3.553711
1	-0.522178	-2.595318	-1.185112
1	-1.420188	-4.743531	-1.991548
1	-1.535326	-4.667463	-0.221586
1	-0.270771	-5.639959	-0.984342
1	1.689009	-2.641013	-2.266824
1	0.480942	-3.540124	-3.205262
1	1.690019	-4.418103	-2.250625
1	0.207638	-0.607222	3.070555
1	3.244977	-0.476621	3.417136
1	2.098103	0.788135	3.902140
1	2.291416	0.381816	2.181868
1	2.002214	-1.953495	5.155696
1	0.298623	-2.360858	4.882316
1	0.756460	-0.734963	5.425004
1	-1.875678	4.986841	1.158644
1	-0.882564	5.743770	-0.988897
1	0.004915	4.170901	-2.598858
1	-2.415567	1.397983	2.010091
1	-3.445555	2.809128	3.658988
1	-3.942572	3.405552	2.063080
1	-2.710479	4.270064	2.996983
1	-0.000156	1.680927	2.572012
1	-1.044741	1.907964	3.996059
1	-0.343146	3.316465	3.166603
1	-1.378104	-0.061894	-2.332343
1	0.230060	-0.733357	-2.055486
1	-0.240676	-0.196744	-3.662967
1	0.147163	2.523695	-4.318137
1	1.425217	1.319600	-4.146509
1	1.576973	2.877563	-3.345659
1	1.044397	3.146017	0.738974
1	2.319391	2.900154	1.965034
1	3.606048	4.754070	1.124980
1	1.993642	5.328861	0.639326
1	3.884059	4.967937	-1.300486
1	2.230179	4.363308	-1.577816
1	3.472358	2.308940	-1.848574

1	4.639100	2.763357	-0.571173
1	3.817240	0.339093	-2.991264
1	2.458968	-0.750645	-3.356493
1	3.973868	-2.606079	-3.280119
1	5.291482	-1.463181	-3.012802
1	5.364867	-2.419829	-0.821686
1	3.710865	-3.038104	-0.970197
1	3.272785	-1.173746	0.484571
1	4.546518	-0.178485	-0.286756
1	-5.787217	1.145049	-0.312810
1	-7.809896	-0.097132	-0.990005
1	-7.678744	-2.535769	-1.487421
1	-5.479844	-3.685638	-1.340741
1	-3.453730	-2.443119	-0.721261
1	-3.406195	1.191280	-0.274255

### **10<sup>Cy</sup>**

6	2.787757	3.208968	-0.461207
6	2.867201	2.126635	0.633989
6	2.599826	2.740691	2.020762
6	3.503747	3.941097	2.308696
6	3.366429	5.005718	1.217786
6	3.686503	4.410628	-0.155700
7	2.083500	0.935483	0.366764
6	0.752181	1.047443	0.345898
6	-0.193530	2.067879	0.351333
7	-1.454787	1.456849	0.251953
6	-1.376564	0.113369	0.187455
7	-0.037042	-0.128385	0.260173
6	-2.676918	2.189496	0.189799
6	-2.997778	2.852562	-1.006819
6	-4.190234	3.582274	-1.053432
6	-5.035998	3.633589	0.049309
6	-4.711703	2.942829	1.214018
6	-3.529423	2.203452	1.310956
6	0.493295	-1.438220	0.500912
6	0.366392	-1.943585	1.796980
6	0.880436	-3.215753	2.108827
6	1.549238	-3.927964	1.107585
6	1.716721	-3.418014	-0.167217
6	1.201757	-2.123940	-0.566356
6	-2.142719	2.666519	-2.250065
6	-2.114146	3.896647	-3.159832
6	-3.177458	1.430831	2.574529
6	-4.390592	1.120712	3.452208
6	-0.285824	-1.128129	2.907975
6	-1.560035	-1.803322	3.428098
6	1.413202	-1.623519	-1.862814
6	0.556005	-0.537543	-2.496950
6	-2.641304	1.434143	-3.022249
6	-2.094653	2.155215	3.387211
6	0.696709	-0.866296	4.056090
6	2.155444	-2.513555	-2.836708
3	2.977334	-0.491533	-0.596561
8	4.334100	-1.224934	0.584582
6	5.049692	-2.436473	0.302832
6	5.079143	-3.229652	1.611947
6	4.906825	-2.132147	2.668359
6	3.933131	-1.196213	1.967813
8	4.289336	-0.019450	-1.970630
6	5.653704	0.334124	-1.763317
6	5.739252	1.780648	-2.230458
6	4.806517	1.777511	-3.452496
6	3.806613	0.642554	-3.147116
3	-2.787038	-1.376707	0.171769
8	-2.683864	-3.130615	-0.533077

6	-1.796561	-4.200050	-0.109458
6	-1.344672	-4.889601	-1.393016
6	-1.409607	-3.746303	-2.410558
6	-2.670017	-3.017473	-1.967827
8	-4.669580	-1.096232	0.019325
6	-5.601419	-2.184578	-0.015493
6	-6.334969	-2.068812	-1.369124
6	-5.896431	-0.690173	-1.912258
6	-5.294027	-0.015282	-0.684763
1	-0.104305	3.139663	0.401406
1	-4.465891	4.106765	-1.963286
1	-5.957609	4.206167	-0.000206
1	-5.395053	2.977645	2.056139
1	-1.117140	2.460276	-1.928439
1	-3.084803	4.075233	-3.635135
1	-1.384066	3.745602	-3.960517
1	-1.833171	4.797318	-2.605682
1	-2.614435	0.544166	-2.383124
1	-2.006928	1.241798	-3.894110
1	-3.671583	1.589933	-3.368350
1	-2.755742	0.472763	2.253409
1	-4.093284	0.448082	4.262465
1	-5.186597	0.632414	2.879559
1	-4.801857	2.024682	3.915033
1	-1.195019	2.328039	2.789138
1	-1.812766	1.552078	4.258312
1	-2.469511	3.121334	3.744926
1	0.774132	-3.628182	3.107150
1	1.940724	-4.920283	1.328419
1	2.229174	-4.027762	-0.903861
1	-0.566404	-0.149908	2.507931
1	-2.283230	-1.974201	2.619246
1	-2.047419	-1.180240	4.187986
1	-1.337902	-2.777654	3.876765
1	0.225550	-0.247348	4.828286
1	1.578887	-0.335026	3.685139
1	1.028093	-1.800174	4.523048
1	-0.525867	-0.744714	-2.429405
1	0.794565	-0.469153	-3.565210
1	0.691049	0.470706	-2.079343
1	3.155675	-2.801730	-2.480643
1	2.300927	-2.003202	-3.794101
1	1.631161	-3.464472	-3.064846
1	-4.534757	0.736490	-0.900917
1	-6.065983	0.430377	-0.041607
1	-5.125879	-0.802825	-2.681851
1	-6.721965	-0.116969	-2.339723
1	-6.053880	-2.875576	-2.049444
1	-7.416973	-2.118597	-1.225546
1	-6.297121	-2.071744	0.825588
1	-5.028863	-3.105714	0.103006
1	-2.362462	-4.852085	0.562324
1	-0.957112	-3.752401	0.426678
1	-2.034834	-5.694836	-1.670783
1	-0.338767	-5.300980	-1.286109
1	-2.677089	-1.951798	-2.229557
1	-3.579985	-3.488522	-2.367017
1	2.798082	1.000166	-2.920811
1	3.746237	-0.083640	-3.965972
1	6.758385	2.092223	-2.471678
1	5.347795	2.436220	-1.447553
1	6.299989	-0.320743	-2.367834
1	5.867617	0.184263	-0.703078
1	6.058733	-2.161999	-0.031734
1	4.537672	-2.969201	-0.504784
1	4.226411	-3.913287	1.650214
1	6.000880	-3.805361	1.726000

1	5.859296	-1.626339	2.863460
1	4.508389	-2.508838	3.613638
1	2.902525	-1.557448	2.046520
1	3.974394	-0.154468	2.295962
1	-1.467827	-4.087757	-3.446821
1	-0.539288	-3.091464	-2.293884
1	4.305611	2.738433	-3.594198
1	5.370329	1.555574	-4.363359
1	3.923610	1.793134	0.647394
1	1.549607	3.055030	2.084371
1	2.734980	1.958973	2.778037
1	3.270061	4.367717	3.291231
1	4.551638	3.608600	2.350307
1	2.334993	5.387155	1.214671
1	4.021795	5.859015	1.427332
1	3.585161	5.171890	-0.938653
1	4.740695	4.095354	-0.157820
1	1.752353	3.554530	-0.568832
1	3.056862	2.750155	-1.421524

### **10<sup>Ph</sup>**

6	5.612143	2.078667	0.056225
8	4.654087	1.011678	0.080043
6	5.263271	-0.083853	-0.615492
6	5.895957	0.576057	-1.835439
6	6.365485	1.940983	-1.284508
3	2.775542	1.342114	0.246689
8	2.718759	3.100005	-0.426219
6	1.840776	4.185267	-0.022670
6	1.444247	4.891665	-1.315532
6	1.522407	3.755092	-2.339320
6	2.752935	2.998990	-1.861707
6	1.327157	-0.121781	0.265272
7	1.393374	-1.470991	0.303547
6	0.133340	-2.064065	0.438400
6	-0.789158	-1.036028	0.488537
7	-0.002281	0.131760	0.386103
7	-2.137931	-0.926776	0.506577
6	-2.916066	-1.983683	0.927805
6	-2.464788	-3.120265	1.643597
6	-3.343033	-4.127995	2.037208
6	-4.703536	-4.061975	1.746008
6	-5.175166	-2.934369	1.067707
6	-4.311506	-1.923923	0.670511
6	2.609087	-2.220323	0.271918
6	2.926993	-2.925518	-0.900915
6	4.106690	-3.676733	-0.914126
6	4.941374	-3.708641	0.197496
6	4.617936	-2.979736	1.338745
6	3.447486	-2.218128	1.404202
6	-0.526843	1.459672	0.536969
6	-0.499211	2.003126	1.823518
6	-1.028274	3.285551	2.048323
6	-1.595877	3.970395	0.966952
6	-1.652907	3.422505	-0.301119
6	-1.136340	2.105549	-0.610115
6	2.084812	-2.766992	-2.156657
6	2.073504	-4.010268	-3.048383
6	3.094914	-1.419384	2.652467
6	4.302153	-1.123496	3.543621
6	0.001613	1.180849	3.004689
6	0.871939	1.987176	3.972385
6	-1.282141	1.546958	-1.895645
6	-0.393859	0.457703	-2.475043
6	2.585177	-1.542764	-2.939930
6	1.987396	-2.111381	3.460875
6	-1.191301	0.538446	3.727740

6	-1.954545	2.385745	-2.962034
3	-2.866869	0.346205	-0.834790
8	-4.352122	1.285258	0.007397
6	-5.075037	2.420253	-0.489675
6	-5.265906	3.363313	0.699168
6	-5.200883	2.403598	1.890753
6	-4.136371	1.417849	1.432196
8	-3.513459	-0.820595	-2.246841
6	-2.850069	-2.054919	-2.524658
6	-3.945636	-3.133132	-2.481523
6	-5.263559	-2.339534	-2.648904
6	-4.798525	-0.890156	-2.849862
1	-5.378928	-4.854519	2.050422
1	0.019907	-3.134728	0.448204
1	4.380026	-4.235921	-1.803493
1	5.852576	-4.299043	0.174153
1	5.291007	-3.004952	2.189231
1	1.053142	-2.562649	-1.853952
1	3.049248	-4.186626	-3.513561
1	1.349032	-3.875236	-3.856883
1	1.794626	-4.905650	-2.484917
1	2.555349	-0.645359	-2.311718
1	1.955101	-1.359937	-3.816819
1	3.617256	-1.702988	-3.278035
1	2.697872	-0.455466	2.316818
1	4.007689	-0.427367	4.334574
1	5.120606	-0.668024	2.975645
1	4.680836	-2.028547	4.031128
1	1.078898	-2.243537	2.866398
1	1.730381	-1.509192	4.339468
1	2.326658	-3.094899	3.805676
1	-1.014201	3.728286	3.038064
1	-1.996625	4.971367	1.121744
1	-2.086846	4.015594	-1.099603
1	0.620097	0.362057	2.625161
1	1.699941	2.478412	3.447498
1	1.293378	1.325205	4.737472
1	0.298265	2.762937	4.489524
1	-0.848936	-0.088638	4.558979
1	-1.769023	-0.083938	3.035218
1	-1.855827	1.312763	4.129907
1	0.653027	0.788411	-2.615548
1	-0.764526	0.185855	-3.470669
1	-0.340232	-0.475260	-1.903159
1	-2.900098	2.830620	-2.629167
1	-2.191114	1.768949	-3.835820
1	-1.339180	3.233214	-3.329082
1	-1.425091	-3.194750	1.937381
1	-2.949317	-4.978465	2.588722
1	-6.235961	-2.841781	0.844246
1	-4.700514	-1.056490	0.142748
1	4.490695	-0.818975	-0.841406
1	6.016583	-0.545982	0.037937
1	5.136239	0.710623	-2.612140
1	6.710193	-0.018258	-2.255518
1	6.122138	2.755804	-1.969730
1	7.445666	1.957276	-1.121376
1	6.290784	1.952997	0.909211
1	5.059148	3.013058	0.162808
1	2.399644	4.821676	0.669418
1	0.976159	3.751896	0.485156
1	2.157857	5.685861	-1.563631
1	0.443128	5.320767	-1.238907
1	2.746028	1.935605	-2.133443
1	3.686078	3.453469	-2.224692
1	-2.070730	-2.184097	-1.769254
1	-2.386930	-1.986963	-3.519915

1	-5.862410	-2.687341	-3.494181
1	-5.869508	-2.422848	-1.743955
1	-4.710193	-0.640958	-3.917784
1	-5.431747	-0.145292	-2.360424
1	-6.035570	2.064498	-0.883594
1	-4.500591	2.876186	-1.301216
1	-4.434420	4.072017	0.749001
1	-6.203416	3.921277	0.636887
1	-6.161218	1.895787	2.033909
1	-4.923127	2.899717	2.823884
1	-3.127612	1.806582	1.601078
1	-4.219325	0.421670	1.872106
1	1.619132	4.102214	-3.370688
1	0.639276	3.113260	-2.253844
1	-3.933072	-3.652862	-1.520444
1	-3.803172	-3.870262	-3.275710

### 11<sup>Cy</sup>

8	6.261070	-2.213767	0.054957
6	5.649195	-1.631733	1.199375
6	5.637107	-2.749837	2.238703
6	5.395502	-4.003381	1.371407
6	5.706214	-3.520600	-0.064575
3	2.512080	0.569985	-0.158138
7	1.132788	1.917698	-0.064002
6	1.328169	3.337563	-0.280719
6	1.430086	4.146223	1.025639
6	1.707647	5.629936	0.771064
6	2.977972	5.812501	-0.064372
6	2.879425	5.036641	-1.379952
6	2.587737	3.557785	-1.122512
6	-0.139276	1.596373	0.224238
6	-1.311920	2.310555	0.424702
7	-2.336344	1.358556	0.572959
6	-1.886539	0.091995	0.512348
7	-0.540184	0.249410	0.332832
6	-3.709283	1.683543	0.780284
6	-4.458230	2.210471	-0.285022
6	-5.807105	2.499362	-0.058541
6	-6.398142	2.248852	1.175340
6	-5.635723	1.727284	2.216256
6	-4.275493	1.453321	2.047767
6	-3.849399	2.458545	-1.654769
6	-4.603112	1.694516	-2.749569
6	-3.456488	0.894293	3.199116
6	-3.713552	1.638257	4.514281
6	0.319817	-0.883225	0.156113
6	1.195133	-1.197463	1.201974
6	2.005574	-2.343728	1.115249
6	1.861302	-3.182293	0.003403
6	0.961452	-2.903727	-1.005246
6	0.110292	-1.738033	-1.000546
6	1.165762	-0.379108	2.490757
6	-0.026794	-0.826850	3.350331
6	-0.862165	-1.553986	-2.011955
6	-0.965021	-2.609193	-3.091586
6	-3.801489	3.959283	-1.967262
6	-3.721957	-0.608329	3.368343
6	2.457163	-0.483749	3.306277
6	-1.310822	-0.196083	-2.529415
8	2.857557	-0.337451	-1.787072
6	2.092135	-0.016927	-2.949837
6	3.160910	0.225705	-4.017607
6	4.289317	-0.755984	-3.611617
6	3.846094	-1.266034	-2.224391
3	-2.484374	-1.656949	-0.435867
8	-4.256220	-1.543363	-1.189905

6	-4.776915	-2.073446	-2.407423
6	-6.253716	-1.628440	-2.471861
6	-6.527860	-1.026436	-1.075602
6	-5.329480	-1.486377	-0.247837
8	-2.622653	-3.293385	0.572848
6	-1.598712	-3.594806	1.547966
6	-1.326091	-5.089822	1.407104
6	-1.615903	-5.324461	-0.078608
6	-2.811096	-4.407293	-0.311392
1	-1.509254	3.368491	0.469684
1	-6.406098	2.912503	-0.866753
1	-7.451200	2.465836	1.329029
1	-6.102761	1.542053	3.179592
1	-2.822466	2.084645	-1.638596
1	-3.319133	4.131526	-2.934793
1	-3.238509	4.502106	-1.202120
1	-4.810656	4.385260	-2.010706
1	-4.607067	0.622610	-2.529980
1	-4.115920	1.844732	-3.718911
1	-5.642242	2.034276	-2.837846
1	-2.399744	1.026152	2.944227
1	-4.781784	-0.785846	3.589851
1	-3.129004	-1.009945	4.198482
1	-3.457035	-1.153558	2.456485
1	-4.725564	1.458718	4.892967
1	-3.580572	2.717390	4.393895
1	-3.012459	1.288077	5.278727
1	2.689503	-2.602700	1.916151
1	2.477282	-4.077951	-0.076858
1	0.918819	-3.577004	-1.855279
1	1.021817	0.674991	2.228027
1	2.464549	0.270710	4.099559
1	3.341110	-0.333693	2.677697
1	2.551590	-1.465699	3.783647
1	-0.962696	-0.761000	2.787817
1	-0.112830	-0.205441	4.249924
1	0.111143	-1.869272	3.664538
1	-0.947301	0.651478	-1.945858
1	-2.406997	-0.099627	-2.595033
1	-0.934173	-0.047187	-3.558226
1	-0.112933	-2.594963	-3.804451
1	-1.865980	-2.444393	-3.696325
1	-1.023035	-3.634401	-2.703638
1	0.473931	3.756142	-0.854832
1	0.514577	4.012264	1.612621
1	2.247262	3.716840	1.623263
1	0.858391	6.071850	0.229896
1	1.792198	6.172410	1.719863
1	3.840236	5.437724	0.509503
1	3.164022	6.875101	-0.258034
1	3.804098	5.147902	-1.959929
1	2.072261	5.466464	-1.989644
1	2.487758	3.005900	-2.066840
1	3.430285	3.108855	-0.579490
1	-0.706265	-3.006116	1.312646
1	-1.978907	-3.301854	2.530897
1	-2.011254	-5.675255	2.030314
1	-0.298783	-5.337708	1.684327
1	-1.835288	-6.366809	-0.322350
1	-0.765340	-4.985906	-0.678158
1	-2.868153	-4.024183	-1.336349
1	-3.760069	-4.900468	-0.058674
1	-4.694520	-3.169177	-2.392474
1	-4.156264	-1.685009	-3.219631
1	-6.413824	-0.888146	-3.259364
1	-6.902664	-2.482356	-2.680863
1	-7.475992	-1.360971	-0.648542

1	-6.537522	0.065461	-1.119093
1	-5.035633	-0.788014	0.539810
1	-5.484693	-2.485896	0.185278
1	1.461028	0.839933	-2.701845
1	1.452885	-0.875064	-3.200543
1	3.511710	1.261557	-3.965202
1	2.784147	0.047269	-5.027200
1	4.385575	-1.583952	-4.317986
1	5.258145	-0.251211	-3.561096
1	3.375073	-2.255194	-2.296487
1	4.642414	-1.301811	-1.476419
1	4.625516	-1.311627	0.954119
1	6.238861	-0.755694	1.486153
1	4.866231	-2.602410	3.000245
1	6.608662	-2.806524	2.737813
1	6.041915	-4.830872	1.671973
1	4.359352	-4.345458	1.445715
1	6.437034	-4.139837	-0.589458
1	4.783154	-3.473621	-0.659601
8	4.389653	1.069849	0.299695
6	5.357498	1.235809	-0.752490
6	6.163038	2.471739	-0.369129
6	6.187630	2.361955	1.157564
6	4.800364	1.798743	1.469391
1	5.991011	0.338786	-0.794914
1	4.808951	1.339579	-1.692869
1	5.639858	3.382166	-0.681159
1	7.159251	2.470999	-0.817062
1	6.364850	3.316183	1.658524
1	6.966596	1.659154	1.472172
1	4.062405	2.588575	1.649170
1	4.803428	1.117892	2.325236

## 11<sup>Ph</sup>

6	-2.041465	-3.526052	0.346805
6	-2.363447	-2.343925	1.051883
6	-3.417306	-2.426364	1.986758
6	-4.107295	-3.613241	2.207746
6	-3.776791	-4.770738	1.499877
6	-2.738270	-4.7111390	0.568094
7	-1.757382	-1.1111290	0.834872
6	-0.405040	-1.103443	0.746636
6	0.576653	-2.062778	0.922769
7	1.805553	-1.406337	0.795896
6	1.670858	-0.090152	0.549470
7	0.312758	0.089219	0.533843
6	3.070079	-2.057815	0.922424
6	3.532327	-2.869236	-0.126153
6	4.778968	-3.485013	0.022898
6	5.547694	-3.282171	1.163684
6	5.067342	-2.474237	2.189846
6	3.814373	-1.861575	2.098817
6	-0.217383	1.406303	0.289722
6	-0.773767	2.095647	1.377409
6	-1.133961	3.443390	1.238339
6	-0.944678	4.070021	0.003264
6	-0.370921	3.402019	-1.060728
6	0.107586	2.044809	-0.970971
6	2.720801	-3.089757	-1.390505
6	3.516621	-2.703410	-2.642225
6	3.304011	-0.982216	3.226639
6	3.533043	-1.602922	4.608569
6	-0.851139	1.435703	2.748179
6	0.515397	1.540639	3.443005
6	0.891036	1.502497	-2.030170
6	1.164411	2.386650	-3.227965
6	2.224127	-4.538483	-1.474157

6	3.946830	0.409513	3.144356
6	-1.936071	2.031162	3.649462
6	0.892272	0.039727	-2.438059
3	-3.055106	0.119733	0.049579
8	-4.927373	-0.918835	-0.399771
6	-5.385240	-2.257138	-0.615371
6	-5.915941	-2.294089	-2.063601
6	-6.026317	-0.804865	-2.459249
6	-5.807791	-0.078231	-1.132330
8	-2.919196	0.273082	-1.915473
6	-2.516952	-1.013511	-2.407671
6	-2.597079	-0.921519	-3.945056
6	-2.826776	0.580338	-4.227508
6	-2.505946	1.238359	-2.886554
3	2.634002	1.310623	-0.643074
8	3.384290	2.898366	0.161991
6	3.765334	3.876716	-0.813401
6	2.829108	5.058916	-0.592511
6	2.624566	5.013336	0.925103
6	2.582420	3.511900	1.198856
8	4.212009	0.621407	-1.545479
6	4.717991	0.856993	-2.857800
6	6.036537	0.059245	-2.958388
6	6.290835	-0.431367	-1.516051
6	5.333246	0.417218	-0.682906
1	0.512780	-3.110164	1.164402
1	5.155948	-4.123489	-0.772584
1	6.519366	-3.758406	1.257286
1	5.670573	-2.325870	3.081099
1	1.845599	-2.436754	-1.344967
1	1.605977	-4.678623	-2.367256
1	1.624307	-4.799329	-0.596682
1	3.064404	-5.240038	-1.529840
1	3.843371	-1.661492	-2.571541
1	2.891537	-2.809374	-3.535511
1	4.401135	-3.338441	-2.772967
1	2.223931	-0.866964	3.091001
1	5.036034	0.332707	3.252402
1	3.568592	1.054371	3.946143
1	3.722507	0.882846	2.182469
1	4.596567	-1.640713	4.867755
1	3.131769	-2.619226	4.660731
1	3.033425	-0.996652	5.370870
1	-1.558045	3.991367	2.072381
1	-1.261007	5.103604	-0.131697
1	-0.269475	3.927016	-2.004739
1	-1.091682	0.379091	2.601193
1	-2.083174	1.394051	4.528107
1	-2.886040	2.114926	3.113288
1	-1.659967	3.028056	4.011220
1	1.311440	1.140435	2.808233
1	0.514683	0.990964	4.392219
1	0.748701	2.591992	3.655944
1	0.522721	-0.642303	-1.671249
1	1.896450	-0.312934	-2.723454
1	0.259462	-0.117703	-3.335988
1	0.274598	2.558845	-3.872622
1	1.916417	1.918626	-3.876632
1	1.544137	3.381257	-2.961225
1	1.564148	3.119891	1.123625
1	3.007948	3.228062	2.166064
1	3.469134	5.483976	1.440660
1	1.700121	5.500660	1.244159
1	3.253450	6.000992	-0.948357
1	1.875874	4.878124	-1.098879
1	3.666319	3.423741	-1.805819
1	4.816134	4.153514	-0.647186

1	4.894155	1.932910	-2.993881
1	3.948446	0.535804	-3.564952
1	5.944309	-0.779672	-3.652399
1	6.846091	0.699866	-3.316636
1	7.330212	-0.309402	-1.202875
1	6.022417	-1.485753	-1.411909
1	4.966782	-0.074421	0.222208
1	5.768429	1.392989	-0.418531
1	-3.188163	-1.753594	-1.965807
1	-1.498533	-1.223743	-2.064617
1	-3.411768	-1.533021	-4.344366
1	-1.665799	-1.274829	-4.394804
1	-2.187083	0.960047	-5.027833
1	-3.867866	0.769194	-4.507197
1	-1.434236	1.432168	-2.776199
1	-3.055500	2.162811	-2.690941
1	-6.182543	-2.478455	0.107841
1	-4.551793	-2.935030	-0.428904
1	-6.881056	-2.804178	-2.112339
1	-5.228088	-2.828801	-2.724702
1	-5.226873	-0.529628	-3.152186
1	-6.984103	-0.552945	-2.920829
1	-5.332763	0.898612	-1.240221
1	-6.755546	0.032462	-0.578209
1	-3.667713	-1.527154	2.543252
1	-4.907507	-3.637770	2.943399
1	-4.309512	-5.699697	1.675670
1	-2.468718	-5.599323	0.001598
1	-1.245806	-3.495276	-0.393659
8	-4.111209	1.422448	1.023034
6	-5.059594	1.021392	2.028010
6	-5.910488	2.259952	2.307160
6	-5.848776	3.000139	0.967621
6	-4.400516	2.752792	0.565783
1	-5.647072	0.189143	1.624512
1	-4.506269	0.670890	2.904173
1	-5.450597	2.869211	3.092902
1	-6.925143	2.002851	2.618880
1	-6.082717	4.064007	1.048258
1	-6.536355	2.544424	0.246547
1	-3.718254	3.453523	1.058904
1	-4.208052	2.788754	-0.511560

## 12

6	-5.288548	0.881401	0.076811
8	-4.074616	0.723048	0.826218
6	-3.822990	1.890917	1.625628
6	-5.153486	2.634247	1.674708
6	-5.722832	2.331684	0.285709
3	-2.452245	0.105299	-0.063490
7	-1.622158	1.486285	-1.106310
6	-2.411953	2.575332	-1.621964
6	-0.346076	1.827807	-0.928114
6	0.369388	3.014038	-1.042752
7	1.695858	2.718611	-0.703415
6	1.876770	1.428314	-0.383903
7	0.621712	0.889486	-0.511006
6	2.745001	3.709424	-0.703677
6	0.393912	-0.518859	-0.366510
6	1.005578	-1.341500	-1.307734
6	0.857322	-2.733328	-1.313524
6	-0.011440	-3.275400	-0.352435
6	-0.649945	-2.485285	0.584396
6	-0.459906	-1.047294	0.688643
6	-1.050711	-0.304814	1.714990
6	-0.525844	1.053277	2.151396
6	-1.899478	-1.045031	2.726119

8	-3.278686	-1.178483	-1.225160
6	-3.916786	-2.382665	-0.780847
6	-3.464853	-3.481456	-1.745011
6	-3.138524	-2.686817	-3.014256
6	-2.521986	-1.424090	-2.427311
3	2.942089	-0.341882	-0.130028
8	3.381613	-0.976972	1.586159
6	2.684127	-2.162999	2.029072
6	1.855095	-1.703228	3.218549
6	2.777034	-0.661029	3.860652
6	3.419705	0.005842	2.643402
8	4.456046	-0.636158	-1.281639
6	5.703329	-0.520016	-0.592128
6	5.977795	0.978645	-0.616259
6	5.524543	1.360445	-2.037181
6	4.506564	0.258876	-2.406113
1	1.583418	-0.852057	-2.092764
1	-2.008312	2.985694	-2.566483
1	-2.487336	3.435659	-0.922692
1	0.050233	4.007954	-1.309049
1	1.356626	-3.349240	-2.051762
1	-0.180636	-4.350619	-0.327322
1	-1.284403	-2.973973	1.316534
1	0.569171	1.061974	2.284004
1	-0.960724	1.314845	3.123034
1	-0.749292	1.882078	1.467527
1	-2.730332	-1.601338	2.268607
1	-2.352186	-0.345260	3.435627
1	-1.332002	-1.783668	3.326749
1	3.495751	0.645750	-2.556001
1	4.818653	-0.308375	-3.290018
1	5.074967	2.354643	-2.075889
1	6.371400	1.347932	-2.728757
1	5.347106	1.469541	0.133699
1	7.022252	1.228441	-0.416686
1	6.475561	-1.080182	-1.138506
1	5.568324	-0.950114	0.401738
1	3.431266	-2.914254	2.317210
1	2.087097	-2.537021	1.191946
1	1.603476	-2.527451	3.890122
1	0.928981	-1.239172	2.864154
1	2.856366	0.881814	2.302396
1	4.464572	0.289979	2.808467
1	-3.039417	2.485535	1.137503
1	-3.458407	1.556384	2.599764
1	-6.806689	2.453671	0.222138
1	-5.255304	2.982113	-0.460562
1	-6.031275	0.179376	0.477238
1	-5.083073	0.624451	-0.966420
1	-5.002429	-2.223874	-0.819765
1	-3.622311	-2.577872	0.255416
1	-2.556276	-3.957254	-1.364036
1	-4.231212	-4.246500	-1.891150
1	-4.053586	-2.449377	-3.568621
1	-2.449923	-3.210861	-3.681073
1	-1.469645	-1.576353	-2.163056
1	-2.605602	-0.531130	-3.050089
1	3.538849	-1.148973	4.478431
1	2.238986	0.060118	4.480109
1	-5.027092	3.701800	1.868005
1	-5.798728	2.212200	2.452969
1	3.655805	3.243468	-0.323123
1	2.918950	4.089162	-1.717086
1	2.474171	4.550052	-0.056867
1	-3.432900	2.229272	-1.826691

**TS<sub>12-13</sub>**

6	-4.801281	-0.662433	-0.328569
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6	-3.597603	-2.039340	-1.800718
6	-4.881099	-2.767247	-1.382970
6	-5.216140	-2.098425	-0.045913
3	-2.115806	-0.050655	-0.023408
7	-1.895452	-0.619570	1.844050
6	-2.845047	-1.279919	2.706831
6	-0.640864	-0.959335	2.160274
6	-0.066196	-1.855522	3.052867
7	1.314150	-1.811922	2.828398
6	1.659589	-0.937934	1.866593
7	0.459230	-0.408833	1.476778
6	2.254509	-2.624446	3.564300
6	0.329347	0.561651	0.433229
6	0.431860	1.893915	0.796843
6	0.349394	2.942203	-0.126672
6	0.171770	2.575553	-1.472264
6	0.054281	1.257177	-1.868329
6	0.051463	0.131870	-0.933850
6	-0.236917	-1.162139	-1.365252
6	-0.297546	-2.410895	-0.497179
6	-0.477525	-1.361459	-2.846230
8	-2.882989	1.699574	0.011636
6	-3.292744	2.491325	-1.104885
6	-3.202643	3.931505	-0.616217
6	-3.616975	3.779723	0.852257
6	-2.975057	2.444647	1.236020
3	3.298061	-0.515991	0.687905
8	4.079353	1.184697	0.250128
6	3.916195	2.091052	1.354039
6	4.180347	3.483033	0.776447
6	3.850012	3.339080	-0.727571
6	3.539433	1.848357	-0.912672
8	4.127563	-1.853416	-0.391095
6	4.619900	-1.411982	-1.660146
6	3.397382	-1.532575	-2.561202
6	2.799564	-2.873384	-2.092250
6	3.347661	-3.036215	-0.656581
1	0.577020	2.097247	1.857228
1	-2.658934	-1.073106	3.777114
1	-2.833030	-2.384857	2.600939
1	-0.509535	-2.518642	3.777089
1	0.426767	3.978842	0.184208
1	0.133701	3.348132	-2.240252
1	-0.072445	1.053987	-2.925698
1	0.554282	-2.532570	0.180243
1	-0.321515	-3.299519	-1.139980
1	-1.188900	-2.468321	0.148854
1	-1.306574	-0.748947	-3.237948
1	-0.722530	-2.405730	-3.067362
1	0.400962	-1.101956	-3.465523
1	2.572968	-3.089748	0.110989
1	4.007935	-3.907125	-0.569006
1	1.709256	-2.848326	-2.109458
1	3.141170	-3.696876	-2.725597
1	2.693737	-0.715658	-2.351128
1	3.643677	-1.521364	-3.625405
1	5.426521	-2.084587	-1.986986
1	5.025267	-0.408423	-1.525751
1	4.625384	1.788070	2.127926
1	2.894143	2.001980	1.738427
1	5.226915	3.764466	0.916741
1	3.557388	4.234418	1.266816
1	2.462527	1.665784	-0.965594
1	4.025548	1.415092	-1.789570

1	-2.698624	-2.584713	-1.501387
1	-3.547572	-1.841499	-2.875810
1	-6.267314	-2.191694	0.237047
1	-4.592876	-2.507868	0.756225
1	-5.564728	-0.136052	-0.920201
1	-4.565264	-0.069331	0.558454
1	-4.325158	2.223745	-1.375635
1	-2.627319	2.258837	-1.940304
1	-2.165972	4.275515	-0.684490
1	-3.845784	4.610175	-1.181941
1	-4.708404	3.721062	0.932470
1	-3.271573	4.599560	1.486235
1	-1.962947	2.565255	1.631328
1	-3.559992	1.858960	1.952227
1	4.700945	3.645681	-1.340625
1	2.983289	3.936893	-1.015734
1	-4.732835	-3.846274	-1.302618
1	-5.682597	-2.585306	-2.106657
1	3.251420	-2.459214	3.152008
1	2.251415	-2.353453	4.625013
1	1.994049	-3.683870	3.470427
1	-3.864176	-0.940636	2.486606

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6	-3.845482	-1.981292	-1.779370
8	-2.988196	-0.855718	-2.001503
6	-1.943023	-1.250825	-2.914769
6	-1.970294	-2.789940	-2.973278
6	-2.902257	-3.174491	-1.814132
3	-2.600210	-0.213248	-0.219880
7	-2.201825	-1.414121	1.209067
6	-2.993767	-2.457575	1.810818
6	-0.982728	-1.332831	1.760277
6	-0.302657	-2.027937	2.748699
7	0.986985	-1.476864	2.803556
6	1.170313	-0.477593	1.925850
7	-0.050156	-0.381819	1.310636
6	2.022398	-1.962768	3.686348
6	-0.279429	0.551079	0.252835
6	-1.115465	1.632985	0.520424
6	-1.296463	2.672999	-0.395942
6	-0.570334	2.605124	-1.594095
6	0.275873	1.546716	-1.872603
6	0.472005	0.431112	-0.978503
6	1.303449	-0.669595	-1.304243
6	0.921608	-2.057603	-0.784499
6	1.878202	-0.690015	-2.708599
8	-4.290779	0.592979	0.226482
6	-4.740245	1.787639	-0.425024
6	-4.940071	2.791212	0.702935
6	-5.474734	1.886870	1.818039
6	-4.649962	0.613716	1.623040
3	2.616774	0.126032	0.537531
8	3.125085	1.979546	0.329236
6	2.327785	2.913832	1.080993
6	2.732757	4.272120	0.530099
6	2.858782	3.958590	-0.965304
6	3.411670	2.528130	-0.968321
8	4.330016	-0.746068	0.936837
6	5.418687	-0.301520	0.131149
6	5.200417	-1.019587	-1.200431
6	4.611055	-2.380163	-0.758049
6	4.250092	-2.159067	0.725542
1	-1.602645	1.657169	1.494836
1	-3.173693	-2.291100	2.890861
1	-2.521037	-3.455644	1.727245
1	-0.612639	-2.840233	3.384832

1	-1.945349	3.513435	-0.175106
1	-0.680983	3.394659	-2.334936
1	0.780949	1.537383	-2.833254
1	1.282485	-2.313912	0.219457
1	1.312588	-2.821950	-1.468003
1	-0.171736	-2.200766	-0.733657
1	1.106859	-0.781670	-3.501024
1	2.556007	-1.540806	-2.840968
1	2.457549	0.207433	-2.961721
1	3.238917	-2.473991	0.992973
1	4.970199	-2.652169	1.392738
1	3.724210	-2.636310	-1.341356
1	5.335459	-3.191412	-0.865889
1	4.467964	-0.466943	-1.798372
1	6.120425	-1.119441	-1.781182
1	6.364434	-0.607304	0.603005
1	5.372354	0.787579	0.087185
1	2.553847	2.754154	2.136940
1	1.264420	2.712446	0.899191
1	3.695915	4.583436	0.948991
1	1.989551	5.044736	0.739814
1	2.940332	1.897573	-1.728975
1	4.499841	2.507732	-1.104050
1	-1.003489	-0.858075	-2.521167
1	-2.141338	-0.793040	-3.889795
1	-3.418902	-4.123409	-1.977434
1	-2.352042	-3.216635	-0.867768
1	-4.596411	-2.032215	-2.581537
1	-4.350055	-1.824029	-0.822397
1	-5.684473	1.579107	-0.945955
1	-3.979373	2.077780	-1.155120
1	-3.975552	3.222074	0.993678
1	-5.620126	3.602579	0.433708
1	-6.539866	1.686457	1.660544
1	-5.349694	2.309475	2.817202
1	-3.723374	0.609630	2.206274
1	-5.201092	-0.303131	1.850883
1	3.509809	4.653033	-1.501432
1	1.868534	3.973072	-1.429465
1	-0.969267	-3.213774	-2.866078
1	-2.386637	-3.132259	-3.925937
1	2.930952	-1.391679	3.486441
1	1.730055	-1.831092	4.733255
1	2.208012	-3.027717	3.505040
1	-3.974701	-2.520786	1.323980

## References

1. A. A. Danopoulos and P. Braunstein, *Chem. Commun.*, 2014, **50**, 3055-3057.
2. APEX2, Bruker AXS Inc., Madison USA, 2006.
3. G. M. Sheldrick, Univeristy of Gottingen, Gottingen, 1999.
4. A. Spek, *J. Appl. Crystallogr.*, 2003, **36**, 7-13.
5. Y. Zhao and D. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
6. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford, CT, USA, 2009.
7. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257-2261.
8. J. D. Dill and J. A. Pople, *J. Chem. Phys.*, 1975, **62**, 2921-2923.
9. P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213-222.
10. G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2010, **132**, 114110.